Perfect Tensors from Multiple Angles and (Quantum) Combinatorial Structures in Category Theory

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Paulina L. A. Goedicke

aus Hamburg,

Institut für theoretische Physik,
Mathematisch-Naturwissenschaftliche Fakultät,
Universität zu Köln

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Abstract

Paulina L. A. Goedicke

Perfect Tensors from Multiple Angles and (Quantum) Combinatorial Structures in Category Theory

This dissertation investigates well-known (quantum) combinatorial structures, such as (quantum) designs and (quantum) orthogonal Latin squares through the lenses of matrix algebras, group theory, and category theory. A central focus is placed on *perfect tensors*, objects that generalise orthogonal Latin squares (OLS), whose existence problem has long been a central topic in combinatorics, exemplified by Euler's classically unsolvable "36 officers" problem. Perfect tensors are examined using representation theory and quasi-orthogonal subalgebras of matrix algebras, yielding a new perspective on the problem of constructing perfect tensors in arbitrary dimensions. In particular, it is shown that the existence of a 2-unitary in dimension d^2 is equivalent to the existence of four mutually quasi-orthogonal subalgebras of $M_{d^2}(\mathbb{C})$ that are each isomorphic to $M_d(\mathbb{C})$. This correspondence is further interpreted in terms of groups and their representations, offering a new structural viewpoint on perfect tensors by relating the existence of perfect tensors to the existence of a group G with a d^2-dimensional irreducible representation and four subgroups on which the representation is also irreducible with multiplicity d and on which the respective character "factorises". A search algorithm implemented in the algebra software GAP is presented that was used to find examples of such groups. Furthermore, additional construction schemes for all dimensions that are of the form 2^m, 2^{2m} or d^n, where m and d are odd integers greater than 1 and n is an arbitrary integer greater than 1, leading to two-unitary complex Hadamard matrices in dimensions 2^{2m}, 2^{4m} and d^{2n}, respectively, are developed, based on the doubly perfect bi-unimodular sequences ansatz introduced by Rather [95]. Using the same ansatz, an analytical resolution of Euler's thirty-six officers problem is provided, which differs from the earlier constructions of perfect tensors in dimension 36 via computer-assisted methods.

Beyond this, the thesis introduces an abstract notion of *categorical designs* formulated via arrow categories. When applied to the categories $\mathbf{Mat}(\mathbb{N})$ and $\mathbf{CP}[\mathbf{FHilb}]$, this framework produces a category-theoretic description of balanced incomplete block designs (BIBDs) and of quantum designs, respectively. The construction generalises Zauner's definition of quantum designs [121] and extends it to a broader concept that can also be interpreted as combinatorial superoperators. These new concepts will be used to define a category of mutually unbiased bases (MUBs) and a category of so-called combinatorial quantum channels.

Together, these contributions provide new mathematical tools and explicit constructions at the intersection of combinatorics, category theory, and quantum information, deepening the structural understanding of designs in both classical and quantum contexts.

Contents

1 Introduction

Combinatorics is a vast field of mathematics with applications in many different areas such as computer science, the design of experiments and ultimately also theoretical physics. One important concept herein is combinatorial design theory which deals with incidence structures (designs) that describe a relation between a given set of points and a set of blocks. A notable example of a combinatorial design is provided by balanced incomplete block designs (BIBDs), an incidence structure that divides a set of v points into a set of b blocks such that each block contains k points, each point is contained in r blocks and each two blocks share exactly λ points. Here a prominent example is given by a complete set of mutually orthogonal Latin squares of order d (MOLS(d)) that can be described by a BIBD consisting of d^2 points and $d(d+1)$ blocks such that each block contains d points, each point is contained in $d+1$ blocks and each two blocks share only one point. This incidence structure happens to be equivalent to a finite affine plane of order d [110].

Zauner extended the concept of BIBDs by introducing the more general notion of quantum design [121], which consists of a set of b trace k projectors on a v-dimensional Hilbert space that satisfy some trace constraints. In the classical limit, where all projectors commute, one obtains classical BIBDs. This concept describes famous quantum structures such as mutually unbiased bases (MUBs) and SIC-POVMs, laying the groundwork for what could be called "quantum combinatorics". Numerous other intersections between quantum theory and combinatorics have been identified. For example, the problem of constructing two orthogonal Latin squares (OLS) of order d has been shown to be equivalent to constructing an absolutely maximally entangled state of four qudits [41]. Moreover, Wocjan and Beth constructed mutually unbiased bases from orthogonal Latin squares [17], and Wootters pointed out that affine planes and mutually unbiased bases actually can be described by the same incidence structure [119]. With the development of quantum computing, it becomes thus relevant to explore how (quantum) combinatorial objects are integrated into quantum information theory.

Apart from Zauner's quantum designs, other combinatorial objects also possess quantum analogues, which can provide new theoretical insights. For instance, Vicary et al. introduced the notion of quantum Latin squares (QLS), a quantum analogue of Latin squares, which enable a novel construction scheme for unitary error bases [83]. Quantum Latin squares also contribute to the classification of other biunitary constructions, including Hadamard matrices [79], quantum teleportation and error correction, and offer a new method for constructing MUBs, as shown by Musto [80]. Building on this, Życzkowski et al. introduced quantum orthogonal arrays (QOA) and demonstrated that their relationship to QLS is analogous to the relationship between classical orthogonal arrays (OA) and LS [40, 41]. Moreover, they introduced the notion of quantum orthogonal Latin squares (QOLS), analogously to its classical counter part OLS [41]. Building on this, in Ref. [99] Życzkowski et al. then presented a quantum solution to Euler's thirty-six officers problem, i.e. classically, no two OLS of order six exist, by constructing a QOLS of order six, using numerical methods.

QOLS are closely related to perfect tensors, i.e. 4-valent tensors that can be reshaped into a unitary matrix $U \in U(d^2)$ for every bipartition of their indices. This structure also goes under the name 2-unitary, indicating that all three, the unitary U itself, its partial transpose U^Γ as well as its reshuffled version U^R, are unitary. In this work the names perfect tensors and 2-unitaries will be used interchangeably. Perfect tensors have their roots in holographic quantum error-correcting codes [90] and are particularly interesting in the theory of tensor networks. Different construction methods have been discussed in Refs. [99, 95, 41, 46, 99] which range from analytical constructions via OLS over numerical constructions to constructions via so-called perfectly perfect bi-unimodular sequences (in this work: doubly perfect bi-unimodular sequences). While construction schemes using OLS do not exist for the special case $d^2 = 36$, since there are no OLS of order six, Życzkowski et al. constructed a 36-dimensional 2-unitary from a QOLS of order six in Ref. [99]. Rather et al. then demonstrated that a solution can also be obtained using bi-unimodular doubly perfect sequences [95]. Although the latter approach has some analytical aspects to it, the question whether it is possible to construct a 2-unitary in dimension 36 without using any numerical tools remained open. This raises the following question:

Problem 1: Can one find an analytic solution to the Euler's thirty-six officers problem, i.e. can one construct a 36-dimensional 2-unitary fully analytically?

A generalisation of 2-unitary matrices to k-unitary matrices, i.e. $2k$-valent tensors that are unitary for all possible bipartitions of their indices, has been given in Ref. [41] and a link between these structures and absolutely maximally entangled states of $2k$ parties with local dimension d, namely AME($2k, d$)-states, has been established, demonstrating that these structures could be a useful tool in constructing AME-states.

Some combinatorial aspects can also be found in the research on quasi-orthogonal systems of subalgebras of matrix algebras that have been widely discussed in the works of Ohno, Weiner and Petz in Refs. [88, 114, 93, 92]. They demonstrated that given a matrix algebra $\mathcal{M}_{p^2}(\mathbb{C})$, finding the maximal number of pairwise quasi-orthogonal subalgebras isomorphic to $\mathcal{M}_p(\mathbb{C})$ is a non-trivial task. Moreover, they established a connection between maximal Abelian subalgebras (MASAs) and MUBs. Some bounds on the number of quasi-orthogonal subalgebras isomorphic to $\mathcal{M}_p(\mathbb{C})$ have been given by Ohno [88] for the case where p is a prime power. In Ref. [86] the authors defined an algebraic analogue of the combinatorial structure resembling an affine plane and showed that this in fact leads to a complete set of MASAs when applied to the matrix algebra $\mathcal{M}_{p^2}(\mathbb{C})$. This reproduces the findings of Zauner who described the same instance in terms of quantum designs. Moreover, they showed that a set of subgroups of an index group of a nice error basis, where all subgroups have pairwise trivial intersections and map to pairwise commutative subalgebras under the respective representation, give rise to a set of mutually quasi-orthogonal MASAs. This establishes a link between combinatorics and representation theory.

Problem 2: How do perfect tensors relate to systems of quasi-orthogonal subalgebras of matrix algebras? Can one describe perfect tensors from a group theoretical point of view? Does that lead to new approaches on making existence statements about perfect tensors in arbitrary dimensions?

The diverse connections between classical combinatorics and quantum combinatorial objects naturally prompt the question of whether one can formulate a more general framework - quantum combinatorics - from which classical combinatorics would emerge as a special (commutative) case that not only encompass quantum designs but also QLS, perfect tensors, k-unitaries and QOA. In fact, while MUBs and SIC-POVMs can be described by Zauner's quantum designs, a description of QLS and perfect tensors and their relation to quantum designs is unknown. An overview about some of the open problems in this area was given by Życzkowski et al. in Ref. [56]. Nevertheless, a unified framework that fully captures the relationship between classical and quantum combinatorics remains to be established.

Problem 3: How does a unified framework of classical and quantum combinatorics that captures all the structures discussed so far look like? Is there a relation between QOLS and MUBs similar to the one between affine planes and MOLS?

One approach towards getting a better understanding of any mathematical structure is by reformulating it in a different "language". Thus it can be instructive to consider (quantum) combinatorial objects in other settings like category theory.

Category-theoretical formulations of quantum combinatorial notions like QLS and MUBs have been made by Musto and Vicary in Refs. [81, 82, 84, 83]. They described QLS and MUBs as objects in a category using special dagger Frobenius algebras. First attempts to find a category-theoretical description of quantum designs have been developed in the present author's master's thesis [36] by defining a category of quantum designs using the arrow category of the category of finite-dimensional Hilbert spaces and completely positive maps, $\mathbf{CP}[\mathbf{FHilb}]$. The same thesis also covers formulation of a category of classical block designs using the arrow categories of the category of relations and the category of matrices and natural numbers, $\mathbf{Mat}(\mathbb{N})$, and the definition of a functor between this category and the category of quantum designs. The similarity in the construction of these categories raises the following questions:

Problem 4: Can one generalise the category theoretical description of classical and quantum block designs to a more general construction scheme that can be applied to any monoidal pointed category? Does such a generalisation lead to new insights or new mathematical objects?

Although this thesis does not aim to fully answer all of these questions, it delivers partial answers by discussing well-known combinatorial structures in the language of matrix algebras, group theory and category theory. Special emphasis will lie on perfect tensors, which will be explored in terms of representation theory and quasi-orthogonal subalgebras of matrix algebras, leading to new approaches to finding perfect tensors in arbitrary dimensions. In particular, it will be shown that the existence of a 2-unitary in dimension d^2 is equivalent to the existence of four mutually quasi-orthogonal subalgebras of $\mathcal{M}_{d^2}(\mathbb{C})$ isomorphic to $\mathcal{M}_d(\mathbb{C})$. This instance will also be described in terms of groups and representations, providing a new way to look at and for perfect tensors. Moreover, construction schemes of perfect tensors from doubly perfect bi-unimodular sequences in all dimensions that are of the form 2^m, 2^{2m} or d^n, where m and d are odd integers greater than 1 and n is an arbitrary integer greater than 1, will be presented and an analytical solution to Euler's thirty-six officers problem based on a doubly perfect bi-unimodular sequence ansatz will be delivered.

Furthermore, a more abstract notion of categorical designs based on arrow categories will be derived that when applied to the categories $\mathbf{Mat}(\mathbb{N})$ and $\mathbf{CP}[\mathbf{FHilb}]$ leads to a category theoretical description of BIBDs and quantum designs respectively. In fact, this construction generalises the notion of quantum designs given by Zauner to a notion of quantum designs that could also be understood as combinatorial superoperator. Special cases are given by the category of MUBs and the category of so-called combinatorial quantum channels. Eventually, it will be discussed how perfect tensors fit into this model.

1.1 Outline

The mathematical concepts that are used throughout the thesis, beginning with (quantum) combinatorial notions such as BIBDs, (quantum) Latin squares, mutually unbiased bases (MUBs), absolutely maximally entangled (AME) states, Hadamard matrices, perfect tensors and the definition of (doubly) perfect sequences will be introduced in Section 2.1 of Chapter 2. The second part of this chapter, Section 2.2, is devoted to quasi-orthogonal systems of subalgebras of matrix algebras, introducing the notions of quasi-orthogonality between subalgebras, factors, maximal Abelian subalgebras (MASAs), and delocalised subalgebras. Building on this, in Section 2.3, selected concepts from the representation theory of finite groups and character theory are discussed. Finally, the last section, Section 2.4, covers basic notions from monoidal category theory, categorical quantum theory, and arrow categories.

Chapter 3 begins with a matrix-algebraic perspective on perfect tensors in Section 3.1, showing that the existence of a 2-unitary in dimension d^2 is equivalent to the existence of four mutually quasi-orthogonal subalgebras of $\mathcal{M}_{d^2}(\mathbb{C})$ isomorphic to $\mathcal{M}_d(\mathbb{C})$. Moreover, a generalisation to k-unitaries will be discussed and it will be demonstrated that, while the existence of a k-unitary implies the existence of k quasi-orthogonal subalgebras of $\mathcal{M}_{d^k}(\mathbb{C})$ isomorphic to $\mathcal{M}_d(\mathbb{C})$, the other direction does not hold. Here a specific example will be given for the case $d^3 = 27$. Building on this, Section 3.2 phrases these concepts in the more abstract framework of groups and representations and it will be shown that the existence of a 2-unitary can be related to the existence of a group G with a d^2-dimensional irreducible representation and four subgroups on which the representation is also irreducible with multiplicity d. As an explicit example of such a group, nice error bases will be discussed. Moreover, a search algorithm implemented in the algebra software GAP, that has been used to look for groups satisfying these criteria, will be presented.

The third part of the chapter, Section 3.3, addresses construction schemes for perfect tensors from doubly perfect sequences in all dimensions that are of the form $2^m, 2^{2m}$ or d^n, where m and d are odd integers greater than 1 and n is an arbitrary integer greater than 1, which lead to 2-unitaries in dimension $2^{2m}, 2^{4m}$ and d^{2n}, respectively. Moreover, an analytic solution for the problem of finding a 2-unitary in dimension $d^2 = 36$ based on a doubly perfect biunimodular sequence of length 36 and period 3 will be presented.

The final section discusses several open questions and observations that were encountered throughout the chapter, including the minimal order of 2-unitaries in dimensions $d^2 = 9, 16, 25, 36$ and the relation between a quasi-orthogonal decomposition of $\mathcal{M}_9(\mathbb{C})$ and different 2-unitaries in dimension 9.

Chapter 4 introduces a categorical framework based on arrow categories that generalises both quantum and block designs by transferring the essential properties of block designs into a pointed monoidal dagger category. The application of this framework to the categories $\mathbf{Mat}(\mathbb{N})$ and $\mathbf{CP}[\mathbf{FHilb}]$ is then discussed, showing that it yields a categorical representation of both block designs and quantum designs, which can be connected via a functor. Furthermore, these techniques are used to define a category of MUBs and to define so-called combinatorial quantum channels. Finally, these concepts are reformulated in the language of matrix algebras and it will be discussed how perfect tensors fit into this model.

Lastly, Chapter 5 summarises the thesis and discusses open questions.

2 Background

In this chapter, the mathematical foundations relevant to this work will be discussed. Beginning with the definitions of combinatorial structures such as balanced incomplete block designs, Latin squares, and affine planes, the first section aims to introduce the relatively new field of *quantum combinatorics* in an exploratory manner. Concepts such as quantum Latin squares, MUBs, AME states, Hadamard matrices, and perfect tensors will be explained. Moreover, the definition of (doubly) perfect sequences will be provided.

The second part of the chapter is devoted to quasi-orthogonal systems of subalgebras of matrix algebras, where the notions of factors, MASAs, and delocalised subalgebras will be defined. In the third section, some concepts from the representation theory of finite groups as well as character theory will be discussed. Finally, the last section of this chapter addresses the basic notions of monoidal categories, category-theoretical quantum theory, and arrow categories.

Familiarity with fundamental concepts of group theory, algebra and quantum theory will be assumed. For an introduction see Refs. [31, 68].

2.1 (Quantum) Combinatorics

Combinatorics is a vast field with applications in many different areas such as computer science, the design of experiments and ultimately also theoretical physics. A substantial part of this chapter is drawn from the definitions in Ref. [37], which are largely adapted from Ref. [110].

One principal concept in this area is the notion of a *design*: a way to relate a given set of objects (points) to another set of objects (blocks).

Definition 2.1. [37] A *design* (V, B, I) is given by a set $V = \{1, .., v\}$ of *points*, and a set $B = \{1, \ldots, b\}$ of *blocks* and an *incidence relation* I between them.

Designs can also be represented as bipartite graphs, where the vertex set is partitioned into disjoint subsets of points and blocks [37]. More precisely, a design (V, B, I) with $|V| = v$ and $|B| = b$ can be encoded in an *incidence matrix* X, which is a $v \times b$ binary matrix defined by

$$X_{i,j} = \begin{cases} 1 & \text{if } (i,j) \in I, \\ 0 & \text{otherwise.} \end{cases}$$

Throughout this work, the incidence matrix representation of designs will be used primarily. In particular, for a design (V, B, I) with associated incidence matrix X, the shorthand notation $X : b \to v$ will be adopted.

2.1.1 Block Designs

Designs can come with extra structure, i.e. certain symmetries within the incidence relations. Prominent examples include *uniformity*- and *regularity*-conditions.

Definition 2.2. [37] A design $X : b \to v$ is called

- *k-uniform*, if every block contains exactly k points: $\sum_{i=1}^{v} X_{i,j} = k$, for all $j = 1, .., b$.
- *r-regular*, if every point appears in exactly r blocks: $\sum_{j=1}^{b} X_{i,j} = r$ for all $i = 1, .., v$.

In other words, every column of X contains exactly k "1"s and every row of X contains exactly r "1"s.

Definition 2.3. [37] A k-uniform and r-regular design $X : b \to v$ is called *λ-balanced*, if any two points are contained in exactly λ blocks. One then has:

$$X \cdot X^T = \lambda \Big(E_{v \times v} - \mathbb{I}_{v \times v} \Big) + r \mathbb{I}_{v \times v}.$$

Here X^T is the transpose incidence matrix, $E_{v \times v}$ denotes the $v \times v$-matrix in which every entry is equal to 1, and $\mathbb{I}_{v \times v}$ denotes the $v \times v$ identity matrix.

Combining these properties, one obtains the notion of a *balanced incomplete block design (BIBD)*.

Definition 2.4. [37] A *balanced incomplete block design (BIBD)*, or a (v, k, r, b, λ)-*design*, is a design $X : b \to v$ which is k-uniform, r-regular and λ-balanced.

By simple counting arguments, one can easily derive the following equational properties ([110], p. 4-5):

Lemma 2.4.1. *For a (v, k, r, b, λ)-design, the following equations hold:*

$$b \cdot k = r \cdot v \tag{2.1}$$

$$\lambda(v-1) = r(k-1) \tag{2.2}$$

To simplify terminology, often the term *block design* will be used throughout this work to refer to BIBDs.

Two block designs can be related via a homomorphism:

Definition 2.5. [37] Consider two designs $X : b \to v$ and $X' : b' \to v'$. A *design homomorphism* $f : X \to X'$ is a pair of functions $f_v : v \to v'$ and $f_b : b \to b'$ such that the following diagram commutes:

$$\begin{array}{ccc} b & \xrightarrow{f_b} & b' \\ \downarrow X & & \downarrow X' \\ v & \xrightarrow{f_v} & v' \end{array}$$

Projective and Affine Planes

Prominent examples of block designs are given by affine and projective planes. The latter are special cases of so-called *symmetric* block designs:

Definition 2.6. ([110], p. 23) A (v, k, r, b, λ)-design is *symmetric* when $v = b$; that is, when there are as many points as blocks.

In this case Lemma 2.4.1 then implies that $r = k$.

Example 1. ([110], p. 27) Consider a finite projective plane of order d. One then has $v = d^2 + d + 1$ points and $b = d^2 + d + 1$ lines (blocks) such that there are $k = d + 1$ points on each line and each point appears on $r = d + 1$ lines. Moreover, every pair of lines intersect in exactly one point. Hence one has a symmetric block design with parameters $v = b = d^2 + d + 1$, $r = k = d + 1$ and $\lambda = 1$.

For $d = 2$, this is equal to the so-called *Fano plane*:

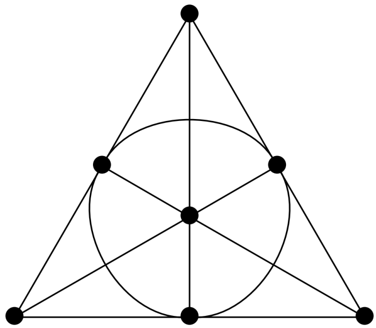


FIGURE 2.1: The Fano plane is a block design with parameters $v = b = 7$, $r = k = 3$ and $\lambda = 1$. This corresponds to a projective plane of order 2.

One can show that the following theorem holds true:

Theorem 2.6.1. *([110], p. 28) For every prime power $q \geq 2$, there exists a (symmetric) $(q^2 + q + 1, q + 1, 1)$-design (i.e. a projective plane of order q).*

For non-prime power dimensions d, the existence problem of projective planes is not fully solved. It was shown that projective planes are known to not exist, if $d = 1 \bmod 4$ or $d = 2 \bmod 4$ and if the square-free part of d contains at least one prime factor of the form $4k + 3$ [19].

Projective planes are equivalent to *affine planes*, which itself are $(d^2, d, d + 1, d, 1)$-designs ([110], p. 106). To see that consider a projective plane of order d. By removing one line (block) and hence d points from the projective plane, one obtains an affine plane. Conversely, given an affine plane, one can construct a projective plane by adding a line (block) with d points that intersects with all other lines in exactly one point to the affine plane [1]. A direct consequence of this fact is the following:

Theorem 2.6.2. *([110], p. 29) For every prime power $q \geq 2$, there exists a $(q^2, q, 1)$-design (i.e. an affine plane of order q).*

[1] See Ref. [110], p. 106 for further details of the proof.

The lines of an affine plane of order d can be grouped into so-called parallel classes. Removing one or more of these parallel classes, such that one is left with k parallel classes, one ends up with an incidence structure known as *k-net* of order d. A k-net with $k = d + 1$ is called *complete* and coincides with an affine plane [86].

Mutually Orthogonal Latin Squares

Affine planes and hence also projective planes are closely related to mutually orthogonal Latin squares which will be introduced in this section.

Definition 2.7. [84] A *Latin square* of order d, in short: LS(d), is a square arrangement of size d such that every entry, taken from the set $\{0, ..., d-1\}$, occurs once in each row and each column.

In the case $d = 3$ for example, the following forms a Latin square:

$$\begin{matrix} 0 & 1 & 2 \\ 2 & 0 & 1 \\ 1 & 2 & 0 \end{matrix}$$

The following definition is well-established and can be found in similar spirit in Ref. [110] on page 131:

Definition 2.8. i) Two Latin squares L and K of size d are called *orthogonal*, if the set of ordered pairs $[L_{ij}, K_{ij}]$ is composed of all possible d^2 combinations of symbols of L and K, where $i, j \in [d]$.

ii) A collection of m LS of order d is called *mutually orthogonal (MOLS)*, if they are pairwise orthogonal.

Example 1. For $d = 3$, the following two Latin squares are orthogonal:

$$\begin{matrix} 0 & 2 & 1 \\ 2 & 1 & 0 \\ 1 & 0 & 2 \end{matrix} \qquad \begin{matrix} 0 & 1 & 2 \\ 2 & 0 & 1 \\ 1 & 2 & 0 \end{matrix} \qquad \rightsquigarrow \qquad \begin{matrix} 00 & 21 & 12 \\ 22 & 10 & 01 \\ 11 & 02 & 20 \end{matrix}$$

Definition 2.9. ([94], p. 96) An OLS(d) with entries from the set $\{0, 1, ..., d-1\}$ is said to be in *normal form*, if every top row is $0, 1, ..., d-1$, in that order and the left column of one of the squares also has $0, 1, ..., d-1$, in that order.

Proposition 2.9.1. *([110], p. 139) A complete set of MOLS(d) is equivalent to an affine plane.*

Proof. Consider an affine plane of order d. Choose an arbitrary parallel class to represent column indices and another arbitrary parallel class to represent row indices. Now, number each line of the column parallel class in arbitrary order and then do the same with the lines of the row parallel class. If one now takes another arbitrary parallel class and label its lines randomly with $0, 1, ..., d-1$, one can assign to each pair of row and column indices a number corresponding to a line of this third parallel class by using the intersection properties of the three corresponding lines of the plane. In this way, the lines of the affine plane can be used as indices for a $d \times d$-matrix where the entries are given by the points of the plane. This matrix is a Latin square. If one chooses a fourth parallel class to construct another Latin square in the same way, both Latin squares are orthogonal. This is merely due to the fact that each line of the third parallel class meets every line of the fourth parallel class at exactly one point. As any affine plane of order d has $d+1$ parallel classes and two of them were chosen to generate matrix indices, one can thus construct $d-1$ mutually orthogonal Latin squares. Conversely, given $d-1$ MOLS(d), one can construct an affine plane of order d in a similar way. See Ref. [110], p. 136-139 for more details. □

One can now establish the following important theorem:

Theorem 2.9.1. *([110], p. 139) Let $d \geq 2$. Then the existence of any one of the following designs implies the existence of the other two designs:*

i) $d-1$ *MOLS*(d),

ii) an affine plane of order d,

iii) a projective plane of order d.

As a consequence, one finds:

Theorem 2.9.2. *(Theorem 4.24 in Ref. [25]) For every prime power p, there exist $p-1$ MOLS of order p, arising from the structure of the finite field $\mathbb{F}_p$.*

What is known about the existence of non-complete sets of MOLS of order d? In 1782, Euler conjectured that there are no two orthogonal Latin squares of order $d \equiv 2 \bmod 4$, the so-called 36 officers problem. This conjecture stood until the beginning of the 20-*th* century, when Tarry proved that there indeed do not exist two orthogonal Latin squares of order 6 in 1900 [111], leaving the other cases open. It was only in 1960 when Bose, Shrikhande, and Parker disproved these other cases [16]. Thus, OLS of order d can be constructed for any $d \neq 2, 6$.

2.1.2 Quantum Designs

The concept of a quantum design was introduced by Zauner in his dissertation [121]. In the following, his definition will be recalled, with minor adjustments in terminology for consistency.

Definition 2.10. A *quantum (v, b)-design* is a set $D = \{p_1, ..., p_v\}$ of complex orthogonal $b \times b$ projection matrices p_i on a b-dimensional Hilbert space $\mathbb{C}^b$, i.e. $p_i = p_i^\dagger = p_i^2$ for all $i \in \{1, \dots, v\}$.

Just as with classical designs, certain structural properties can also be defined for quantum designs.

Definition 2.11. A quantum (v, b)-design is called

- *r-regular*, if there exists some $r \in \mathbb{N}$ with $\mathrm{tr}(p_i) = r$ for all $i \in \{1, \dots, v\}$,
- *k-uniform*, if there exists some $k \in \mathbb{R}$ with $\sum_{i=1}^{v} p_i = k \cdot \mathbb{I}_{b \times b}$.

Definition 2.12. [121] Given a quantum (v, b)-design, its *degree* is the cardinality of the set $\{\mathrm{tr}(p_i p_j) | i, j \in \{1, \dots, v\}, i \neq j\}$.

It follows that a quantum design has degree 1 just when there exists some $\lambda \in \mathbb{R}$ such that

$$\mathrm{tr}(p_i p_j) = \lambda \qquad \forall i, j = 1, ..., v \qquad \text{with} \qquad i \neq j. \tag{2.3}$$

Such a quantum design will be called *λ-balanced* in the course of this work. That λ is real in this case follows from a simple argument: $\lambda = \mathrm{tr}(p_i p_j) = \mathrm{tr}((p_i p_j)^\dagger)^* = \mathrm{tr}(p_j^\dagger p_i^\dagger)^* = \mathrm{tr}(p_j p_i)^* = \mathrm{tr}(p_i p_j)^* = \lambda^*$.

The following lemma can then be established analogous to Lemma 2.4.1 for classical designs.

Lemma 2.12.1. *[121] For a k-uniform, r-regular and λ-balanced quantum design $D = \{p_1, ..., p_v\}$ with $p_i \in \mathbb{C}^b$ the following equations hold:*

$$b \cdot k = v \cdot r, \tag{2.4}$$

$$\lambda(v - 1) = r(k - 1). \tag{2.5}$$

Proof. This proof is also part of the present author's paper [37].

Consider an r-uniform, k-regular and λ-balanced quantum design $D = \{p_1, ..., p_v\}$ with $p_i \in \mathbb{C}^b$. By applying the trace function to the uniformity condition, one gets:

$$\mathrm{tr}\Big(\sum_{i=0}^{v} p_i\Big) = \sum_{i=0}^{v} \mathrm{tr}(p_i) = k \cdot \mathrm{tr}(\mathbb{I}_{b\times b}). \tag{2.6}$$

Using the regularity condition this expression becomes:

$$\sum_{i=0}^{v} \mathrm{tr}(p_i) = \sum_{i=0}^{v} r = v \cdot r = k \cdot \mathrm{tr}(\mathbb{I}_{b\times b}) = k \cdot b. \tag{2.7}$$

This proves Eq. 2.4.

In order to prove Eq. 2.5, start with the following expression:

$$b = \mathrm{tr}(\mathbb{I}_{b\times b}) = \mathrm{tr}(\mathbb{I}^2_{b\times b}). \tag{2.8}$$

Using the uniformity condition, one gets:

$$\mathrm{tr}(\mathbb{I}^2_{b\times b}) = \frac{1}{k^2}\mathrm{tr}\Big(\sum_{i=0}^{v} p_i \sum_{j=0}^{v} p_i\Big) = \frac{1}{k^2}\sum_{i,j=0}^{v} \mathrm{tr}(p_i p_j) \tag{2.9}$$

$$= \frac{1}{k^2}\sum_{i,j=0,j\neq i}^{v} \lambda + \frac{1}{k^2}\sum_{i}^{v} r = \frac{1}{k^2}(\lambda v(v-1) + vr). \tag{2.10}$$

Here the uniformity and the λ-condition have been used in the third step. Hence one has:

$$b = \frac{1}{k^2}(\lambda v(v-1) + vr) \Leftrightarrow \tag{2.11}$$

$$\frac{b \cdot k}{v} \cdot k = \lambda(v-1) + r. \tag{2.12}$$

Using Eq. 2.4, one obtains:

$$r \cdot k = \lambda(v-1) + r. \tag{2.13}$$

This is equivalent to Eq. 2.5. □

Definition 2.13. [121] A quantum design is *commutative* when all projection matrices pairwise commute.

Theorem 2.13.1 ([121], Theorem 1.10)**.** *A commutative quantum design is equivalent to a classical block design.*

The proof is based on the fact that every commutative design is unitarily equivalent to a design comprised of diagonal matrices (as the projections are idempotent, the diagonal entries must therefore be 0 or 1) and can be found in Ref. [121].

Example 1. Let $\mathcal{A}$ be an affine plane of order d, i.e. $\mathcal{A}$ has d^2 points and $d(d+1)$ lines that can be grouped into $d+1$ parallel classes that contain d lines each. Each line contains d points and each point is contained in $d+1$ lines. Moreover, each two lines from different parallel classes intersect in exactly one point. In other words, consider a block design with parameters $b = d^2$, $v = d(d+1)$, $r = d$, $k = d+1$ and $\lambda = 1$. According to Theorem 2.13.1 this block design gives rise to a commutative quantum design, i.e. set of commuting orthogonal projectors p_i, of the form:

$$D_{\mathcal{A}} = \{p_1, ..., p_{d(d+1)}\}, \text{ with } p_i \in \mathcal{M}_{d^2}(\mathbb{C}) \tag{2.14}$$

The projectors can be grouped into $d+1$ so-called *parallel classes* $A_1 = \{p_1^1,...,$ $p_d^1\},..., A_{d+1} = \{p_1^{d+1}, ..., p_d^{d+1}\}$ and fulfil:

i) $\mathrm{tr}(p_i^a) = d \;\; \forall \;\; i = 1, ..., d(d+1)$,

ii) $\sum_{a=1}^{(d+1)} \sum_{i=1}^{d} p_i^a = (d+1)\mathbb{I}_{d^2}$,

iii) $\mathrm{tr}(p_i^a, p_j^b) = (1-\delta_{ab}) + d \cdot \delta_{ab}\delta_{ij}$ for all $i, j \in [d]$ and $a, b \in [d+1]$.

This construction can also be seen as $d+1$ d-outcome measurements in the Hilbert space $\mathbb{C}^{d^2}$, each consisting of orthogonal projectors of rank d. Each parallel class can be seen as a subalgebra of $\mathcal{M}_{d^2}(\mathbb{C})$. One has that $tr(pq) = 1$ for p, q not lying in the same parallel class and hence each two parallel classes are quasi-orthogonal [2] subalgebras of $\mathcal{M}_{d^2}(\mathbb{C})$. In total, one has $d+1$ of them.

This example actually describes a complete set of *MUBs*. These structures will be introduced in the next section.

[2]See Section 2.2.1 for more details.

MUBs

Notable examples of uniform and regular quantum designs are *mutually unbiased bases (MUBs)* which play a crucial role in quantum information theory.

Definition 2.14. [86] A set of k bases $\{\{|f_i^1\rangle\}_{i\in[d]},..,\{|f_i^k\rangle\}_{i\in[d]}\}$ in a d-dimensional Hilbert space H is called *mutually unbiased*, if the the following holds for any pair of bases:

$$\langle f_i^a|f_j^b\rangle = \delta_{a,b}\frac{1}{d}\ \ \forall\, i,j \in [d]. \tag{2.15}$$

In other words, the inner product between any two vectors from different bases is constant.

A set of $d+1$ MUBs in a Hilbert space of dimension d is called *complete*. The following example is taken from Ref. [37] and has originally been made in Ref. [121]

Example 1. [121] A uniform and regular quantum design of degree 2 with parameters $r=1, b=d, v=d\cdot k$ and $\Lambda = \{\frac{1}{d},0\}$ defines a set of k MUB's in a d-dimensional Hilbert space H. Indeed, the $d\cdot k$ projectors all have trace one and satisfy the following condition, where a labels the different orthogonal classes, and i labels the projectors within an orthogonal class:

$$\sum_{a=1}^{k}\sum_{i=1}^{d} p_i^a = k\cdot \mathbb{I} \tag{2.16}$$

Moreover, the following holds:

$$\mathrm{tr}(p_i^a p_j^b) = \frac{1}{d}(1-\delta_{ab}) + \delta_{ij}\delta_{ab}$$

It is easy to see that one gets a complete set of MUBs if v equals $d\,(d+1)$, as one then has $k=d+1$.

2.1.3 Orthogonal Quantum Latin Squares, Perfect Tensors, and AME-States

Let K be a Latin square of order d. One can construct a *quantum Latin square* by replacing the classical entries with elements of the computational basis:

$$K_{ij} \mapsto |K_{ij}\rangle\,. \tag{2.17}$$

Due to the properties of Latin squares, every row and every column of the corresponding quantum Latin square forms an orthonormal basis in $\mathbb{C}^d$.

This motivates the following definition:

Definition 2.15. [42] A *quantum Latin square* (QLS) of order d is a $d \times d$ array of quantum states $\{|\Psi_{ij}\rangle\}_{i,j\in[d]}$ in a Hilbert space H_d such that each row and each column forms an orthonormal basis:

$$\mathrm{QLS}(d) = \begin{bmatrix} |\Psi_{0,0}\rangle & \cdots & |\Psi_{0,d-1}\rangle \\ \vdots & \ddots & \vdots \\ |\Psi_{d-1,0}\rangle & \cdots & |\Psi_{d-1,d-1}\rangle \end{bmatrix}.$$

The concept of QLS was first introduced in Ref. [83] and later generalised to *quantum orthogonal Latin squares (QOLS)* in Ref. [42]:

Definition 2.16. Two QLS(d)s Φ and Ψ are called *orthogonal* if the set $\{|\phi_{ij}\rangle = |\Phi_{ij}\rangle \otimes |\Psi_{ij}\rangle\}_{i,j\in[d]}$ forms an orthonormal basis of $H_d^{\otimes 2}$ and

i) All rows satisfy

$$\mathrm{tr}_B\left(\sum_{k=0}^{d-1} |\phi_{ik}\rangle\langle\phi_{jk}|\right) = \delta_{ij}\mathbb{I}_d \tag{2.18}$$

ii) All columns satisfy

$$\mathrm{tr}_B\left(\sum_{k=0}^{d-1} |\phi_{ki}\rangle\langle\phi_{jk}|\right) = \delta_{ij}\mathbb{I}_d \tag{2.19}$$

One can show that this is equivalent to the following condition:

Proposition 2.16.1. *[82] Two QLS(d)s Φ and Ψ are orthogonal if and only if one, and hence both, of the following equivalent conditions hold:*

$$\sum_{i,j=0}^{d-1} |\Phi_{ij}\rangle\langle\Phi_{ij}| \otimes |\Psi_{ij}\rangle\langle\Psi_{ij}| = \mathbb{I}_{d^2}, \tag{2.20}$$

$$\sum_{i,j,p,q=0}^{d-1} \langle\Phi_{ij}|\Phi_{pq}\rangle\langle\Psi_{ij}|\Psi_{pq}\rangle\,|ij\rangle\langle pq| = \mathbb{I}_{d^2}. \tag{2.21}$$

Analogously to the classical case, one can construct a quantum orthogonal Latin square of order d from two orthogonal classical Latin squares K and L by making the following assertion:

$$K_{ij}L_{ij} \mapsto |K_{ij}L_{ij}\rangle\,. \tag{2.22}$$

Now each row and each column of the resulting array forms an orthonormal basis of $H_d^{\otimes 2}$.

Every pair of orthogonal Latin squares gives rise to a QOLS, but the converse is not true in general. In fact, QOLS can consist of entangled states, that is, they need not be product states. In this thesis, such QOLS will be referred to as *genuinely quantum* following previous notions by Życzkowski.

Perfect Tensors

Let V be a finite-dimensional vector space over a field $\mathbb{F}$, and let V^* be its dual space. A *tensor of type* (m,n) on V is a multilinear map

$$T : \underbrace{V^* \times \cdots \times V^*}_{m \text{ times}} \times \underbrace{V \times \cdots \times V}_{n \text{ times}} \to \mathbb{F}.$$

A tensor of rank (k,k) can be reshaped into a matrix of dimension d^k [3]. Since there are $\frac{1}{2}\binom{2k}{k}$ bipartitions of the $2k$ indices (excluding global transpositions), there are $\frac{1}{2}\binom{2k}{k}$ matrices that can be constructed from this tensor [41]. Consider for example the case $k = 2$. The indices of the $(2,2)$-tensor A can be reshaped into a matrix in three inequivalent ways, each of which corresponding to one of the following matrices:

$$\langle ij|\, A\, |kl\rangle \rightsquigarrow A, \tag{2.23}$$

$$\langle ik|\, A\, |jl\rangle \rightsquigarrow A^R \quad \text{(reshuffling)}, \tag{2.24}$$

$$\langle il|\, A\, |kj\rangle \rightsquigarrow A^\Gamma \quad \text{(partial transpose)}. \tag{2.25}$$

Definition 2.17. A $(2,2)$-tensor T is called *perfect* if its reshaping into a matrix $U \in U(d^2)$ is unitary for every possible bipartition of its four indices. The resulting matrix U is then called a *2-unitary*.

A unitary U that remains unitary under reshuffling is also known as *dual unitary*. Similarly, a unitary U whose partial transpose is also unitary is called Γ-*dual unitary*.

[3] See Ref. [10], p. 239 for more details

For a bipartite matrix $U \in U(d^2)$ that can be written as a tensor product of two sub-matrices $U = U_1 \otimes U_2$, the following holds [46]:

$$U^R = U_1^R \otimes U_2^R \quad \text{and} \quad U^\Gamma = U_1^\Gamma \otimes U_2^\Gamma. \tag{2.26}$$

Thus, if U is 2-unitary, its sub-matrices are also 2-unitary [46].

Proposition 2.17.1. *If $U \in U(d^2)$ is 2-unitary, then its partial transpose is also 2-unitary.*

Proof. Let $U \in U(d^2)$ be 2-unitary, then U^Γ and $(U^\Gamma)^\Gamma = U$ are unitary per definition. Moreover, one has $(U^\Gamma)^R = (U^R)S$, where S denotes the partial swap[4]. Since U^R is unitary per definition, $(U^\Gamma)^R = (U^R)S$ is also unitary, and hence U^Γ is 2-unitary. □

For higher-order tensors one can make the following generalisation:

Definition 2.18. [41] A (k, k)-tensor T is called *k-unitary* if its reshaping into a matrix $U \in U(d^k)$ is unitary for every possible bipartition of its $2k$ indices.

A weaker condition is given by *multiunitarity*:

Definition 2.19. [41] A (k, k)-tensor T is called *multiunitary* if its reshaping into a matrix $U \in U(d^k)$ is unitary for some, but not all, of the $\frac{1}{2}\binom{2k}{k}$ possible index permutations.

These concepts and there applications are extensively discussed from a geometric point of view in Ref. [74].

Proposition 2.19.1. *[41] Every pair of orthogonal Latin squares of order d gives rise to a 2-unitary matrix in dimension d^2.*

2-unitaries are closely related to so-called *absolutely maximally entangled (AME)-states*:

Definition 2.20. [41] An *absolutely maximally entangled* state of N parties, each with local dimension d, i.e. an AME(N, d) state, is a pure state whose reduced density matrices are maximally mixed for every bipartition into $k \leq N/2$ subsystems:

$$\rho_k = \frac{1}{d^k} \mathbb{I}_{d^k}, \quad \forall k \leq \frac{N}{2}. \tag{2.27}$$

[4] US corresponds to the following index change: $\langle ij| U |kl\rangle \to \langle ij| U |lk\rangle$.

Example 1. [33] For $N = 2 = d$ the Bell-states are AME-states:

$$|\Phi^+\rangle = \frac{1}{\sqrt{2}}\big(|0\rangle_A \otimes |0\rangle_B + |1\rangle_A \otimes |1\rangle_B\big), \tag{2.28}$$

$$|\Phi^-\rangle = \frac{1}{\sqrt{2}}\big(|0\rangle_A \otimes |0\rangle_B - |1\rangle_A \otimes |1\rangle_B\big), \tag{2.29}$$

$$|\Psi^+\rangle = \frac{1}{\sqrt{2}}\big(|0\rangle_A \otimes |1\rangle_B + |1\rangle_A \otimes |0\rangle_B\big), \tag{2.30}$$

$$|\Psi^-\rangle = \frac{1}{\sqrt{2}}\big(|0\rangle_A \otimes |1\rangle_B - |1\rangle_A \otimes |0\rangle_B\big) \tag{2.31}$$

$$\tag{2.32}$$

Another key example is when $N = 4$. Consider a state on four subsystems of local dimension d (labeled A, B, C, D):

$$|\Phi(4,d)\rangle = \frac{1}{d}\sum_{i,j=0}^{d-1} |i\rangle_A\, |j\rangle_B \otimes |\Psi_{ij}\rangle_{CD}\,. \tag{2.33}$$

Theorem 2.20.1. *[41] The existence of a 2-unitary matrix is equivalent to the existence of an AME(4, d) state.*

Proof. Consider a state on four subsystems of local dimension d :

$$|\Phi(4,d)\rangle = \frac{1}{d}\sum_{i,j=0}^{d-1} |i\rangle_A\, |j\rangle_B \otimes |\Psi_{ij}\rangle_{CD}\,, \tag{2.34}$$

where

$$|\Psi_{ij}\rangle_{CD} = U_{ij}\, |i\rangle_C\, |j\rangle_D\,, \tag{2.35}$$

and $U_{ij} = \sum_{k,l=0}^{d-1} T^{ij}_{kl}\, |kl\rangle\, \langle ij|$ is a 2-unitary. By slight abuse of notation, the corresponding perfect tensor will be denoted by T^{kl}_{ij}. The full state can then be written as:

$$|\Phi(4,d)\rangle = \frac{1}{d}\sum_{i,j,k,l=0}^{d-1} T_{ijkl}\, |i\rangle_A\, |j\rangle_B\, |k\rangle_C\, |l\rangle_D\,. \tag{2.36}$$

The density operator associated to this state is given by:

$$\rho = |\Phi\rangle\langle\Phi| = \frac{1}{d^2}\sum_{i,j,k,l,m,n,r,s=0}^{d-1} T_{ijkl}T^{mnrs\dagger}|i\rangle_A|j\rangle_B|k\rangle_C|l\rangle_D\,\langle m|_A\,\langle n|_B\,\langle r|_C\,\langle s|_D\,. \tag{2.37}$$

The state described by this operator can be partitioned into two subsystems of size two in three different ways: $AB|CD$, $AD|CB$ and $AC|BD$. Tracing out the subsystem AB one finds:

$$\mathrm{tr}_{AB}(\rho) = \frac{1}{d^2}\sum_{m,n,k,l,r,s=0}^{d-1} T_{mnkl}T^{mnrs\dagger}|k\rangle_C|l\rangle_D\,\langle r|_C\,\langle s|_D\,.$$

This is equal to

$$\frac{1}{d^2}\mathbb{I}_{CD}, \tag{2.38}$$

if and only if

$$(TT^\dagger)^{rs}_{kl} = \delta^r_k\delta^s_l \tag{2.39}$$

which means that the tensor T^{kl}_{ij} reshaped into a matrix has to be unitary. Since one can do this for all three bipartitions,one finds that the state $|\Phi\rangle$ is an AME(4, d)-state if and only if the tensors T^{kl}_{ij}, T^{ki}_{lj} and T^{jl}_{ik} reshaped into a matrix are unitary, i.e. T^{kl}_{ij} is perfect. □

Theorem 2.20.2. *[41] The existence of a QOLS(d) is equivalent to the existence of an AME(4, d) state.*

Proof. AME ⇒ OQLS(d).

Consider an AME(4, d)-state which, following the proof of the previous theorem, can be written as:

$$|\Phi(4,d)\rangle = \frac{1}{d}\sum_{i,j=0}^{d-1}|i\rangle_A|j\rangle_B|\Psi_{ij}\rangle_{CD}, \tag{2.40}$$

where $|\Psi_{ij}\rangle \in H_{CD}$. By considering the vectors corresponding to the subsystems A and B as index sets, one can arrange the $|\Psi_{ij}\rangle$ in a $d \times d$ grid. Due to the AME-properties, one finds that for every bipartition the following holds:

$$\frac{1}{d^2}\mathbb{I}_{AC} = \mathrm{tr}_{BD}(|\Psi_{ij}\rangle \langle \Psi_{ij}|). \tag{2.41}$$

But this is equivalent to

$$\begin{aligned}
\frac{1}{d^2}\mathbb{I}_{AC} &= \frac{1}{d^2}\mathrm{tr}_{BD}\left(\sum_{i,j,k,l=0}^{d-1} |ij\rangle \langle kl| \otimes |\Psi_{ij}\rangle \langle \Psi_{kl}|\right) \\
&= \frac{1}{d^2}\sum_{i,k=0}^{d-1} |i\rangle \langle k| \otimes \mathrm{tr}_D\left(\sum_{j=0}^{d-1} |\Psi_{ij}\rangle \langle \Psi_{kj}|\right) \\
&= \frac{1}{d^2}\left(\mathbb{I}_A \otimes \mathrm{tr}_D\left(\sum_{j=0}^{d-1} |\Psi_{ij}\rangle \langle \Psi_{ij}|\right) + \sum_{i\neq k,i,k=0}^{d-1} |i\rangle \langle k| \otimes \mathrm{tr}_D\left(\sum_{j=0}^{d-1} |\Psi_{ij}\rangle \langle \Psi_{kj}|\right)\right).
\end{aligned}$$

This is only true, if

$$\mathrm{tr}_D\left(\sum_{j=0}^{d-1} |\Psi_{ij}\rangle \langle \Psi_{ij}|\right) = \mathbb{I}_C \text{ and} \tag{2.42}$$

$$\mathrm{tr}_D\left(\sum_{j=0}^{d-1} |\Psi_{ij}\rangle \langle \Psi_{kj}|\right) = 0. \tag{2.43}$$

This proves condition i) of Def. 2.16. Analogously, one can prove condition ii) of Def. 2.16. Condition i) holds because every bipartition of $|\Phi(4,d)\rangle$ is maximally entangled: Consider the setting from above and choose the OQLS entries to be given by the states associated to the subsystem CD. Due to the AME-property one then finds

$$\rho_\Psi = \sum_{m,n=0}^{d-1} |\Psi_{mn}\rangle \langle \Psi_{mn}| = \frac{1}{d^2}\mathbb{I}_{CD} \tag{2.44}$$

via tracing out the subsystem AB.

QOLS(d) $\Rightarrow$ AME.

Conversely, if one has two orthogonal quantum Latin squares forming a $d \times d$ grid with entries $|\Psi\rangle$, one can use each entry to construct a state

$$|\Phi\rangle = \frac{1}{d} \sum_{i,j=0}^{d-1} |i\rangle_A |j\rangle_B |\Psi_{ij}\rangle_{CD}.$$

Analogously to the calculation above, one can show that this state is an AME(4, d)-state using condition i) and ii) of Def. 2.16. □

It follows that the existence of MOLS, QOLS, AME(4, d) states, and 2-unitaries are intimately related.

This correspondence can be generalised to higher rank tensors:

Proposition 2.20.1. *[41] Every k-unitary of dimension d^k corresponds to an AME(2k, d) state.*

The existence of $\mathrm{AME}(4, d)$- states for arbitrary dimensions d is a widely discussed topic. Refs. [58, 59] give a broad overview with the most important cases summarised below:

For $d = 2$ no $\mathrm{AME}(4, 2)$ and hence no 2-unitary of dimension 4 exists. This is has been proven by Higuchi and Sudbery in Ref. [55]. For the cases $d = 3, 4, 5$ a standard constructive route is via combinatorial designs (orthogonal arrays, OLS and MOLS). These can be used to produce 2-unitary matrices and thus $\mathrm{AME}(4, d)$-states. For prime-power dimensions one usually gets constructions from stabilizer codes and finite-field methods [58]. The case $d = 6$ is tied to Euler's "36 officers" problem and the non-existence of a pair of orthogonal Latin squares of order 6 showing that there cannot exist a 2-unitary and hence an $\mathrm{AME}(4, 6)$-state that arises from a classical combinatorial structure (compare to the discussion on the existence of MOLS in the previous section). However, the explicit construction of a 2-unitary of dimension 36 in Ref. [99] being equivalent to a genuinely quantum orthogonal Latin square proved the existence of $\mathrm{AME}(4, 6)$-states demonstrating the usefulness of quantum combinatorics.

2.1.4 Hadamard Matrices

Hadamard matrices have a wide range of applications: from combinatorics and signal processing, to error-correcting codes and quantum computing [8]. In this work, they are primarily of interest in the context of 2-unitary matrices.

Definition 2.21. [20] A *complex Hadamard matrix* of order n is a square matrix $H \in \mathbb{C}^{n \times n}$ such that the following holds:

$$|H_{ij}| = 1 \text{ for all } i, j \in [n],$$
$$HH^\dagger = n\mathbb{I}_n.$$

If all entries are powers of q-th roots of unity, i.e. $(H_{ij})^q = 1$ for all $i, j \in [n]$, then the Hadamard matrix is said to be of *Butson-type* [20].

2.1.5 Doubly Perfect Sequences

The study of unimodular sequences originates in harmonic analysis and combinatorics and plays an important role in signal processing, where *bi-unimodular* sequences, i.e. unimodular sequences whose discrete Fourier transform is also unimodular, are relevant in communication systems and radar systems [5].

Let $\omega_d = \exp(2\pi i/d)$ be a primitive d-th root of unity. A *unimodular sequence* of length d^{2n} and phase d is a sequence defined as:

$$\Lambda(\mathbf{a}) = \omega_d^{f(a_0,\dots,a_{2n-1})} = [\lambda_0, \dots, \lambda_{d^{2n-1}}], \tag{2.45}$$

where $f(\mathbf{a}) = f(a_0, \dots, a_{2n-1})$ is a function $f : \mathbb{Z}_d^{2n} \to \mathbb{Z}$. Throughout this thesis, vectors will be denoted by using bold font.

Definition 2.22. Given a sequence $\Lambda(\mathbf{a}) = \omega_d^{f(a_0,\dots,a_{n-1})}$, its *discrete Fourier transform (DFT)* is given by:

$$\mathcal{F}(\Lambda)(\mathbf{k}) = \Lambda(\mathbf{a})\omega_d^{-[\mathbf{k},\mathbf{a}]}, \tag{2.46}$$

where

$$[\mathbf{k}, \mathbf{a}] = \mathbf{k}^T J\mathbf{a}, \quad \text{with} \quad J = \begin{pmatrix} 0 & \mathbb{I}_n \\ -\mathbb{I}_n & 0 \end{pmatrix} \tag{2.47}$$

defines the *symplectic product* on $\mathbb{Z}_d^{2n}$.

In the following, the *absolute value of a sequence* is defined as:

$$|\Lambda| := [|\lambda_0|, \dots, |\lambda_{d^{2n-1}}|]. \tag{2.48}$$

For a unimodular sequence Λ it is easy to verify that its absolute value is given by the all-one array:

$$|\Lambda| = [1, \ldots, 1]. \tag{2.49}$$

A bi-unimodular sequence Λ additionally satisfies:

$$|\mathcal{F}(\Lambda)| = [1, \ldots, 1]. \tag{2.50}$$

Definition 2.23. Given a sequence Λ of length d^{2n} and phase d, its *auto-correlation* is defined as:

$$(\Lambda \star \Lambda)(\mathbf{a}) = \sum_{\mathbf{b} \in \mathbb{Z}_d^{2n}} \Lambda(\mathbf{a} + \mathbf{b})\overline{\Lambda(\mathbf{b})}. \tag{2.51}$$

One important concept that can be derived from this is the concept of *perfect sequences*, i.e. sequences with zero auto-correlation (also known as ZAC or CAZAC sequences), having their roots in radar and communication theory [5][5].

Definition 2.24. A sequence Λ of length d^{2n} is called *perfect* if its auto-correlation satisfies:

$$(\Lambda \star \Lambda)(\mathbf{a}) = \delta(\mathbf{a})\lambda_0 = [\lambda_0, 0, \ldots, 0], \tag{2.52}$$

i.e., the auto-correlation vanishes for all off-peak values of $\mathbf{a}$.

Similarly, one can define a *twisted* auto-correlation:

Definition 2.25. Given a sequence Λ of length d^{2n} and phase d, its *twisted auto-correlation* is defined as:

$$(\Lambda \tilde{\star} \Lambda)(\mathbf{a}) = \sum_{\mathbf{b} \in \mathbb{Z}_d^{2n}} \omega_d^{[\mathbf{a},\mathbf{b}]} \Lambda(\mathbf{a} + \mathbf{b})\overline{\Lambda(\mathbf{b})}. \tag{2.53}$$

The twisted auto-correlation can vanish on all off-peak elements. This motivates the following definition:

Definition 2.26. A perfect sequence Λ of length d^{2n} is called *doubly perfect*, if the following holds:

$$(\Lambda \tilde{\star} \Lambda)(\mathbf{a}) = \delta(\mathbf{a})\tilde{\lambda_0} = [\tilde{\lambda}_0, 0, \ldots, 0].$$

[5] The property of the sequences that all entries of the autocorrelation except from the peak are zero, ensures that the incoming radar signals do not interfere with the outgoing signals.

For a bi-unimodular doubly perfect sequence, it is straightforward to verify that $\lambda_0 = \tilde{\lambda}_0 = d^{2n}$.

Example 1. [95] The following bi-unimodular sequence of length 36 and period 3 is doubly perfect:

$$\Lambda = \exp\left(\frac{2\pi i}{3}[0,2,2,0,0,1,0,1,1,1,2,1,0,2,0,2,2,2,2,0,2,2,2,1,1,1,2,0,\right.$$
$$\left. 2,2,0,1,2,2,1,0]\right).$$

Theorem 2.26.1. *[46] If Λ is a bi-unimodular, doubly perfect sequence, then so is $\mathcal{F}(\Lambda)$.*

Proof. Since Λ is bi-unimodular, its Fourier transform is unimodular:

$$|\mathcal{F}(\Lambda)| = [1, \ldots, 1].$$

- **Auto-correlation:** Let Λ be perfect, i.e., $(\Lambda \star \Lambda)(\mathbf{a}) = \delta(\mathbf{a})d^{2n}$. Using the convolution theorem:

$$\mathcal{F}(\Lambda \star \Lambda)(\mathbf{a}) = d^n\, \overline{\mathcal{F}(\Lambda)}(\mathbf{a})\, \mathcal{F}(\Lambda)(\mathbf{a}), \tag{2.54}$$

  and applying the Fourier transform again, one obtains:

$$\begin{aligned} \mathcal{F}(\mathcal{F}(\Lambda) \star \mathcal{F}(\Lambda))(\mathbf{a}) &= d^n\, \overline{\mathcal{F}^2(\Lambda)}(\mathbf{a})\, \mathcal{F}^2(\Lambda)(\mathbf{a}) & (2.55)\\ &= \delta(\mathbf{a})d^n, & (2.56) \end{aligned}$$

  which implies:

$$(\mathcal{F}(\Lambda) \star \mathcal{F}(\Lambda))(\mathbf{a}) = \mathcal{F}^{-1}(\delta(\mathbf{a})) \cdot d^n = \delta(\mathbf{a})d^{2n}. \tag{2.57}$$

- **Twisted auto-correlation:** Let $(\Lambda\tilde{\star}\Lambda)(\mathbf{a}) = \delta(\mathbf{a})d^{2n}$. Then:

$$(\mathcal{F}(\Lambda)\tilde{\star}\mathcal{F}(\Lambda))(\mathbf{a}) = \sum_{\mathbf{b}} \mathcal{F}(\Lambda)(\mathbf{a}+\mathbf{b})\overline{\mathcal{F}(\Lambda)(\mathbf{b})}\omega_d^{[\mathbf{a},\mathbf{b}]} \tag{2.58}$$

$$= \sum_{\mathbf{b},\mathbf{l},\mathbf{k}} \Lambda(\mathbf{k})\overline{\Lambda(\mathbf{l})}\omega_d^{[\mathbf{b},\mathbf{l}]-[\mathbf{a}+\mathbf{b},\mathbf{k}]+[\mathbf{a},\mathbf{b}]} \tag{2.59}$$

$$= \sum_{\mathbf{l},\mathbf{k}} \Lambda(\mathbf{k})\overline{\Lambda(\mathbf{l})}\omega_d^{-[\mathbf{a},\mathbf{k}]} \sum_{\mathbf{b}} \omega_d^{[\mathbf{k}+\mathbf{a}-\mathbf{l},\mathbf{b}]} \tag{2.60}$$

$$= \sum_{\mathbf{l},\mathbf{k}} \Lambda(\mathbf{l}-\mathbf{a})\overline{\Lambda(\mathbf{l})}\omega_d^{-[\mathbf{a},\mathbf{l}]} \tag{2.61}$$

$$= \delta(\mathbf{a})d^{2n}. \tag{2.62}$$

Thus, $\mathcal{F}(\Lambda)$ is also bi-unimodular and doubly perfect. □

There are additional transformations under which doubly perfect sequences remain invariant. The following proposition can be found in a similar spirit in Ref. [46]:

Proposition 2.26.1. *Let $\Lambda(\mathbf{a})$ be a bi-unimodular doubly perfect sequence. Then the sequences*

i) $\tilde{\Lambda}(\mathbf{a}) = \Lambda(\mathbf{a}) \cdot \omega_d^{[\mathbf{b},\mathbf{a}]}$

ii) $\tilde{\Lambda}(\mathbf{a}) = \Lambda(\mathbf{a}-\mathbf{b})$

are also bi-unimodular doubly perfect.

Proof. Let $\Lambda(\mathbf{a})$ be a bi-unimodular doubly perfect sequence.

i) Consider $\tilde{\Lambda}(\mathbf{a}) = \Lambda(\mathbf{a}) \cdot \omega_d^{[\mathbf{b},\mathbf{a}]}$. Then:

$$|\tilde{\Lambda}(\mathbf{a})| = |\Lambda(\mathbf{a})| \cdot |\omega_d^{[\mathbf{b},\mathbf{a}]}| = 1. \tag{2.63}$$

Hence $\tilde{\Lambda}(\mathbf{a}) = \Lambda(\mathbf{a}) \cdot \omega_d^{[\mathbf{b},\mathbf{a}]}$ is also unimodular. The Fourier transformation of $\tilde{\Lambda}(\mathbf{a}) = \Lambda(\mathbf{a}) \cdot \omega_d^{[\mathbf{b},\mathbf{a}]}$ is given by:

$$\mathcal{F}(\tilde{\Lambda})(\mathbf{a}) = \tilde{\Lambda}(\mathbf{k})\omega_d^{-[\mathbf{a},\mathbf{k}]} = \Lambda(\mathbf{k}) \cdot \omega_d^{[\mathbf{b},\mathbf{k}]-[\mathbf{a},\mathbf{k}]} = \Lambda(\mathbf{k}) \cdot \omega_d^{[\mathbf{b}-\mathbf{a},\mathbf{k}]} \tag{2.64}$$

which leads to:

$$|\mathcal{F}(\tilde{\Lambda})(\mathbf{a})| = |\Lambda(\mathbf{k})| \cdot |\omega_d^{[\mathbf{b}-\mathbf{a},\mathbf{k}]}| = 1. \tag{2.65}$$

The auto-correlation picks up a global phase factor yielding:

$$(\tilde{\Lambda} \star \tilde{\Lambda})(\mathbf{a}) = \sum_{\mathbf{k}\in\mathbb{Z}_d^n} \Lambda(\mathbf{a}+\mathbf{k})\omega^{[\mathbf{b},\mathbf{a}+\mathbf{k}]}\overline{\Lambda(\mathbf{k})}\omega^{-[\mathbf{b},\mathbf{k}]} \tag{2.66}$$

$$= \sum_{\mathbf{k}\in\mathbb{Z}_d^n} \Lambda(\mathbf{a}+\mathbf{k})\overline{\Lambda(\mathbf{k})}\omega^{[\mathbf{b},\mathbf{a}]} \tag{2.67}$$

$$= \delta(\mathbf{a}) \cdot \omega_d^{[\mathbf{b},\mathbf{a}]}. \tag{2.68}$$

Hence the auto-correlation vanishes on all elements except the peak element. Similarly, for the twisted auto-correlation one gets:

$$(\tilde{\Lambda}\tilde{\star}\tilde{\Lambda})(\mathbf{a}) = \sum_{\mathbf{k}\in\mathbb{Z}_d^n} \Lambda(\mathbf{a}+\mathbf{k})\omega^{[\mathbf{b},\mathbf{a}+\mathbf{k}]}\overline{\Lambda(\mathbf{k})}\omega^{-[\mathbf{b},\mathbf{k}]}\omega^{[\mathbf{k},\mathbf{a}]} \tag{2.69}$$

$$= \sum_{\mathbf{k}\in\mathbb{Z}_d^n} \Lambda(\mathbf{a}+\mathbf{k})\overline{\Lambda(\mathbf{k})}\omega^{[\mathbf{k},\mathbf{a}]}\omega^{[\mathbf{b},\mathbf{a}]} \tag{2.70}$$

$$= \delta(\mathbf{a}) \cdot \omega_d^{[\mathbf{b},\mathbf{a}]}. \tag{2.71}$$

ii) Now consider $\tilde{\Lambda}(\mathbf{a}) = \Lambda(\mathbf{a}-\mathbf{b})$. First note that:

$$|\tilde{\Lambda}(\mathbf{a})| = |\Lambda(\mathbf{a}-\mathbf{l})| = 1, \tag{2.72}$$

since the shift only permutes the entries in the array Λ and does not change their values. For the DFT one finds :

$$|\mathcal{F}(\tilde{\Lambda})(\mathbf{a})| = |\mathcal{F}(\Lambda(\mathbf{a}-\mathbf{l}))| = |\Lambda(\mathbf{k})| \cdot |\omega_d^{-[\mathbf{a}-\mathbf{l},\mathbf{k}]}| = 1. \tag{2.73}$$

Moreover, for the auto correlation one finds:

$$(\tilde{\Lambda} \star \tilde{\Lambda})(\mathbf{a}) = \sum_{\mathbf{k}\in\mathbb{Z}_d^n} \Lambda(\mathbf{a}+\mathbf{k}-\mathbf{b})\overline{\Lambda(\mathbf{k}-\mathbf{b})}. \tag{2.74}$$

$$\tag{2.75}$$

Now setting : $\mathbf{k}-\mathbf{b}=\mathbf{l}$, one gets:

$$(\tilde{\Lambda} \star \tilde{\Lambda})(\mathbf{a}) = \sum_{\mathbf{l}-\mathbf{b}\in\mathbb{Z}_d^n} \Lambda(\mathbf{a}+\mathbf{l})\overline{\Lambda(\mathbf{l})} \tag{2.76}$$

$$= \delta(\mathbf{a}). \tag{2.77}$$

Analogously, for the twisted auto-correlation one finds:

$$(\tilde{\Lambda}\tilde{\star}\tilde{\Lambda})(\mathbf{a}) = \sum_{\mathbf{k}\in\mathbb{Z}_d^n} \Lambda(\mathbf{a}+\mathbf{k}-\mathbf{b})\overline{\Lambda(\mathbf{k}-\mathbf{b})}\omega^{[\mathbf{a},\mathbf{k}-\mathbf{b}]} \tag{2.78}$$

$$= \sum_{\mathbf{l}-\mathbf{b}\in\mathbb{Z}_d^n} \Lambda(\mathbf{a}+\mathbf{l})\overline{\Lambda(\mathbf{l})}\omega^{[\mathbf{a},\mathbf{l}]} \tag{2.79}$$

$$= \delta(\mathbf{a}). \tag{2.80}$$

□

In particular, Λ remains doubly perfect under multiplication by a scalar $z \in \mathbb{C}$ with $|z| = 1$.

2.2 Algebras

Algebras serve not only as a bridge between linear algebra and abstract algebra in terms of representation theory (see Section 2.3), they also play a significant role in quantum theory. Throughout this thesis, it will be assumed that an algebra $\mathcal{A}$ over a field $\mathbb{F}$ with multiplication $\cdot : \mathcal{A} \times \mathcal{A} \to \mathcal{A}$ is associative and unital:

- *associative* if $(A \cdot B) \cdot C = A \cdot (B \cdot C)$ for all $A, B, C \in \mathcal{A}$,
- *unital* if there exists an element $\mathbf{1} \in \mathcal{A}$ such that $\mathbf{1} \cdot A = A \cdot \mathbf{1} = A$ for all $A \in \mathcal{A}$.

In the following the $\cdot$ will be omitted and instead of $A \cdot B$ the shorthand notation AB will be adopted.

To model quantum theory, one requires an operation corresponding to complex conjugation and transposition. This is achieved by introducing an anti-linear involution on $\mathcal{A}$, namely $\dagger : \mathcal{A} \to \mathcal{A}$, satisfying:

- $(A^\dagger)^\dagger = A$
- $(AB)^\dagger = B^\dagger A^\dagger$

for all $A, B \in \mathcal{A}$. This concept leads to what is known as a $*$-algebra [86], where the star stems from the fact, that the dagger operation is often denoted with a star in the literature. A closely related concept is that of a C^*-algebra:

Definition 2.27. [86] A C^*-algebra is an algebra $\mathcal{A}$ together with an anti-linear involution $\dagger : \mathcal{A} \to \mathcal{A}$ and a norm $\|\cdot\|$ such that:

- $\|A \cdot B\| \leq \|A\|\|B\|$
- $\|A^\dagger A\| = \|A\|^2$

for all $A, B \in \mathcal{A}$, and such that $\mathcal{A}$ is complete with respect to the metric induced by the norm.

Since in this thesis only finite dimensions are considered, the latter property, i.e. the norm being complete with respect to the metric, is irrelevant for now.

Every finite-dimensional C^*-algebra is unital and possesses a canonical trace [86], i.e. a linear functional $\mathrm{tr} : \mathcal{A} \to \mathbb{C}$ satisfying $\mathrm{tr}(AB) = \mathrm{tr}(BA)$ for all $A, B \in \mathcal{A}$, which scaled by $1/\mathrm{tr}(\mathbf{1})$ leads to the notion of the *canonical normalised trace*: $\tau = (1/\mathrm{tr}(\mathbf{1}))\mathrm{tr}$.

In quantum theory, operators can be described using C^*-algebras:

Example 1. Let H be a finite dimensional Hilbert space with inner product $\langle \cdot, \cdot \rangle : H \otimes H \to \mathbb{C}$. This induces a Hilbert space $L(H) \cong H \otimes H^*$ whose elements are bounded linear maps from H to itself: $X \in L(H)$. The inner product of this space is given by the *Hilbert-Schmidt inner product*

$$\langle X, Y \rangle_{HS} = \tau(X^\dagger Y),$$

where $X^\dagger, Y \in L(H)$ and τ denotes the normalised trace: $\tau(A) = \mathrm{tr}(A)/\mathrm{tr}(\mathbf{1})$. Together with the anti-linear involution $\dagger : X \mapsto X^\dagger$ and the *Hilbert-Schmidt norm*

$$\|X\|_{HS} = \sqrt{\tau(X^\dagger X)},$$

this space forms a C^*-algebra.[6]

Finite-dimensional C^*-algebras can be described in terms of matrices, as the following theorem suggests:

Theorem 2.27.1. *[86] Every d-dimensional C^*-algebra $\mathcal{C}$ is $*$-isomorphic[7] to a direct sum of full matrix algebras:*

$$\mathcal{C} \cong \bigoplus_{i=1}^{k} \mathcal{M}_{n_i}(\mathbb{C}) \tag{2.81}$$

[6] This norm coincides with the Schatten 2-norm, which satisfies the Cauchy-Schwarz inequality: $\|XY\|_2 \leq \|X\|_2\|Y\|_2$ for $X, Y \in L(H)$.

[7] That means that the isomorphism preserves the dagger structure.

for some $n_1, \dots, n_k$ *satisfying* $\sum_{j=1}^{k} n_j^2 = d$.

The elements of $L(L(H))$, i.e. bounded linear maps from $H \otimes H^*$ to itself, again form a $*$-algebra, the algebra of *superoperators*, with inner product given by

$$\langle S, R \rangle_S = \mathrm{Tr}(SR^\dagger),$$

where $S^\dagger, R \in L(L(H))$.

One can associate to each subalgebra $\mathcal{A} \subseteq L(H)$ a superoperator $P_\mathcal{A} \in L(L(H)) \cong H \otimes H^* \otimes H^* \otimes H$ that projects onto $\mathcal{A}$. This is also referred to as the *trace-preserving expectation onto* $\mathcal{A}$.

2.2.1 Quasi-orthogonal Systems of Subalgebras

In the following, the orthogonality relations between two subalgebras of $L(H)$ will be discussed. This has also been addressed in Refs. [114, 88, 92].

Definition 2.28. Let $\mathcal{A}, \mathcal{B}$ be two $*$-subalgebras of $L(H)$, and let $P_\mathcal{A}, P_\mathcal{B} \in L(L(H))$ be the corresponding projection operators. Then $\mathcal{A}$ and $\mathcal{B}$ are said to be *quasi-orthogonal*, if

$$\mathrm{Tr}(P_\mathcal{A} P_\mathcal{B}^\dagger) = 1. \tag{2.82}$$

Since any two subalgebras $\mathcal{A}, \mathcal{B}$ always contain the unit element, they cannot be orthogonal. However, their trace-free parts

$$\mathcal{A}_0 = \{A \in \mathcal{A} \mid \mathrm{tr}(A) = 0\}, \quad \mathcal{B}_0 = \{B \in \mathcal{B} \mid \mathrm{tr}(B) = 0\}$$

can be orthogonal with respect to the Hilbert-Schmidt inner product. Therefore, $\mathcal{A}$ and $\mathcal{B}$ are quasi-orthogonal if and only if their trace-free parts are orthogonal. To see this, decompose each subalgebra into the orthogonal sum of its trace-free part and the identity:

$$\mathcal{A} = \mathcal{A}_0 \oplus \mathbb{C}\mathbf{1}, \quad \mathcal{B} = \mathcal{B}_0 \oplus \mathbb{C}\mathbf{1}.$$

The corresponding projectors are then given by:

$$P_\mathcal{A} = P_{\mathcal{A}_0} + P_\mathbf{1}, \quad P_\mathcal{B} = P_{\mathcal{B}_0} + P_\mathbf{1}.$$

Taking the trace of their product yields:

$$\begin{aligned} \mathrm{Tr}(P_\mathcal{A} P_\mathcal{B}^\dagger) &= \mathrm{Tr}(P_{\mathcal{A}_0} P_{\mathcal{B}_0}^\dagger) + \mathrm{Tr}(P_{\mathcal{A}_0} P_\mathbf{1}) + \mathrm{Tr}(P_{\mathcal{B}_0} P_\mathbf{1}) + \mathrm{Tr}(P_\mathbf{1} P_\mathbf{1}) \\ &= \mathrm{Tr}(P_{\mathcal{A}_0} P_{\mathcal{B}_0}^\dagger) + 1, \end{aligned}$$

where the fact that $\mathcal{A}_0$ and $\mathcal{B}_0$ are orthogonal to $\mathbb{C}\mathbf{1}$ was used in the second step. This expression equals 1 if and only if $\mathrm{Tr}(P_{\mathcal{A}_0}P_{\mathcal{B}_0}) = 0$, i.e. if $\mathcal{A}_0$ and $\mathcal{B}_0$ are orthogonal.

A third characterisation is given by the following:

Proposition 2.28.1. *[114] Two $*$-subalgebras $\mathcal{A}, \mathcal{B} \subseteq L(H)$ are quasi-orthogonal if and only if*

$$\tau(AB) = \tau(A)\tau(B) \tag{2.83}$$

for all $A \in \mathcal{A}$ and $B \in \mathcal{B}$.

Proof. Let $A \in \mathcal{A}$ and $B \in \mathcal{B}$. Define their trace-free parts as:

$$A_0 = A - \tau(A)\mathbf{1} \in \mathcal{A}_0, \quad B_0 = B - \tau(B)\mathbf{1} \in \mathcal{B}_0.$$

Then:

$$\begin{aligned} \tau(A_0B_0^\dagger) &= \tau(AB^\dagger) - \tau(\tau(A)B^\dagger) - \tau(\tau(B)^*A) + \tau(\tau(A)\tau(B)^*\mathbf{1}) \\ &= \tau(AB^\dagger) - \tau(A)\tau(B^\dagger), \end{aligned}$$

since τ is linear and $\tau(\mathbf{1}) = 1$. Therefore, $\tau(A_0B_0^\dagger) = 0$ holds, if and only if $\tau(AB^\dagger) = \tau(A)\tau(B^\dagger)$, which is equivalent to Eq. (2.83). □

Before giving an explicit example for quasi-orthogonal subalgebras, it is instructive to introduce two important types of subalgebras, namely *factors* and *maximal Abelian subalgebras (MASAs)*, that are useful to model quantum systems consisting of multiple parties. This will be done in the next section.

2.2.2 Local and Delocalised Subalgebras

Let $\mathcal{A} \subseteq L(H)$ be a subalgebra. The *commutant* of $\mathcal{A}$ is defined as

$$\mathcal{A}' = \{Y \in L(H) \mid XY = YX \ \ \forall X \in \mathcal{A}\}.$$

Each subalgebra $\mathcal{A}$ has a commutant $\mathcal{A}'$ which can be used to define its *center*:

$$Z(\mathcal{A}) = \mathcal{A} \cap \mathcal{A}'. \tag{2.84}$$

Depending on the form of its center, i.e. on how one can characterise the relation between the subalgebra and its commutant, a subalgebra has a particular structure.

Definition 2.29. [114] A subalgebra $\mathcal{A} \subseteq L(H)$ is called a *factor*, if $Z(\mathcal{A}) = \mathcal{A} \cap \mathcal{A}' = \mathbb{C}\mathbf{1}$, i.e. $\mathcal{A}$ has a trivial center.

The counterpart to this is the notion of a *maximal Abelian subalgebra (MASA)*, i.e. a maximal set of commuting operators that is closed under taking adjoints. Since commuting self-adjoint matrices are simultaneously diagonalisable, a MASA corresponds to the set of all diagonal matrices [86]. Now it is straightforward to verify that the commutant of a MASA is given by the whole algebra and thus one can characterise MASAs also as follows:

Proposition 2.29.1. *A subalgebra $\mathcal{A} \subseteq L(H)$ is a MASA, if and only if it is equal to its own center: $Z(\mathcal{A}) = \mathcal{A}$.*

One can show that a set of quasi-orthogonal MASAs of the matrix algebra $\mathcal{M}_d(\mathbb{C})$ that spans $\mathcal{M}_d(\mathbb{C})$, corresponds to a collection of $d+1$ MUBs in $\mathbb{C}^d$ [86].

The following example relates quasi-orthogonality of MASAs to affine quantum designs:

Example 1. Consider Example 1 from Section 2.1 again, i.e. consider the affine quantum design that resembles the combinatorial structure of an affine plane. Since $\mathcal{M}_{d^2}(\mathbb{C}) \cong \mathcal{M}_d(\mathbb{C}) \otimes \mathcal{M}_d(\mathbb{C})$, one can try to decompose the projectors into a tensor product of elements of $\mathcal{M}_d(\mathbb{C})$ via:

$$p_i^a = \sum_{m,k=1}^{d} c_{k,m,i}^a e_{k,i}^a \otimes f_{m,i}^a, \tag{2.85}$$

where $c_{k,m}^a \in \mathbb{C}$ and $e_k^a, f_m^a \in \mathcal{M}_d(\mathbb{C})$ for all k, m and a. Since the p_i^a's are orthogonal projectors, i.e. $(p_i^a)^2 = p_i^a = (p_i^a)^\dagger$, it is easy to see that the following has to hold:

- $c_{k,m,i}^a = 1$ for all k, m and a.
- The elements $e_{k,i}^a$ and $f_{m,i}^a$ also have to be orthogonal projectors for all k, m and a.

Hence the expression reduces to:

$$p_i^a = \sum_{k,m=1}^{d} e_{k,i}^a \otimes f_{m,i}^a. \tag{2.86}$$

Imposing the conditions $i)$-$iii)$ from above, one further gets:

i) $\Rightarrow \sum_{k,m=1}^{d} \mathrm{tr}(e_{k,i}^{a})\mathrm{tr}(f_{m,i}^{a}) = d$,

ii) $\Rightarrow \sum_{k,m=1}^{d} \sum_{a=1}^{d+1} \sum_{i=1}^{d} e_{k,i}^{a} \otimes f_{i,m}^{a} = (d+1)(\mathbb{I}_d \otimes \mathbb{I}_d)$,

iii) $\Rightarrow \sum_{k,l,m,n=1}^{d} \mathrm{tr}(e_{k,i}^{a} e_{l,j}^{b})\mathrm{tr}(f_{m,i}^{a} f_{n,j}^{b}) = (1-\delta_{ab}) + d \cdot \delta_{ab}\delta_{ij}$.

Moreover, commutativity of the p_i^a's implies:

$$\sum_{k,l,m,n=1}^{d} [e_{l,i}^{a} \otimes f_{m,i}^{a}, e_{l,j}^{b} \otimes f_{n,j}^{b}] = 0. \tag{2.87}$$

One obvious choice would be to set $f_{m,i}^{a} := \mathbb{I}_d$ for all $i \in [d]$, $a \in [d+1]$ and to assume that the $e_{l,i}^{a}$ form $d+1$ MUBs in $\mathcal{M}_d(\mathbb{C})$. Then the resulting set of orthogonal classes $\{A_1, ..., A_{d+1}\}$, where $A_a = \{p_1^a, ..., p_d^a\}$, actually form $d+1$ quasi-orthogonal subalgebras of $\mathcal{M}_{d^2}(\mathbb{C}) \cong \mathcal{M}_d(\mathbb{C}) \otimes \mathcal{M}_d(\mathbb{C})$ and would be of the form

$$A_a \cong M_a \otimes \mathbb{I}, \quad \forall a \in [d+1]. \tag{2.88}$$

Here the M_a are mutually quasi-orthogonal MASAs.

This example is closely related to the combinatorial k-nets over an algebra which have been discussed by Nietert et al. in Ref. [86].

Recall that every finite-dimensional $*$-algebra is $*$-isomorphic to a direct sum of matrix algebras. In this context, one finds:

Proposition 2.29.2. *[114] Let $\mathcal{A}$ be a factor of a matrix algebra $\mathcal{M}_n(\mathbb{C}) \cong \mathcal{M}_k(\mathbb{C}) \otimes \mathcal{M}_l(\mathbb{C})$ with $k \cdot l = n$. Then*

$$\mathcal{A} \cong \mathcal{M}_k(\mathbb{C}) \otimes \mathbb{I}_l.$$

Coming back to quantum theory, one can now give the following example:

Example 2. Consider the Hilbert space $H = H_L \otimes H_R$, where $\dim(H_L) = n = \dim(H_R)$. That is, H is the tensor product of a "left" and a "right" space. Then the space of superoperators $L(H)$ can be associated with the tensor product of two *local* algebras: a "left" and a "right" subalgebra:

$$L(H) \cong L(H_L) \otimes L(H_R).$$

In terms of matrix algebras this can be written as follows:

$$L(H) \cong \mathcal{M}_{n^2}(\mathbb{C}) \cong \mathcal{M}_n(\mathbb{C}) \otimes \mathcal{M}_n(\mathbb{C}),$$

with $L(H_L) \cong \mathcal{M}_n(\mathbb{C}) \cong \mathcal{M}_n(\mathbb{C}) \otimes \mathbb{I}_n$ and $L(H_R) \cong \mathcal{M}_n(\mathbb{C}) \cong \mathbb{I}_n \otimes \mathcal{M}_n(\mathbb{C})$. Hence the left and the right space give rise to left and right factors in $\mathcal{M}_{n^2}(\mathbb{C})$. It is straightforward to verify that $\mathcal{L} := L(H_L)$ and $\mathcal{R} := L(H_R)$ are each others commutant, and that the following holds:

$$Z_L(\mathcal{L}) = \mathcal{L} \cap \mathcal{L}' = \mathcal{L} \cap \mathcal{R} = \mathbb{C}\mathbf{1} = \mathcal{R}' \cap \mathcal{R} = Z_R(\mathcal{R}). \tag{2.89}$$

Throughout this thesis, the terms *left (right) factor* or *left (right) subalgebra* will be used when referring to $L(H_L)$ and $L(H_R)$, respectively.

Proposition 2.29.3. *Let $\mathcal{A}$ be a factor of the matrix algebra $\mathcal{M}_n(\mathbb{C})$ and let $\mathcal{A}'$ be its commutant. Then $\mathcal{A}$ and $\mathcal{A}'$ are quasi-orthogonal.*

Proof. Let $\mathcal{A}$ be a factor of $\mathcal{M}_n(\mathbb{C})$. According to Prop. 2.29.2, $\mathcal{A}$ is isomorphic to $\mathcal{M}_k(\mathbb{C}) \otimes \mathbb{I}_l$ where $k \cdot l = n$. But then $\mathcal{A}'$ has to be isomorphic to $\mathbb{I}_{l'} \otimes \mathcal{M}_{k'}(\mathbb{C})$ where $k' \cdot l' = n$. It it now easy to verify that:

$$\tau(AA') = \tau(A)\tau(A') \tag{2.90}$$

for each choice of $A \in \mathcal{A}$ and $A' \in \mathcal{A}'$. □

In particular, the two local subalgebras $\mathcal{L}$ and $\mathcal{R}$ in Example 2 are quasi-orthogonal.

Definition 2.30. A subalgebra $\mathcal{A} \subseteq L(H_L \otimes H_R)$ is called *delocalised* if it is quasi-orthogonal to both the left and right subalgebra, $\mathcal{L}$ and $\mathcal{R}$.

2.3 Representation Theory of Finite Groups

As many physical processes inhabit symmetries that can be traced back to groups, the representation of these groups via matrices play a crucial role in quantum physics. This section will give a brief review of some fundamental concepts in representation theory with special emphasis on irreducible representations of finite groups and character theory. Familiarity with the basic notions of group theory will be assumed (see Ref. [101] for an introduction).

Definition 2.31. ([31], p. 3) Let G be a finite group. A *representation of* G on a $\mathbb{K}$-vector space V is a group homomorphism

$$\rho : G \to \mathrm{GL}(V), \tag{2.91}$$

where $\mathrm{GL}(V)$ denotes the general linear group on V. The dimensions of the representation is given by the dimension of the vector space V.

If V is a Hilbert space, a representation of a group G is a group homomorphism from G to $L(H)$. Two representations can be linked via a morphism:

Definition 2.32. ([31], p. 3) Let (ρ, V) and (ρ', W) be two representations of a group G. A map $\phi : V \to W$ such that $\rho' \circ \phi = \phi \circ \rho$ holds is called an *intertwiner* or equivalently a morphism between representations.

2.3.1 Irreducible representations

Definition 2.33. ([31], p. 4) A *subrepresentation* of a representation (ρ, V) is a representation $\rho|_W$ on a subspace $W \subset \mathrm{GL}(V)$ such that $\rho|_W(g) = \rho(g)|_W$. A representation is called *irreducible* if there exists no non-zero subspace of $\mathrm{GL}(V)$.

In the course of this thesis, for the term "irreducible representation" often the acronym "irrep" will be adopted. In fact, both terms will be used interchangeably.

Proposition 2.33.1. *([31], p. 4) Given two representations (ρ, V) and (ρ', W) of a group G, their tensor product $(\rho \otimes \rho', V \otimes W)$ and their direct sum $(\rho \oplus \rho', V \oplus W)$ are again representations.*

The proof can be found on p. 4 in [31].

Theorem 2.33.1. *([31], p. 7) Any representation (ρ, V) of a finite group G, where V is a $\mathbb{K}$-vector space, can be decomposed into a direct sum of distinct irreducible representations.*

The proof can be found on p. 7 in [31].

The following theorem is a direct consequence from Burnside's theorem and has been proven in Ref. [107].

Proposition 2.33.2. *Let H be a Hilbert space and G be a finite group with representation ρ on H. Then the linear span of $\{\rho(g)\}_{g\in G}$ is equal to $L(H)$, if and only if ρ is irreducible.*

2.3.2 Character Theory

Representation theory can also be rephrased in terms of character theory, which bears the advantage that the irrelevant information that is contained in a representation is neglected by only considering the traces of the matrices that lie in the image of the representation homomorphism ([60], p. 14).

Definition 2.34. ([60], p. 14) Let (ρ, V) be a representation of a group G. Its *character* χ is defined to be

$$\chi(g) = \mathrm{tr}(\rho(g)), \tag{2.92}$$

where $\mathrm{tr}(.)$ denotes the trace on $\mathrm{GL}(V)$. The *degree* of χ is given by $\chi(e)$ and equals the dimension of ρ.

One also says that χ is *afforded* by ρ. The following lemma and its proof can be found in similar spirit in Ref. [60] on page 20.

Lemma 2.34.1. *Let χ be a character afforded by a representation (ρ, V) of the group G. Then the following holds for any $g \in G$ with order n:*

i) $\chi(g) = \sum \epsilon_i$, *where* $\epsilon_i^n = 1$,

ii) $|\chi(g)| \leq \chi(e)$,

iii) $\chi(e) = \dim(V)$.

Proof. i) Let $g \in G$ have order n, i.e. $g^n = e$. Then: $\mathbb{I} = \rho(e) = \rho(g^n) = \rho(g)^n$ and hence $\rho(g)$ also has order n. Since ρ is unitary, one can diagonalise $\rho(g)$ with all eigenvalues being on the main diagonal. From $\rho(g)^n = \mathbb{I}$ it then follows, that all eigenvalues ϵ_i have to be n^{th}-roots of unity, i.e. $\epsilon^n = 1$. Now taking the trace one gets: $\chi(g) = \mathrm{tr}(\rho(g)) = \sum_i \epsilon_i$.

ii) $|\chi(g)| = |\sum_i \epsilon_i| \leq \sum_i |\epsilon_i| = \chi(e)$.

iii) $\chi(e) = \mathrm{tr}(\rho(e)) = \mathrm{tr}(\mathbb{I}) = \dim(V)$.

□

Since characters are constant on the conjugacy classes of a group[8], a character can also be understood as a *class function* $\chi : G \to \mathbb{C}$. One can define a scalar product on the space of class functions:

[8]This can easily be verified using the cyclic properties of the trace.

Definition 2.35. ([60], p. 20) Given a group G and two characters χ_1 and χ_2, their scalar product is defined to be:

$$\langle \chi_1, \chi_2 \rangle = \frac{1}{|G|} \sum_{g \in G} \chi_1(g) \overline{\chi_2(g)}. \tag{2.93}$$

The characters of all irreducible representations of a group are orthonormal with respect to this scalar product:

Proposition 2.35.1. *([60], p. 21) Let G be a group. Then*

$$\langle \chi_i, \chi_j \rangle = \delta_{ij} \quad \forall \quad \chi_i, \chi_j \in \mathrm{Irr}(G). \tag{2.94}$$

It follows that the irreducible characters form a basis on the space of class functions. With that one can determine any representation by its character via a *character table*, i.e. a table that displays the values of all characters of a certain group G for each conjugacy class of G.

Theorem 2.35.1. *([60], p. 19) Let G be a group with character χ. Then the following holds for all $h \in G$:*

$$\frac{1}{|G|} \sum_{g \in G} \chi(gh) \overline{\chi(g)} = \frac{\chi(h)}{\chi(e)}. \tag{2.95}$$

The proof can be found in Ref. [60] on page 19.

For $h = e$ this implies:

$$\frac{1}{|G|} \sum_{g \in G} \chi(g) \overline{\chi(g)} = \frac{1}{|G|} \sum_{g \in G} |\chi(g)|^2 = 1. \tag{2.96}$$

Definition 2.36. Let G be a group and χ be a character. One says that χ *factorises*, if

$$\chi(e)\chi(gh) = \chi(g)\chi(h) \quad \forall \quad g, h \in G. \tag{2.97}$$

Proposition 2.36.1. *Let G be a group with d-dimensional representation (ρ, V) and let A, B be subgroups of G. The algebras $\mathcal{A} = \langle \rho(A) \rangle$ and $\mathcal{B} = \langle \rho(B) \rangle$ are quasi-orthogonal, if and only if the character afforded by ρ factorises.*

Proof. Let $N \in \mathcal{A} = \langle \rho(A) \rangle$ and $M \in \mathcal{B} = \langle \rho(B) \rangle$ such that $N = \rho(a)$ and $M = \rho(b)$ for some $a \in A$ and $b \in B$. Since ρ is a group homomorphism one finds: $N' = \rho(ab) = \rho(a) \cdot \rho(b) = N \cdot M$. Thus, one has: $\tau(N') = \tau(\rho(ab)) = \tau(\rho(a) \cdot \rho(b)) = \tau(N \cdot M)$. One can now apply Prop. 2.28.1 and get that $\chi(e)\chi(ab) = d \cdot \chi(ab) = d \cdot \mathrm{tr}(\rho(a) \cdot \rho(b)) = d \cdot \mathrm{tr}(N \cdot M) = \mathrm{tr}(N)\mathrm{tr}(M) = \mathrm{tr}(\rho(a))\mathrm{tr}(\rho(b)) = \chi(a)\chi(b)$ iff $\mathcal{A}$ and $\mathcal{B}$ are quasi-orthogonal. □

Given a representation ρ of a group G, its kernel is defined by: $\ker(\rho) = \{g \in G \mid \rho(g) = \mathbb{I}\}$ ([60], p. 23). In particular, the kernel is a normal subgroup of G ([60], p. 23). It is straightforward to see that, in the language of character theory, the kernel of a character χ is given by $\{g \in G \mid \chi(g) = \chi(e)\}$([60], p. 23).

Definition 2.37. ([60], p. 28) A representation (ρ, G) is called *faithful*, if its kernel is the trivial group $\{e_G\}$.

In particular, a character is called faithful, if the set $\{g \in G \mid \chi(g) = \chi(e)\}$ only contains the identity element of G.

Proposition 2.37.1. *Let G be a compact group with d^2-dimensional representation (ρ, V) and let R, L be two subgroups, the following are equivalent*

- $\chi(l^{-1}rlr^{-1}) = \chi(e) = d^2$ *for all $r \in R, l \in L$, i.e. $l^{-1}rlr^{-1} \in \ker(\chi)$ for all $r \in R, l \in L$.*
- $\langle\rho(L)\rangle$ *and* $\langle\rho(R)\rangle$ *are each others commutant.*

Proof. To see that, first assume that all elements of $\langle\rho(R)\rangle$ and $\langle\rho(L)\rangle$ commute. One then finds for all $l \in L$ and $r \in R$:

$$\begin{aligned}\chi(l^{-1}rlr^{-1}) &= \mathrm{tr}(\rho(l^{-1}rlr^{-1})) = \mathrm{tr}(\rho(l^{-1})\rho(r)\rho(l)\rho(r^{-1})) \\ &= \mathrm{tr}(\rho(l^{-1})\rho(l)\rho(r)\rho(r^{-1})) = \chi(e) = d^2.\end{aligned}$$

On the other hand, for a compact group G with representation ρ on a Hilbert space, one can assume that ρ is unitary. Now, if

$$\chi(l^{-1}rlr^{-1}) = \chi(e) = d^2$$

holds for all $l \in L$ and $r \in R$, one finds that the following has to hold:

$$d^2 = \chi(l^{-1}rlr^{-1}) = \mathrm{tr}(\rho(l^{-1}rlr^{-1})).$$

Since ρ is unitary, $\rho(l^{-1}rlr^{-1}) = \rho(l)^{-1}\rho(r)\rho(l)\rho(r)^{-1}$ has to be the identity, as a unitary U has trace equal to its dimension iff it is the identity. But this means that $\rho(l)$ and $\rho(r)$ have to commute for all pairs of l, r and in particular, that $l^{-1}rlr^{-1} \in \ker(\chi)$. □

Similarly to the the algebraic case, one can define the center of a group G, $Z(G)$, as the set of elements of G that commute with all elements of G. It is easy to see, that the image of any element of $Z(G)$ under a representation has to be proportional to the identity matrix. Thus, the elements of $Z(G)$ all have a character whose absolute value is equal to $\chi(e)$. This motivates the following definition:

Definition 2.38. ([60], p. 26) Let χ be a character of a group G. Then $Z(\chi) = \{g \in G \mid |\chi(g)| = \chi(e)\}$.

Lemma 2.38.1. *([60], p. 27) Let χ be a character of a group G and ρ be the representation associated to χ. Then*

- $Z(\chi) = \{g \in G \mid \rho(g) = \epsilon \mathbb{I}$ *for some* $\epsilon \in \mathbb{C}\}$
- $Z(G) = \bigcap\{Z(\chi) \mid \chi \in \mathrm{Irr}(G)\}$

The proof can be found on page 27 in Ref. [60]

Proposition 2.38.1. *Let G be a group and χ be a character afforded by the representation $\rho : G \to L(H)$. Within the subgroup $Z(\chi)$ the character factorises.*

Proof. Consider $Z(\chi) = \{g \in G \mid \rho(g) = \epsilon\mathbb{I},\ \epsilon \in \mathbb{C}\}$. Then for any $l, r \in Z(\chi)$ one can find $\epsilon, \epsilon' \in \mathbb{C}$ such that

$$\rho(l) = \epsilon\mathbb{I} \quad \text{and} \quad \rho(r) = \epsilon'\mathbb{I}.$$

From this one can conclude that

$$\rho(l \cdot r) = \rho(l) \cdot \rho(r) = \epsilon\epsilon'\mathbb{I}. \tag{2.98}$$

Taking the trace one finds

$$\chi(l \cdot r) = \epsilon\epsilon'\chi(e) = \frac{1}{\chi(e)}\epsilon\epsilon'\chi(e)^2 = \frac{1}{\chi(e)}\chi(l)\chi(r) \tag{2.99}$$

and thus the character factorises. □

Proposition 2.38.2. *([60], p. 28) Let $\chi \in \mathrm{Irr}(G)$. Then*

$$\chi(e)^2 \leq |G : Z(\chi)| \tag{2.100}$$

with equality, if and only if χ vanishes on $G - Z(\chi)$.

The proof can be found on page 28 in [60]. When equality holds in the above equation, one has: $Z(\chi) = Z(G)$ [60]. This motivates the following definition:

Definition 2.39. [63] A group G with irreducible character χ is said to be of *central type*, if $\chi(e)^2 = |G : Z(G)|$.

The last two theorems of this section turn out to be useful in Section 3.2 . Their proofs can be found in [60] on page 38.

Theorem 2.39.1. *([60], p. 38) Let* $\chi \in \mathrm{Irr}(G)$*. Then* $\chi(e) \mid |G|$.

Theorem 2.39.2. *([60], p. 38) Let* $\chi \in \mathrm{Irr}(G)$*. Then* $\chi(e) \mid |G : Z(\chi)|$.

2.3.3 The Clifford Group

Since processes in quantum mechanics are modelled by unitary operators, one of the main interests here lies in unitary representations, i.e. representations of the form $\rho : G \to U(H)$ where $U(H)$ denotes the unitary group of a Hilbert space H. One prominent example of such a representation is the representation of $\mathbb{Z}_d^n$ that generates the *Weyl-Heisenberg group (WH-group)*, which is a subgroup of $U(H)$. The WH-group can be used to characterise quantum kinematics and quantum states [112].

For an n-qudit system, this group is defined as follows:

Definition 2.40. (Generalised Weyl-Heisenberg group)
Let $Z = \mathrm{diag}(1, \omega_d, \omega_d^2, ..., \omega_d^{d-1})$, where $\omega_d = \exp(2\pi i/d)$ and

$$X = \begin{pmatrix} 0 & 0 & ... & 0 & 1 \\ 1 & 0 & ... & 0 & 0 \\ 0 & 1 & ... & 0 & 0 \\ . & . & ... & . & . \\ 0 & 0 & ... & 1 & 0 \end{pmatrix} \tag{2.101}$$

be the discrete Weyl-Heisenberg operators in $\mathcal{M}_d(\mathbb{C})$, defining an orthogonal basis in $\mathcal{M}_d(\mathbb{C})$ via $\{X^i Z^j\}_{i,j\in[d]}$. One can generalise this to higher dimensions, i.e. $\mathcal{M}_{d^n}(\mathbb{C}) \cong (\mathcal{M}_d(\mathbb{C}))^{\bigotimes^n}$ by defining a basis

$$\{\bigotimes_{i=1}^{n} X^{k_i} Z^{l_i}\} \text{ where } k_i, l_i \in \mathbb{Z}_d \ \forall \ i \in [n]. \tag{2.102}$$

One can now define a projective homomorphism $\pi : \mathbb{Z}_d^{2n} \cong \mathbb{Z}_d^n \times \mathbb{Z}_d^n \to \mathcal{M}_{d^n}(\mathbb{C})$ by

$$\pi : \mathbf{u} = (k_1, .., k_n, l_1, .., l_n) \mapsto \bigotimes_{i=1}^{n} X^{k_i} Z^{l_i}. \tag{2.103}$$

Setting

$$J = \begin{pmatrix} 0 & \mathbb{I}_n \\ -\mathbb{I}_n & 0 \end{pmatrix}, \tag{2.104}$$

a symplectic product in $\mathbb{Z}_d^{2n}$ can be defined by:

$$[\mathbf{u}, \mathbf{u}'] = \mathbf{u} J \mathbf{u}' \mod d. \tag{2.105}$$

Now, setting

$$\tau_d = \exp(\pi i / d), \tag{2.106}$$

i.e. $\tau_d^2 = \omega_d$, one can show that the following has to hold:

$$\pi(\mathbf{u})\pi(\mathbf{u}') = \tau_d^{[\mathbf{u},\mathbf{u}']} \pi(\mathbf{u} + \mathbf{u}'). \tag{2.107}$$

Thus, $\pi(\mathbf{u})$ and $\pi(\mathbf{u}')$ commute if and only if the symplectic of $\mathbf{u}$ and $\mathbf{u}'$ is equal to zero or d.

Denoting the Weyl-Heisenberg group by $H(d^n)$, its normaliser $N_{U(d^n)}(H(d^n))$ in $U(d^n)$ is given by the so-called *Clifford group*:

Definition 2.41. [112] The Clifford group consists of all unitary operators $X \in U(d^n)$ for which the following holds

$$X H(d^n) X^{-1} = H(d^n). \tag{2.108}$$

Prominent examples of unitaries that lie in the Clifford group are given by the Hadamard, $\pi/4$-phase and controlled-X gates, all of which are elementary quantum gates used in quantum computing [112].

Chinese Remaindering of the Clifford Group

The construction in Def. 2.40 is based on the assumption that the Hilbert space has dimension d. If d can be realised as the product of two smaller numbers d_1, d_2 that are coprime, one can apply the *Chinese remainder theorem* to the phase space $\mathbb{Z}_d^4 = \mathbb{Z}_{d_1 d_2}^4$:

Theorem 2.41.1 (Chinese Remainder Theorem). *([85], p. 629) Let $n = n_1, ..., n_k$ with $n_i \in \mathbb{N}/\{0\}$ for all $i \in [k]$. If the n_i are pairwise coprime for all $i \in [k]$, then there exists an isomorphism*

$$\mathbb{Z}_n \cong \mathbb{Z}_{n_1} \times .. \times \mathbb{Z}_{n_k}, \quad x \bmod n \mapsto (x \bmod n_1, ..., x \bmod n_k). \tag{2.109}$$

The following discussion is inspired by Ref.s [2, 28].

Let $d = d_1 \cdot d_2$, where d_1 and d_2 are coprime, and $\pi : \mathbb{Z}_d^4 \to \mathcal{M}_{d^2}(\mathbb{C})$ be a projective representation of $\mathbb{Z}_d^4$ on $\mathcal{M}_{d^2}(\mathbb{C})$ such that

$$\pi : (a_1, a_2, a_3, a_4) \mapsto X_d^{a_1} Z_d^{a_2} \otimes X_d^{a_3} Z_d^{a_4} \tag{2.110}$$

with

$$\pi(\mathbf{u})\pi(\mathbf{u}') = \tau_d^{[\mathbf{u},\mathbf{u}']} \pi(\mathbf{u} + \mathbf{u}'), \tag{2.111}$$

where $\tau = \omega_d^2 = \exp(\pi i/d)$ and $[\mathbf{u}, \mathbf{u}'] = \mathbf{u}^T J \mathbf{u}'$. According to the Chinese remainder theorem one can define an isomorphism

$$\mathbb{Z}_d \cong \mathbb{Z}_{d_1} \times \mathbb{Z}_{d_2}, \quad a_i \bmod d \mapsto (k_i \bmod d_1, x_i \bmod d_2) \tag{2.112}$$

for each component a_i of a tuple $\mathbf{u} = (a_1, a_2, a_3, a_4) \in \mathbb{Z}_d^4$. Moreover, the following holds

$$\mathcal{M}_{d^2}(\mathbb{C}) = \mathcal{M}_{(d_1 \cdot d_2)^2}(\mathbb{C}) \cong \mathcal{M}_{d_1^2}(\mathbb{C}) \otimes \mathcal{M}_{d_2^2}(\mathbb{C}) \cong (\mathcal{M}_{d_1}(\mathbb{C}) \otimes \mathcal{M}_{d_2}(\mathbb{C}))^{\otimes 2}.$$

Let d_i^{-1} denote the multiplicative inverse of d_i. One can then show that:

$$\omega_d = \omega_{d_1}^{d_2^{-1}} \omega_{d_2}^{d_1^{-1}}. \tag{2.113}$$

The representation homomorphism π can thus be redefined as follows:

$$\begin{aligned} \pi : (\mathbb{Z}_{d_1} \times \mathbb{Z}_{d_2})^4 &\to (\mathcal{M}_{d_1}(\mathbb{C}) \otimes \mathcal{M}_{d_2}(\mathbb{C}))^{\otimes 2}, \\ (\mathbf{k}, \mathbf{x}) &\mapsto (X_{d_1}^{k_1} Z_{d_1}^{d_2^{-1} k_2} \otimes X_{d_2}^{x_1} Z_{d_2}^{d_1^{-1} x_2}) \otimes (X_{d_1}^{k_3} Z_{d_1}^{d_2^{-1} k_4} \otimes X_{d_2}^{x_3} Z_{d_2}^{d_1^{-1} x_4}). \end{aligned}$$

The Weyl-Heisenberg actually provides an example of a *nice error basis*, a concept that was first introduced as unitary error bases in a representation-theoretic setting by Knill [65] and further discussed by Klappenecker and Roettler in Ref. [63].

Definition 2.42. [63] Let G be a group of order d^2 and $\pi : G \to U(d)$ be a projective unitary representation such that $\pi(g)\pi(h) = \omega(g,h)\pi(gh)$ for all $g, h \in G$ and a scalar function $\omega : G \times G \to \mathbb{C}^\times$. The set of unitary matrices $\{\pi(g) \in U(d) | g \in G\}$ is called a *nice error basis*, if

$$\mathrm{tr}(\pi(g)) = 0 \quad \forall\, g \in G \quad \text{with}\, g \neq e_G. \tag{2.114}$$

Given a nice error basis $\mathcal{E} = \{\pi(g) \in U(d) | g \in G\}$, one calls G its *index group* and the values of the function $\omega : G \times G \to \mathbb{C}^\times$ its *factor system*. Consider the cyclic group W, generated by the values of $\omega(g,h)$. Set $H := W \times G$ with group multiplication:

$$(a,g) \circ (b,h) = (ab\omega(g,h), gh), \quad \forall a,b \in W, g,h \in G. \tag{2.115}$$

One can show that H is a finite group with respect to this multiplication [63]. Every group isomorphic to such kind of group is called *abstract error group* [65, 63].

Theorem 2.42.1. *[63] A group H is an abstract error group, if and only if H is a group of central type with cyclic center $Z(H)$.*

2.4 Category Theory

Category theory is a branch of mathematics that organises mathematical objects by abstracting away from their internal structure and focusing instead on the relationships (morphisms) between them [73]. While playing a major role in abstract mathematics, like homological algebra and topology, it is also important in computer science and in theoretical physics. In fact, the field of categorical quantum theory provides a neat framework to model quantum processes and quantum protocols for quantum computations [54]. Categorical quantum theory distills quantum mechanics down to its compositional structure, capturing the essence of quantum processes in terms of objects, morphisms, and their interaction [54]. One of the most practical benefits of categorical quantum theory is its use of string diagrams to reason visually about quantum processes. Complex quantum protocols such as teleportation, entanglement swapping, or error correction become diagrams [54].

Moreover, categorical quantum theory formalises the interface between classical and quantum information [54].

In this section, the basic notions of categorical quantum theory will be explained. Starting with a brief recap of monoidal categories and monoidal functors, dagger structures and Frobenius algebras will be then explained, laying the foundation for categorical quantum theory. Building on this, it will be explained how complete positivity of algebraic maps can be modelled in a category theoretical context and how this can be used to define a category of quantum channels. The author refers to Maclane [73] and Heunen and Vicary [54] for further background on category theory and categorical quantum theory and to Ref. [118] for more details on the graphical calculus for open quantum systems.

Definition 2.43. ([54], p. 2) A *category* $\mathcal{C}$ consists of the following:

- a class of *objects* $\mathrm{obj}(\mathcal{C})$
- for every pair of objects A and B, a class of *morphisms* $\mathrm{Hom}_{\mathcal{C}}(A, B)$
- for every pair of morphisms $f : A \to B$, $g : B \longrightarrow C$, a composite $g \circ f : A \to C$
- for every object $A \in \mathrm{obj}(\mathcal{C})$, an identity morphism $\mathrm{id}_A : A \to A$

such that for all $A, B, C, D \in \mathrm{obj}(\mathcal{C})$ and all $f : A \to B$, $g : B \to C$, $h : C \to D$ $\in \mathrm{Hom}_{\mathcal{C}}$, the following holds

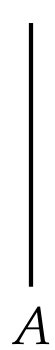
- *associativity*:

$$h \circ (g \circ f) = (h \circ g) \circ f, \tag{2.116}$$

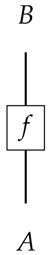
- *identity*:

$$\mathrm{id}_B \circ f = f \circ \mathrm{id}_A. \tag{2.117}$$

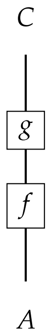
Graphically, one can represent objects as



and a morphism $f : A \to B$ as



where one reads the diagram from bottom to top. The concatenation of two morphisms $f : A \to B$ and $g : B \to C$ can be represented via:



The categories that will be mostly used in this thesis are the category of matrices and natural numbers, **Mat**($\mathbb{N}$), and the category of finite-dimensional Hilbert spaces and bounded linear maps, **FHilb**:

Example 1.

(i) ([54], p. 16) The category **FHilb** has as objects finite-dimensional Hilbert spaces and as morphisms bounded linear maps between Hilbert spaces. The composition is the composition of linear maps as ordinary functions and the identity morphisms are given by identity linear maps.

(ii) ([102], p. 4) The category **Mat**($\mathbb{N}$) of matrices over $\mathbb{N}$ has objects equal to the set of natural numbers and for $m, n \in \mathbb{N}$, a hom-set $\mathrm{Hom}_{\mathbf{Mat}(\mathbb{N})}(m, n)$ that is equal to the set of all $n \times m$-matrices over $\mathbb{N}$. The composition is defined by matrix multiplication and the identity morphism is given by the identity matrix. [9]

[9] One can exchange the field of natural numbers into an arbitrary number field.

Given two categories, one can define a map between them that relates objects to objects and morphisms to morphisms:

Definition 2.44. ([54], p. 9) Given two categories $\mathcal{C}$ and $\mathcal{D}$, a *functor* between these two categories is defined by the following data:

- for each object $A \in \mathrm{Obj}(\mathcal{C})$, there is an object $\mathcal{F}(A) \in \mathrm{Obj}(\mathcal{D})$
- for each morphism $f : A \to B$ in $\mathcal{C}$, there is a morphism $\mathcal{F}(f) : \mathcal{F}(A) \to \mathcal{F}(B)$ in $\mathcal{D}$

such that $\mathcal{F}$ respects composition

$$\mathcal{F}(g \circ f) = \mathcal{F}(g) \circ \mathcal{F}(f) \tag{2.118}$$

for all morphisms $f : A \to B$ and $g : B \to C$ in $\mathcal{C}$ and the following holds for every object A in $\mathcal{C}$:

$$\mathcal{F}(\mathrm{id}_A) = \mathrm{id}_{\mathcal{F}(A)}. \tag{2.119}$$

The above definition defines a *covariant* functor. There also exist *contravariant* functors that reverse the direction of the morphisms, such that $\mathcal{F}(g \circ f) = \mathcal{F}(f) \circ \mathcal{F}(g)$ holds ([54], p. 9).

Definition 2.45. ([54], p. 10) Let $\mathcal{F}, \mathcal{G} : \mathcal{C} \to \mathcal{D}$ be two functors. A *natural transformation* $\zeta : \mathcal{F} \to \mathcal{G}$ assigns to each object A in $\mathcal{C}$ a morphism

$$\zeta_A : \mathcal{F}(A) \to \mathcal{G}(A)$$

in $\mathcal{D}$, such that the following diagram commutes for every morphism $f : A \to B$ in $\mathcal{C}$:

$$\begin{array}{ccc} \mathcal{F}(A) & \xrightarrow{\zeta_A} & \mathcal{G}(A) \\ {\scriptstyle \mathcal{F}(f)}\big\downarrow & & \big\downarrow{\scriptstyle \mathcal{G}(f)} \\ \mathcal{F}(B) & \xrightarrow{\zeta_B} & \mathcal{G}(B) \end{array}$$

Definition 2.46. ([54], p. 10) A *natural isomorphism* is a natural transformation, where every component ζ_A is an isomorphism.

Definition 2.47. ([73], p. 93) A functor $\mathcal{F} : \mathcal{C} \to \mathcal{D}$ defines an equivalence of categories, if it is

- *essentially surjective*: for every object D in $\mathcal{D}$,there exists an object C in $\mathcal{C}$, such that $\mathcal{F}(C) \cong D$ in $\mathcal{D}$.
- *fully faithful*: for any pair C, C' of objects in $\mathcal{C}$, the map

$$\mathcal{F} : \mathrm{Hom}_{\mathcal{C}}(C, C') \longrightarrow \mathrm{Hom}_{\mathcal{D}}(\mathcal{F}(C), \mathcal{F}(C')) \tag{2.120}$$

  is bijective.

2.4.1 Monoidal Categories

In ordinary category theory, morphisms describe relationships between objects that can be composed in a sequential manner, but many systems (physical, computational, or logical) require parallel composition: putting things together not in sequence, but side by side. Monoidal categories do exactly this and hence provide a framework to model quantum systems.

Definition 2.48. ([54], p. 30) A *monoidal category* $(\mathcal{C}, \otimes_{\mathcal{C}}, \mathbb{I}_{\mathcal{C}})$ is comprised of the following data:

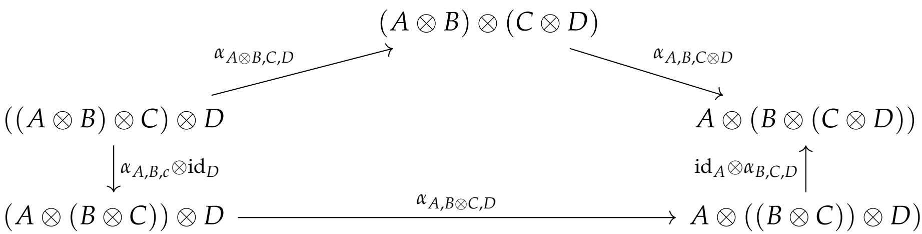
- a category $\mathcal{C}$,
- a functor $\otimes_{\mathcal{C}} : \mathcal{C} \times \mathcal{C} \to \mathcal{C}$ called the *tensor product* which associates to every pair of objects (A, B) in $\mathcal{C}$, an object $A \otimes_{\mathcal{C}} B$ in $\mathcal{C}$, and to every pair of morphism (f, g) in $\mathcal{C}$, a morphism $f \otimes_{\mathcal{C}} g$ in $\mathcal{C}$ with source and target given by the tensor products of the source and target objects,
- an object $\mathbb{I}_{\mathcal{C}}$ in $\mathcal{C}$ called the *tensor unit*,
- a natural isomorphism

$$\alpha : \otimes_{\mathcal{C}}(\otimes_{\mathcal{C}} \times \mathrm{id}) \to \otimes_{\mathcal{C}}(\mathrm{id} \times \otimes_{\mathcal{C}}) \tag{2.121}$$

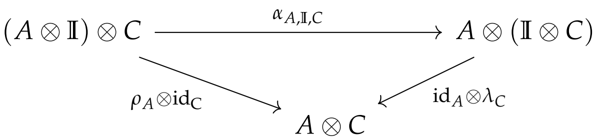
  called the *associator*,
- natural isomorphisms

$$\rho : \mathrm{id} \otimes_{\mathcal{C}} \mathbb{I}_{\mathcal{C}} \to \mathbb{I}_{\mathcal{C}}, \tag{2.122}$$
$$\lambda : \mathbb{I}_{\mathcal{C}} \otimes \mathrm{id} \to \mathbb{I}_{\mathcal{C}}, \tag{2.123}$$

  called *right- and left-unitor* respectively, such that the pentagon relation

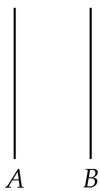


and the triangle identity

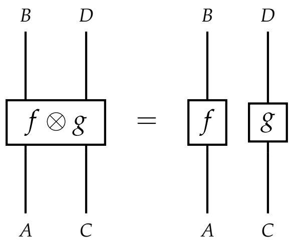


hold.

Graphically, the monoidal product of two objects $A, B \in \mathrm{obj}(\mathcal{C})$ will be expressed as two lines parallel to each other:



On two morphisms $f : A \to A', g : B \to B' \in \mathrm{Hom}_{\mathcal{C}}$, the monoidal product looks as follows:



The following example discusses the monoidal product in the categories $\mathbf{Mat}(\mathbb{N})$ and **FHilb**:

Example 1.

(i) ([54], p. 16) The category **FHilb** has as objects finite-dimensional Hilbert spaces and as morphisms bounded linear maps between Hilbert spaces. Composition is the composition of linear maps as ordinary functions and the identity morphisms are given by identity linear maps. The monoidal product is given by the tensor product on Hilbert spaces and the unit object is the one-dimensional Hilbert space $\mathbb{C}$.

(ii) ([102], p. 4) The category $\mathbf{Mat}(\mathbb{N})$ of matrices over $\mathbb{N}$ has objects given by natural numbers. For $m, n \in \mathbb{N}$, the Hom-set $\mathrm{Hom}_{\mathbf{Mat}(\mathbb{N})}(m, n)$ is the set of all $n \times m$-matrices over $\mathbb{N}$, composition being matrix multiplication. The monoidal product on objects is given by the multiplication of numbers and on morphisms by the Kronecker product of matrices. The monoidal unit is the natural number 1.

2.4.2 Special Dagger Frobenius Algebras

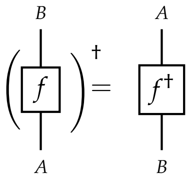
In order to define adjoint maps, one needs a categorical analogue that implements this. This is achieved by a so-called dagger functor:

Definition 2.49. ([54], p. 74) A *dagger category* is a category $\mathcal{C}$ equipped with a contravariant, involutive functor $(-)^\dagger : \mathcal{C}^{\mathrm{op}} \to \mathcal{C}$ such that:

- For every morphism $f : A \to B$, there exists a morphism $f^\dagger : B \to A$,
- $(f^\dagger)^\dagger = f$ for all morphisms $f \in \mathrm{Hom}_{\mathcal{C}}(A, B)$,
- $(g \circ f)^\dagger = f^\dagger \circ g^\dagger$ for all composable morphisms $f : A \to B, g : B \to C$,
- $\mathrm{id}_A^\dagger = \mathrm{id}_A$ for all objects $A \in \mathcal{C}$.

On objects the functor acts as the identity.

Graphically, the dagger-functor corresponds to a vertical reflection of the diagram:

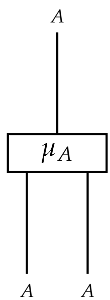


In order to fully model quantum theory, one needs a structure that models operations like discarding or initialising a quantum state and copying or deleting a quantum state. This can be achieved by *(co)monoids*:

Definition 2.50. ([54], p. 129) In a monoidal category, a *monoid* is a triple (M, μ, η) consisting of an object M and morphisms $\mu_M : M \otimes M \to M$ (multiplication) and $\eta_M : I \to M$ (unit) such that the following conditions are satisfied:

- *associativity:* $\mu_M \circ (\mu_M \otimes \mathrm{id}_M) = \mu_M \circ (\mathrm{id}_M \otimes \mu_M)$,
- *unitality:* $\mu_M \circ (\mathrm{id}_M \otimes \eta_M) = \mathrm{id}_M = \mu_M \circ (\eta_M \otimes \mathrm{id}_M)$.

One also refers to η as a *state*. Graphically, the multiplication and unit correspond to the following diagrams:

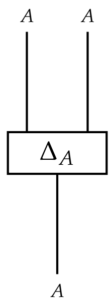


The dual concept is given by *comonoids*:

Definition 2.51. ([54], p. 128) In a monoidal category, a *comonoid* is a triple (M, Δ, ϵ) consisting of an object M and morphisms $\Delta_M : M \to M \otimes M$ (comultiplication) and $\epsilon_M : M \to I$ (counit) such that the following conditions are satisfied:

- *coassociativity:* $(\Delta_M \otimes \mathrm{id}_M) \circ \Delta_M = (\mathrm{id}_M \otimes \Delta_M) \circ \Delta_M$,
- *counitality:* $(\mathrm{id}_M \otimes \epsilon_M) \circ \Delta_M = \mathrm{id}_M = (\epsilon_M \otimes \mathrm{id}_M) \circ \Delta_M$.

One also refers to Δ as the copy map and to ϵ as an *effect*. Graphically, the comultiplication and counit correspond to the following diagrams:

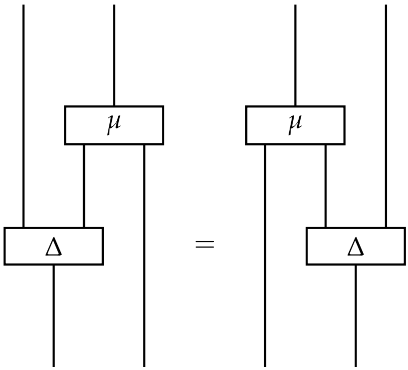


Combining these two notions gives rise to the following structure:

Definition 2.52. ([54], p. 148) In a monoidal category, a *Frobenius structure* consists of a pair of a monoid and a comonoid $A, \mu, \Delta, \eta, \epsilon$ such that the *Frobenius law* is satisfied:

$$\Delta \circ \mu = (\mu \otimes \mathrm{id}_A) \circ (\mathrm{id}_A \otimes \Delta) = (\mathrm{id}_A \otimes \mu) \circ (\Delta \otimes \mathrm{id}_A).$$

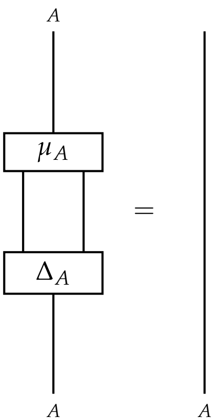
Graphically, the Frobenius law is given by:



Definition 2.53. ([54], p. 150) Let $(A, \mu, \eta, \Delta, \epsilon)$ be a Frobenius structure in a monoidal category. It is called *special* if the following condition holds:

$$\mu \circ \Delta = \mathrm{id}_A.$$

Graphically this is equivalent to



Special commutative dagger Frobenius structures provide the categorical framework to model classical data inside quantum systems:

Definition 2.54. ([54], p. 151) In a braided monoidal category, a *classical structure* is a special commutative dagger Frobenius algebra (†-SCFA).

They enable a diagrammatic, and algebraically rich way to represent measurement, copying, basis structures, and controlled operations.

Example 1. ([54], p. 147-151) In **FHilb**, special commutative dagger Frobenius structures correspond precisely to orthonormal bases. The comultiplication copies basis elements: $\Delta(|i\rangle) = |i\rangle \otimes |i\rangle$ and the counit $\epsilon(|i\rangle) = 1$ deletes elements.

A concept, that is closely related to units and counits is given by so-called *pointed structures*:

Definition 2.55. A *pointed* monoidal category is a monoidal category for which every object A is equipped with a canonical morphism $p_A : \mathbb{I} \to A$.

The counit in a Frobenius structure corresponds to a pointed structure in a pointed category. However, not every pointed structure corresponds to a counit of a Frobenius structure.

Example 1.

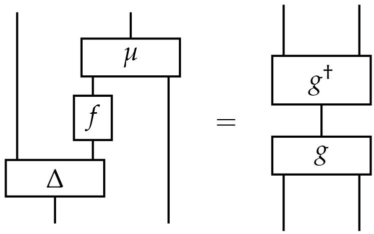
i) The category $\mathbf{CP}[\mathcal{C}]$ has a pointed structure given by the adjoint of the trace map $V \otimes V^* \to \mathbb{I}$.

ii) In **Mat**($\mathbb{N}$) a pointed structure is given by a column matrix with a 1 at every entry: $p_n : 1 \to n$.

2.4.3 Completely Positive Maps in Category Theory

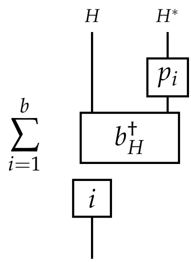
The concept of completely positive maps is well-established [77] and plays a significant role in quantum theory. Here Selinger's categorical description of completely positive maps [106], will be considered, exploiting the notion of dagger Frobenius structures, which was introduced in the previous section.

Definition 2.56. Let (A, μ_A, η_A) and (B, μ_B, η_B) be dagger Frobenius structures in a monoidal dagger category. A morphism $f : A \to B$ satisfies the *CP-condition*, if there exists some object X and some morphism $g : A \otimes B \to X$, such that the following equation holds:



One can show that, in a symmetric monoidal dagger category, a morphism that satisfies this condition constitutes a CP-map [54].

Example 1. In **FHilb**, consider a POVM consisting of b projections $p_i : H \to H$. One can define a completely positive map $\varphi : \mathbb{C}^b \to H \otimes H^*$ that sends the computational basis vector $|i\rangle$ to p_i. Graphically, one can represent φ as follows, where $b_H : \mathbb{C} \to H^* \otimes H$ is the evaluation map:



Proposition 2.56.1. *Let $(\mathcal{C}, \otimes_{\mathcal{C}}, \mathbb{I}_{\mathcal{C}})$ be a monoidal dagger category. There is a category* $\mathbf{CP}[\mathcal{C}]$ *in which*

- *objects are special symmetric dagger Frobenius structures in $\mathcal{C}$,*
- *morphisms are morphisms of $\mathcal{C}$ that satisfy the CP-condition.*

Example 2. In $\mathbf{CP}[\mathbf{FHilb}]$ objects are finite dimensional H^*-algebras, i.e. an algebra A that is also a Hilbert space with an anti-linear involution $\dagger$:

$A \to A$ satisfying $\langle ab|c\rangle = \langle b|a^\dagger c\rangle = \langle a|cb^\dagger\rangle$, and morphisms are completely positive maps.

A special case is the following subcategory of $\mathbf{CP}[\mathcal{C}]$:

Definition 2.57. The category $\mathbf{CP_c}[\mathcal{C}]$ has *classical structures* special commutative dagger Frobenius structures in $\mathcal{C}$, as objects and completely positive maps between these structures as morphisms. It is a subcategory of $\mathbf{CP}[\mathcal{C}]$.

Proposition 2.57.1 ([54], p. 241)**.** *The category* $\mathbf{CP_c}[\mathbf{FHilb}]$ *is monoidally equivalent to* $\mathbf{Mat}(\mathbb{N})$.

An interpretation of these constructions is the following: while $\mathcal{C}$ models pure state quantum mechanics and $\mathbf{CP}[\mathcal{C}]$ models mixed state quantum mechanics, $\mathbf{CP_c}[\mathcal{C}]$ describes statistical mechanics [54].

2.4.4 Arrow Categories

Just as ordinary categories describe how objects relate via arrows, arrow categories describe how arrows relate to each other via commuting squares. Hence they treat the morphisms of a category as objects in their own right. This shift in perspective is fundamental when reasoning about diagrams, natural transformations, and higher-order structures. Moreover, arrow categories are particularly useful in categorical quantum theory, as they describe transformations between processes.

Definition 2.58 ([102], p. 23-24)**.** For a category $\mathcal{C}$, its *arrow category* $\mathbf{Arr}[\mathcal{C}]$ is defined as follows:

- objects are triples (A, B, h) with $h : A \to B$ in $\mathcal{C}$,
- morphisms $\phi : (A, B, h) \to (A', B', h')$ are pairs of morphisms $\phi_A : A \to A'$ and $\phi_B : B \to B'$ in $\mathcal{C}$, such that the following diagram commutes:

$$\begin{array}{ccc} A & \xrightarrow{\phi_A} & A' \\ {\scriptstyle h}\downarrow & & \downarrow{\scriptstyle h'} \\ B & \xrightarrow{\phi_B} & B' \end{array}$$

Example 1. The arrow category of $\mathbf{Mat}(\mathbb{N})$, namely $\mathbf{Arr}[\mathbf{Mat}(\mathbb{N})]$, has objects that are matrices over the natural numbers $M_i : v_i \to b_i$ and morphisms that are pairs of matrices $N_v : v_1 \to v_2$, $N_b : b_1 \to b_2$ over the natural numbers, such that the following diagram commutes:

$$\begin{array}{ccc} v_1 & \xrightarrow{N_v} & v_2 \\ {\scriptstyle M_1}\downarrow & & \downarrow{\scriptstyle M_2} \\ b_1 & \xrightarrow{N_b} & b_2 \end{array}$$

In what follows, it will be shown, that arrow categories inherit certain structures from their underlying category. This includes functors, natural transformations and the monoidal product. These results are part of the present author's Master's thesis and can also be found in Appendix A of Ref. [37].

Proposition 2.58.1. *[37] Given a functor $F : \mathcal{C} \to \mathcal{D}$, applying the arrow construction to this functor, gives another functor $\widetilde{F} : \mathbf{Arr}[\mathcal{C}] \to \mathbf{Arr}[\mathcal{D}]$.*

Proof. Given a functor $F : \mathcal{C} \to \mathcal{D}$, one can define a functor $\widetilde{F} : \mathbf{Arr}[\mathcal{C}] \to \mathbf{Arr}[\mathcal{D}]$ as follows. On objects, one maps $f : A \to B$ in $\mathbf{Arr}[\mathcal{C}]$ to an object $F(f) : F(A) \to F(B)$ in $\mathbf{Arr}[\mathcal{D}]$. On morphisms, one maps $(\phi, \psi) : f \to f'$ in $\mathbf{Arr}[\mathcal{C}]$ to a morphism $\tilde{F}(\phi, \psi) = (F(\phi), F(\psi)) : F(f) \to F(f')$ in $\mathbf{Arr}[\mathcal{D}]$. This is valid because the diagram

$$\begin{array}{ccc} F(A) & \xrightarrow{F(\phi)} & F(A') \\ {\scriptstyle F(f)}\downarrow & & \downarrow{\scriptstyle F(f')} \\ F(B) & \xrightarrow{F(\psi)} & F(B') \end{array}$$

commutes due to functoriality of F. Moreover, one has

$$\widetilde{F}(\mathrm{id}_A, \mathrm{id}_B) = (F(\mathrm{id}_A), F(\mathrm{id}_B)) = (\mathrm{id}_{F(A)}, \mathrm{id}_{F(B)}), \tag{2.124}$$

where $(\mathrm{id}_A, \mathrm{id}_B)$ is the identity morphism in $\mathbf{Arr}[\mathcal{C}]$. Due to functoriality of F and because the concatenation of two commuting diagrams yields again a commuting diagram, $\tilde{F}$ also preserves composition. □

Similarly, a contravariant functor $F : \mathcal{C} \to \mathcal{D}$ gives rise to a contravariant functor $\widetilde{F} : \mathbf{Arr}[\mathcal{C}] \to \mathbf{Arr}[\mathcal{D}]$ [37].

Proposition 2.58.2. *[37] Let $F, G : \mathcal{C} \to \mathcal{D}$ be two functors between two categories $\mathcal{C}$ and $\mathcal{D}$, and let $\widetilde{F}, \widetilde{G} : \mathbf{Arr}[\mathcal{C}] \to \mathbf{Arr}[\mathcal{D}]$ be the induced functors on the arrow categories. A natural transformation $\eta : F \Rightarrow G$ induces a natural transformation $\tilde{\eta} : \tilde{F} \Rightarrow \tilde{G}$.*

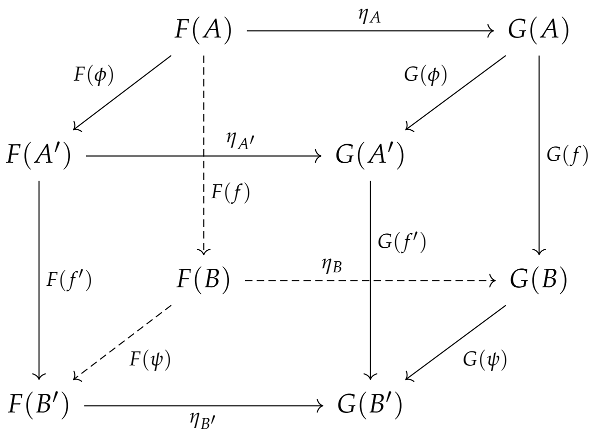
Proof. Let $\eta : F \Rightarrow G$ be a natural transformation that assigns to every object A in $\mathcal{C}$, a morphism $\eta_A : F(A) \to G(A)$, such that for any morphism $f : A \to B$ in $\mathcal{C}$ the following diagram (naturality condition) commutes:

$$\begin{array}{ccc} F(A) & \xrightarrow{\eta_A} & G(A) \\ {\scriptstyle F(f)}\big\downarrow & & \big\downarrow{\scriptstyle G(f)} \\ F(B) & \xrightarrow{\eta_B} & G(B) \end{array}$$

One can use the naturality of η to define a natural transformation $\widetilde{\eta} : \widetilde{F} \Rightarrow \widetilde{G}$ that assigns to every object $f : A \to B$ in $\mathbf{Arr}[\mathcal{C}]$ a morphism $\widetilde{\eta}_f = (\eta_A, \eta_B) : \widetilde{F}(f) \to \widetilde{G}(f)$ via the commutative diagram from above, such that for any morphism $(\phi, \psi) : f \to f'$ in $\mathbf{Arr}[\mathcal{C}]$:

$$\begin{array}{ccc} A & \xrightarrow{\phi} & A' \\ {\scriptstyle f}\big\downarrow & & \big\downarrow{\scriptstyle f'} \\ B & \xrightarrow{\psi} & B' \end{array}$$

the following diagram (naturality condition in the arrow category) commutes:



Here the the top, the back, the front and the bottom face commute due to naturality of η and the two side faces commute by definition. Hence the whole diagram commutes and one has defined a natural transformation $\widetilde{\eta} : \widetilde{F} \Rightarrow \widetilde{G}$. □

Proposition 2.58.3. *[37] If $\eta : F \Rightarrow G$ is a natural isomorphism, then so is $\tilde{\eta} : \widetilde{F} \Rightarrow \widetilde{G}$.*

The proof can be found in Ref. [38].

Theorem 2.58.1. *[37] Let $\mathcal{C}$ and $\mathcal{D}$ be equivalent categories; that is, there exist functors $F : \mathcal{C} \to \mathcal{D}$ and $G : \mathcal{D} \to \mathcal{C}$ and natural isomorphisms $F \circ G \cong \mathrm{id}_{\mathcal{D}}$ and $G \circ F \cong \mathrm{id}_{\mathcal{C}}$. Then Arr($\mathcal{C}$) and Arr($\mathcal{D}$) are also equivalent.*

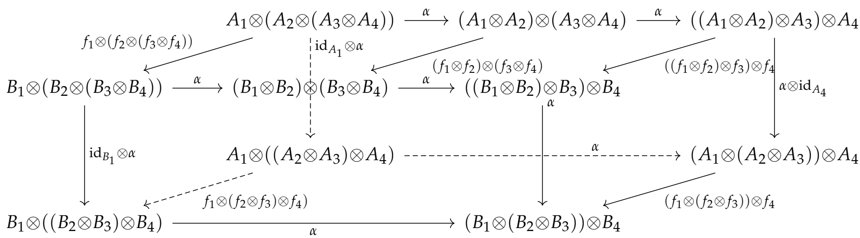
Proof. By Proposition 2.58.1 the functors $F : \mathcal{C} \to \mathcal{D}$ and $G : \mathcal{D} \to \mathcal{C}$ give rise to functors $\widetilde{F} : \mathbf{Arr}[\mathcal{C}] \to \mathbf{Arr}[\mathcal{D}]$ and $\widetilde{G} : \mathbf{Arr}[\mathcal{D}] \to \mathbf{Arr}[\mathcal{C}]$. From Proposition 2.58.3 one knows that the natural isomorphisms $F \circ G \cong \mathrm{id}_{\mathcal{D}}$ and $G \circ F \cong \mathrm{id}_{\mathcal{C}}$ give rise to natural isomorphisms $\widetilde{F} \circ \widetilde{G} \cong \mathrm{id}_{\mathbf{Arr}[\mathcal{D}]}$ and $\widetilde{G} \circ \widetilde{F} \cong \mathrm{id}_{\mathbf{Arr}[\mathcal{C}]}$. Hence one has an equivalence. □

One can show that the same theorems apply to monoidal functors and monoidal natural transformations [38]. Furthermore, given a monoidal category, it is possible to define a monoidal product for its arrow category as the following proposition will demonstrate. However, this result is not necessarily new and can be in fact found in a similar notion in [116].

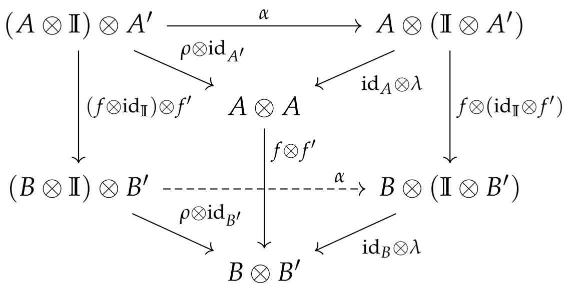
Proposition 2.58.4. *[37] For a monoidal category $\mathcal{C}$, one can define a monoidal product on $\mathbf{Arr}[\mathcal{C}]$, written $\boxtimes$, as follows:*

- *on objects, $f \boxtimes g := f \otimes g$;*
- *on morphisms, $(p,q) \boxtimes (p',q') := (p \otimes p', q \otimes q')$.*

Proof. It will be shown that the pentagon and the triangle axiom are satisfied. The pentagon axiom holds, due to the following diagram, where the front and the back face commute, because α satisfies the ordinary pentagon axiom. The two side faces commute due to the definition of the monoidal product and naturality of the associator, and the top and bottom faces commute due to naturality of the associator:



The triangle axiom for $\mathbf{Arr}[\mathcal{C}]$ is given by the following diagram:



Here the top and the bottom faces commute due to the the triangle identity and the two side faces commute due to the definition of the monoidal product in $\mathbf{Arr}[\mathcal{C}]$ and due to naturality of the left and right unitors in $\mathcal{C}$. Finally, the back face commutes because of the naturality of the associator. $\square$

3 Perfect Tensors from Multiple Angles

This chapter aims to shed light on the existence problem of perfect tensors from multiple angles, as the title already indicates. Starting with the most natural way[1] to look at perfect tensors, namely from the algebraic point of view, in Section 3.1, the existence problem of perfect tensors will be linked to the existence problems of systems of four factors of a matrix algebra $\mathcal{M}_{d^2}(\mathbb{C})$, which form two pairs of commuting subalgebras. This will in parts be generalised to multiunitaries. In Section 3.2 these concepts will then be put in the more abstract language of groups and representations. After this, construction schemes of perfect tensors from doubly perfect bi-unimodular sequences in arbitrary dimensions and in particular an analytic solution for $d^2 = 36$ will be presented in Section 3.3. Finally, in the last section the minimal order[2] of 2-unitaries up to dimension 36 as well as a diagonal decomposition of $\mathcal{M}_9(\mathbb{C})$ into factors isomorphic to $\mathcal{M}_3(\mathbb{C})$ will be discussed.

Some of the results presented in this chapter have been previously published in Ref. [46] (c.f. *Teilpublikationen* listed on page iii). In particular, the algebraic characterisation of 2-unitarity presented in Sec. 3.1 appears in [46] (Sec. VII), though additional examples have been added here. Moreover, the pen-and-paper construction of a 2-unitary of dimension 36 detailed in Section 3.3 has been published as Sec. IV of Ref. [46]. However, the paper left some constructions implicit. Most notably, Theorem 5 uses the existence of trace-orthonormal bases in finite extension fields, but does not describe an algorithm for constructing them concretely. Such an algorithm is presented

[1]Of course, "most natural" is subjective.

[2]The term order refers here, and everywhere else in this chapter to the smallest positive integer that, when used as an exponent for a matrix (or for an element of any kind of group), gives the identity matrix (or the identity element of the group).

in Section 3.3.2 of this chapter. An implementation in the computer algebra system SageMath appears in Appendix B.1 and in the present author's GitHub repository [35]. This section also contains further concrete examples beyond those that have appeared in [46]. The generalisation to k-unitaries in Section 3.1.3, all results of Section 3.2 except from the no-go theorem for Clifford 2-unitaries in dimension 36, and all of Section 3.4 have not been previously published.

3.1 The Algebraic Point of View

In this section the existence problem of 2-unitaries in dimension d^2 will be considered in a matrix algebraic context. The underlying mathematical concepts were introduced in Section 2.2.1. For this, the action of a 2-unitary $U \in \mathcal{M}_{d^2}(\mathbb{C})$ as automorphism $A \to UAU^\dagger$ on $\mathcal{M}_{d^2}(\mathbb{C})$ on the local subalgebras $\mathcal{R}, \mathcal{L}$ of $\mathcal{M}_{d^2}(\mathbb{C})$ will be investigated. As it turns out, the resulting subalgebras $U\mathcal{R}U^\dagger, U\mathcal{L}U^\dagger$ are delocalised. Moreover, the converse is also true: every delocalised subalgebra gives rise to a 2-unitary. Building on that, the existence of multiunitary matrices will be linked to the existence of delocalised subalgebras in $\mathcal{M}_{d^k}(\mathbb{C})$ in the second part of the section. It will be shown that, while the existence of a multiunitary in dimension d^k implies the existence of k delocalised subalgebras in $\mathcal{M}_{d^k}(\mathbb{C})$, the converse is not true.

3.1.1 Related Work

Quasi-orthogonal systems of matrix algebras have already been widely discussed in the works of Ohno, Weiner and Petz (see Refs. [88, 93, 92, 114]), where it was demonstrated that given a matrix algebra $\mathcal{M}_{d^2}(\mathbb{C})$, finding the maximal number of pairwise quasi-orthogonal subalgebras isomorphic to $\mathcal{M}_d(\mathbb{C})$ is a non-trivial task. In Ref. [88] the author shows that, if p is a prime, the maximal number of pairwise quasi-orthogonal subalgebras isomorphic to $\mathcal{M}_p(\mathbb{C})$ in $\mathcal{M}_{p^2}(\mathbb{C})$ is p^2+1 for $p \geq 3$. Furthermore, the author proves that the left factor is quasi-orthogonal to a factor obtained by conjugating the left factor with a unitary, if and only if this unitary can be decomposed into a tensor product of two orthonormal bases where all prefactors are equal to 1. Although not stated in the paper, one can deduce that the unitary has to be dual unitary in that case, since this property is directly linked to the matrix having a Schmidt decomposition into a tensor product of two orthonormal bases with all Schmidt coefficients being equal to 1 (see Ref. [10], p. 241).

3.1.2 Delocalised Subalgebras of $\mathcal{M}_{d^2}(\mathbb{C})$ and the Existence of 2-unitaries

In this section, the relation between perfect tensors and systems of four quasi-orthogonal subalgebras in $\mathcal{M}_{d^2}(\mathbb{C})$, where two of them will correspond to the left and the right subalgebra, will be discussed. As a start, Proposition 3.0.1 will relate the reshuffle and partial transpose of a unitary $U \in U(d^2)$, corresponding to the dual and the Γ-dual unitary, to the *overlap* of the subalgebra $\mathcal{A}_L := U\mathcal{L}U^\dagger$ with the two local subalgebras. The overlap of two subalgebras was introduced independently in Ref. [88] and Ref. [48] and basically describes how far two subalgebras are away from being quasi-orthogonal.

Proposition 3.0.1. *Consider the matrix algebra $\mathcal{M}_{d^2}(\mathbb{C}) \cong \mathcal{M}_d(\mathbb{C}) \otimes \mathcal{M}_d(\mathbb{C})$ and let $U \in U(d^2)$. Set $\mathcal{A} := U\mathcal{L}U^\dagger$, where $\mathcal{L} \cong \mathcal{M}_d(\mathbb{C}) \otimes \mathbb{I}_d$. Then the following holds:*

i) $\mathrm{Tr}(P_{\mathcal{A}_L} P_{\mathcal{L}}^\dagger) = ||U^R (U^R)^\dagger||_{2,\tau}^2$,

ii) $\mathrm{Tr}(P_{\mathcal{A}_L} P_{\mathcal{R}}^\dagger) = ||U^\Gamma (U^\Gamma)^\dagger||_{2,\tau}^2$.

Proof. i). Let $\sqrt{d}E_{ij} = \sqrt{d}\,|i\rangle\langle j|$ be an ONB in $\mathcal{L} \cong \mathcal{M}_d(\mathbb{C})$ and $\mathbb{I}_d$ be the identity operator of $\mathcal{M}_d(\mathbb{C})$. Then $P_{\mathcal{L}} = d\sum_{i,j=1}^d |E_{ij} \otimes \mathbb{I}_d\rangle\langle E_{ij} \otimes \mathbb{I}_d|$ is the projection onto the left subalgebra. Similarly,

$$P_{U\mathcal{L}U^\dagger} = d\sum_{i,j=1}^{d} |U(E_{ij} \otimes \mathbb{I}_d)U^\dagger\rangle\langle U(E_{ij} \otimes \mathbb{I}_d)U^\dagger| \tag{3.1}$$

is a projection onto $\mathcal{A}$. One then has:

$$\begin{aligned}
\mathrm{Tr}(P_{U\mathcal{L}U^\dagger} P_{\mathcal{L}}^\dagger) &= d^2 \sum_{i,j,k,l=1}^{d} |\langle (UE_{ij} \otimes \mathbb{I}_d U^\dagger)|E_{kl} \otimes \mathbb{I}_d\rangle|^2 \\
&= d^2 \sum_{i,j,k,l=1}^{d} |\tau\big((UE_{ij} \otimes \mathbb{I}_d U^\dagger)(E_{kl} \otimes \mathbb{I}_d)\big)|^2 \\
&= d^2 \sum_{i,j,k,l=1}^{d} |\frac{1}{d^2}\mathrm{tr}\big((UE_{ij} \otimes \mathbb{I}_d U^\dagger)(E_{kl} \otimes \mathbb{I}_d)\big)|^2 \\
&= \frac{1}{d^2} \sum_{i,j,k,l=1}^{d} |\mathrm{tr}\big((UE_{ij} \otimes \mathbb{I}_d U^\dagger)(E_{kl} \otimes \mathbb{I}_d)\big)|^2
\end{aligned}$$

Now compute:

$$\begin{aligned}
\mathrm{tr}\Big((UE_{ij}\otimes \mathbb{I}_d U^\dagger)(E_{kl}\otimes \mathbb{I}_d)\Big) &= \mathrm{tr}\Big(\sum_{r,s=1}^{d}(UE_{ij}\otimes E_{rr}U^\dagger)(E_{kl}\otimes E_{ss})\Big)\\
&= \mathrm{tr}\Big(\sum_{r,s=1}^{d} U\left|ir\right\rangle\left\langle jr\right| U^\dagger \left|ks\right\rangle\left\langle ls\right|\Big)\\
&= \sum_{r,s=1}^{d}\left\langle ls\right| U\left|ir\right\rangle\left\langle jr\right| U^\dagger\left|ks\right\rangle\\
&= \sum_{r,s=1}^{d} U_{ir}^{ls}U^{\dagger\,jr}_{ks} = \sum_{r,s=1}^{n} U_{ir}^{ls}(U^*)_{jr}^{ks}\\
&= \sum_{r,s=1}^{d}(U^R)_{sr}^{li}(U^{R*})_{sr}^{kj} = \sum_{r,s=1}^{d}(U^R)_{sr}^{li}((U^R)^\dagger)_{kj}^{sr}\\
&= (U^R(U^R)^\dagger)_{kj}^{li}
\end{aligned}$$

With that one gets:

$$\begin{aligned}
\mathrm{Tr}(P_{U\mathcal{L}U^\dagger}P_{\mathcal{L}}^\dagger) &= \frac{1}{d^2}\sum_{i,j,k,l=1}^{d}|(U^R(U^R)^\dagger)_{kj}^{li})|^2\\
&= \frac{1}{d^2}||U^R(U^R)^\dagger||_2^2\\
&= ||U^R(U^R)^\dagger||_{2,\tau}^2.
\end{aligned}$$

A similar argument can be made for *ii*). □

Based on this, one can make the following statement:

Proposition 3.0.2. *Consider the matrix algebra* $\mathcal{M}_{d^2}(\mathbb{C}) \cong \mathcal{M}_d(\mathbb{C})\otimes\mathcal{M}_d(\mathbb{C})$ *and let* $U\in U(d^2)$. *Set* $\mathcal{A} := U\mathcal{L}U^\dagger$, *where* $\mathcal{L}\cong\mathcal{M}_d(\mathbb{C})\otimes\mathbb{I}_d$. *Then the following holds:*

i) $\mathcal{A}$ *is quasi-orthogonal to* $\mathcal{L}$ *iff* U^R *is unitary,*

ii) $\mathcal{A}$ *is quasi-orthogonal to* $\mathcal{L}' = \mathcal{R}$ *iff* U^Γ *is unitary,*

iii) $\mathcal{A}$ *is delocalised iff* U *is a 2-unitary.*

Proof. Recall that two subalgebras $\mathcal{A}_L$ and $\mathcal{L}$ are quasi-orthogonal, if and only if $\mathrm{Tr}(P_{U\mathcal{L}U^\dagger} P_{\mathcal{L}}^\dagger) = 1$, where $P_{\mathcal{A}_L}$ is the projection onto $\mathcal{A}_L$ and $P_{\mathcal{L}}$ is the projection onto $\mathcal{L}$. Therefore, *i*) and *ii*) reduce to the following statements:

i) $||U^R(U^R)^\dagger||_{2,\tau}^2 = 1 \quad \Leftrightarrow U^R$ is unitary,

ii) $||U^\Gamma(U^\Gamma)^\dagger||_{2,\tau}^2 = 1 \quad \Leftrightarrow U^\Gamma$ is unitary.

So assuming that U^R is a unitary in dimension d^2, one directly sees that:

$$\begin{aligned}\mathrm{Tr}(P_{U\mathcal{L}U^\dagger} P_{\mathcal{L}}^\dagger) &= \frac{1}{d^2} \sum_{i,j,k,l=1}^{d} |(U^R(U^R)^\dagger)_{kj}^{li})|^2 \\ &= \frac{1}{d^2} \sum_{i,j,k,l=1}^{d} |(\mathbb{I}_{d^2})_{kj}^{li})|^2 = \frac{1}{d^2} \cdot d^2 = 1\end{aligned}$$

and thus $\mathcal{A}$ and $\mathcal{L}$ are quasi-orthogonal. A similar argument can be made for U^Γ.

Now for the other direction, assume that $\mathcal{L}$ and $\mathcal{A}$ are quasi-orthogonal, i.e. that $\mathrm{Tr}(P_{U\mathcal{L}U^\dagger} P_{\mathcal{L}}^\dagger) = 1$. One then finds:

$$\mathrm{Tr}(P_{U\mathcal{L}U^\dagger} P_{\mathcal{L}}^\dagger) = ||U^R(U^R)^\dagger||_{2,\tau}^2 = 1. \tag{3.2}$$

The 2-norm satisfies the following inequality

$$||X \cdot Y||_{2,\tau} \leq ||X||_{4,\tau} \cdot ||Y||_{4,\tau} \tag{3.3}$$

for all $X, Y \in L(H)$, where $||X||_{4,\tau}$ denotes the normalised Schatten-4-norm. With that one gets:

$$1 = ||U^R(U^R)^\dagger||_{2,\tau}^2 \leq ||U^R||_{4,\tau}^4 \leq ||U^R||_{2,\tau}^4. \tag{3.4}$$

Since the two norm is just a reordering of matrix entries, it holds that

$$||U^R||_{2,\tau} = ||U||_{2,\tau} = 1. \tag{3.5}$$

Hence one gets:

$$1 = ||U^R(U^R)^\dagger||_{2,\tau}^2 \leq ||U^R||_{4,\tau}^4 \leq ||U^R||_{2,\tau}^4 = ||U||_{2,\tau} = 1. \tag{3.6}$$

From that one can conclude that the Schatten-2-norm and the Schatten-4-norm of U^R are equal. Write the Schatten norms in terms of Eigenvalues:

$$||U||_{p,\tau} = \Big(\frac{1}{d}\sum_i \lambda_i^{p/2}(UU^\dagger)\Big)^{1/p} \tag{3.7}$$

Then Eq. 3.6 implies that the following has to be true:

$$\Big(\frac{1}{d^2}\sum_i \lambda_i(U^R(U^R)^\dagger)\Big)^2 = \frac{1}{d^2}\sum_j \lambda_j^2(U^R(U^R)^\dagger) \tag{3.8}$$

Using Jensen's inequality, one can deduce that all the eigenvalues of $U^R(U^R)^\dagger$ have to be equal. There can be at most d^2 eigenvalues and since the sum over all the eigenvalues has to be equal to d^2, one can conclude that all of them have to be equal to 1. But this means that $U^R(U^R)^\dagger$ is the identity matrix. Because the 2-norm is invariant under transpositions one can equally conclude that $(U^R)^\dagger U^R$ is the identity matrix. Therefore, U^R has to be unitary. Analogously, one can prove that $||U^\Gamma(U^\Gamma)^\dagger||^2_{2,\tau} = 1$ implies that U^Γ is unitary.

From *i*) and *ii*) one can then conclude that $\mathcal{A}_L$ is delocalised, which proves *iii*). □

A proof using the other characterisation of quasi-orthogonality defined in Proposition 2.28.1, can be found in Appendix A.

Example 1. Consider the matrix algebra $\mathcal{M}_9(\mathbb{C}) \cong \mathcal{M}_3(\mathbb{C}) \otimes \mathcal{M}_3(\mathbb{C})$ with left and right factors given by $\mathcal{L} = \mathcal{M}_3(\mathbb{C}) \otimes \mathbb{I}$ and $\mathcal{R} = \mathbb{I} \otimes \mathcal{M}_3(\mathbb{C})$ respectively.

A basis for $\mathcal{M}_3(\mathbb{C})$ is given by the WH-basis:

$$\{X^iZ^j\} \text{ for } i,j \in [3]. \tag{3.9}$$

The left and right factors expressed in terms of this basis are given by:

$$\mathcal{L} = \langle \mathbb{I}_9, X\otimes\mathbb{I}_3, Z\otimes\mathbb{I}_3, X^2\otimes\mathbb{I}_3, Z^2\otimes\mathbb{I}_3, XZ\otimes\mathbb{I}_3, X^2Z^2\otimes\mathbb{I}_3, \\ XZ^2\otimes\mathbb{I}_3, X^2Z\otimes\mathbb{I}_3\rangle$$

and

$$\mathcal{R} = \langle \mathbb{I}_9, \mathbb{I}_3\otimes X, \mathbb{I}_3\otimes Z, \mathbb{I}_3\otimes X^2, \mathbb{I}_3\otimes Z^2, \mathbb{I}_3\otimes XZ, \mathbb{I}_3\otimes X^2Z^2, \\ \mathbb{I}_3\otimes XZ^2, \mathbb{I}_3\otimes X^2Z\rangle.$$

Now consider the 2-unitary permutation matrix of order 4:

$$U_{OLS} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}. \tag{3.10}$$

This matrix corresponds to the following MOLS(3) which is in normal form:

$$\begin{vmatrix} 11 & 22 & 33 \\ 23 & 31 & 12 \\ 32 & 13 & 21 \end{vmatrix}. \tag{3.11}$$

One obtains U by replacing each entry of the above Latin square by a 3×3 block with a single one at the place indexed by the Latin square entry and zero everywhere else.

Now the following subalgebras are delocalised:

$$\begin{aligned} U\mathcal{L}U^\dagger &= \langle \mathbb{I}_9, XZ \otimes X^2Z^2, X^2Z^2 \otimes XZ, XZ^2 \otimes X^2Z, X^2 \otimes X, \\ &\quad Z \otimes Z^2, X^2Z \otimes XZ^2, Z^2 \otimes Z, X \otimes X^2 \rangle, \\ U\mathcal{R}U^\dagger &= \langle \mathbb{I}_9, X \otimes X, X^2 \otimes X^2, Z^2 \otimes Z^2, XZ \otimes XZ, Z \otimes Z, \\ &\quad X^2Z^2 \otimes X^2Z^2, X^2Z \otimes X^2Z, XZ^2 \otimes XZ^2 \rangle. \end{aligned}$$

The calculations can be found in the Sage notebook on the present author's GitHub repository [35].

3.1.3 Generalisation to k-Unitaries

Given that the notion of 2-unitaries can be generalised to k-unitaries, it is natural to ask, if one can generalise Proposition 3.0.5 to matrix algebras isomorphic to a k-fold tensor product of $\mathcal{M}_d(\mathbb{C})$ with k local subalgebras and k delocalised subalgebras isomorphic to $\mathcal{M}_d(\mathbb{C})$. As it turns out, this will in general not work, as the case $k = 3$ already demonstrates.

Multiunitaries and Delocalised Subalgebras in Dimension 9

Consider the matrix algebra $\mathcal{M}_{d^3}(\mathbb{C}) \cong \mathcal{M}_d(\mathbb{C}) \otimes \mathcal{M}_d(\mathbb{C}) \otimes \mathcal{M}_d(\mathbb{C})$. This algebra has three local subalgebras: the left subalgebra $\mathcal{L} = \mathcal{M}_d(\mathbb{C}) \otimes \mathbb{I}_{d^2}$, the right subalgebra $\mathcal{R} = \mathbb{I}_{d^2} \otimes \mathcal{M}_d(\mathbb{C})$, and the "middle" subalgebra $\mathcal{M} = \mathbb{I}_d \otimes \mathcal{M}_d(\mathbb{C}) \otimes \mathbb{I}_d$. All of these subalgebras clearly commute with each other. Consider $\mathcal{L} = \mathcal{M}_d(\mathbb{C}) \otimes \mathbb{I}_{d^2}$. Its commutant is given by: $\mathcal{L}' = \mathcal{R} \cdot \mathcal{M}$. Now since $\mathcal{L}$ and $\mathcal{R} \cdot \mathcal{M}$ have trivial intersection, these subalgebras are factors where one factor is isomorphic to $\mathcal{M}_d(\mathbb{C})$ and the other is isomorphic to $\mathcal{M}_{d^2}(\mathbb{C})$. The same holds for $\mathcal{R}$ and $\mathcal{L} \cdot \mathcal{M}$ and for $\mathcal{M}$ and $\mathcal{R} \cdot \mathcal{L}$. Now it is easy to verify that the following pairs of subalgebras are quasi-orthogonal:

- $\mathcal{L}$ and $\mathcal{R}$
- $\mathcal{L}$ and $\mathcal{M}$
- $\mathcal{R}$ and $\mathcal{M}$
- $\mathcal{L}$ and $\mathcal{R} \cdot \mathcal{M}$
- $\mathcal{R}$ and $\mathcal{L} \cdot \mathcal{M}$
- $\mathcal{M}$ and $\mathcal{R} \cdot \mathcal{L}$

In this context, one says that a subalgebra is *delocalised* if and only if it is quasi-orthogonal to $\mathcal{L}$, $\mathcal{R}$ and $\mathcal{M}$.

Proposition 3.0.3. *Consider the matrix algebra $\mathcal{M}_{d^3}(\mathbb{C}) \cong \mathcal{M}_d(\mathbb{C}) \otimes \mathcal{M}_d(\mathbb{C}) \otimes \mathcal{M}_d(\mathbb{C})$ and let $\mathcal{L} = \mathcal{M}_d(\mathbb{C}) \otimes \mathbb{I}_{d^2}$, $\mathcal{R} = \mathbb{I}_{d^2} \otimes \mathcal{M}_d(\mathbb{C})$ and $\mathcal{M} = \mathbb{I}_d \otimes \mathcal{M}_d(\mathbb{C}) \otimes \mathbb{I}_d$. Now consider $U \in U(d^3)$ and set $\mathcal{A}_L := U\mathcal{L}U^\dagger$. The following holds:*

i)

$$\mathrm{Tr}(P_{U\mathcal{L}U^\dagger} P_{\mathcal{L}}^\dagger) = \begin{cases} \left\| \mathrm{tr}_3 \left(U^{R_{2,4}} (U^{R_{2,4}})^\dagger \right) \right\|_2^2 \\ \left\| \mathrm{tr}_2 \left(U^{R_{3,4}} (U^{R_{3,4}})^\dagger \right) \right\|_2^2 \\ \left\| \mathrm{tr}_3 \left(U^{R_{1,5}} (U^{R_{1,5}})^\dagger \right) \right\|_2^2 \\ \left\| \mathrm{tr}_2 \left(U^{R_{1,6}} (U^{R_{1,6}})^\dagger \right) \right\|_2^2 \end{cases} \tag{3.12}$$

ii)

$$\mathrm{Tr}(P_{U\mathcal{L}U^\dagger} P_{\mathcal{R}}^\dagger) = \begin{cases} ||\mathrm{tr}_2(U^{\Gamma_{3,6}}(U^{\Gamma_{3,6}})^\dagger)||_2^2 \\ ||\mathrm{tr}_3(U^{R_{3,5}}(U^{R_{3,5}})^\dagger)||_2^2 \\ ||\mathrm{tr}_2(U^{\Gamma_{1,4}}(U^{\Gamma_{1,4}})^\dagger)||_2^2 \\ ||\mathrm{tr}_1(U^{R_{2,4}}(U^{R_{2,4}})^\dagger)||_2^2 \end{cases} \tag{3.13}$$

iii)

$$\mathrm{Tr}(P_{U\mathcal{L}U^\dagger} P_{\mathcal{M}}^\dagger) = \begin{cases} ||\mathrm{tr}_3(U^{\Gamma_{2,5}}(U^{\Gamma_{2,5}})^\dagger)||_2^2 \\ ||\mathrm{tr}_3(U^{\Gamma_{1,4}}(U^{\Gamma_{1,4}})^\dagger)||_2^2 \\ ||\mathrm{tr}_1(U^{R_{3,4}}(U^{R_{3,4}})^\dagger)||_2^2 \\ ||\mathrm{tr}_2(U^{R_{2,6}}(U^{R_{2,6}})^\dagger)||_2^2 \end{cases} \tag{3.14}$$

Proof. The proof starts with discussing the trace conditions for the subalgebra $\mathcal{A}_L$.

I. Trace condition for $\mathcal{A}_L$ and $\mathcal{L}$

Let $\sqrt{d}E_{ij} = \sqrt{d}\,|i\rangle\,\langle j|$ be an ONB in $\mathcal{M}_d(\mathbb{C})$. Then

$$P_{\mathcal{L}} = d \sum_{i,j=1}^{d} |E_{ij} \otimes \mathbb{I}_{d^2}\rangle \, \langle E_{ij} \otimes \mathbb{I}_{d^2}|$$

is the projection onto the left subalgebra. Similarly, one has

$$P_{U\mathcal{L}U^\dagger} = d \sum_{i,j=1}^{d} |U(E_{ij} \otimes \mathbb{I}_{d^2})U^\dagger\rangle \, \langle U(E_{ij} \otimes \mathbb{I}_{d^2})U^\dagger|$$

as projection onto $\mathcal{A}_L$. Following the proof of Prop. 3.0.2, one can then compute:

$$\begin{aligned}
\mathrm{Tr}(P_{U\mathcal{L}U^\dagger}P_{\mathcal{L}}^\dagger) &= d^2 \sum_{i,j,k,l=1}^{d} |\langle (UE_{ij}\otimes \mathbb{I}_{d^2}U^\dagger)|E_{kl}\otimes \mathbb{I}_{d^2}\rangle|^2 \\
&= d^2 \sum_{i,j,k,l=1}^{d} |\tau\big((UE_{ij}\otimes \mathbb{I}_{d^2}U^\dagger)(E_{kl}\otimes \mathbb{I}_{d^2})\big)|^2 \\
&= d^2 \sum_{i,j,k,l=1}^{d} |\frac{1}{d^3}\mathrm{tr}\big((UE_{ij}\otimes \mathbb{I}_{d^2}U^\dagger)(E_{kl}\otimes \mathbb{I}_{d^2})\big)|^2 \\
&= \frac{1}{d^4} \sum_{i,j,k,l=1}^{d} |\mathrm{tr}\big((UE_{ij}\otimes \mathbb{I}_{d^2}U^\dagger)(E_{kl}\otimes \mathbb{I}_{d^2})\big)|^2.
\end{aligned}$$

Further compute:

$$\begin{aligned}
\mathrm{tr}\Big((UE_{ij}\otimes \mathbb{I}_{d^2}U^\dagger)(E_{kl}\otimes \mathbb{I}_{d^2})\Big) &= \mathrm{tr}\Big(\sum_{r,s,t,u=1}^{d} (UE_{ij}\otimes E_{rr}\otimes E_{tt}U^\dagger)(E_{kl}\otimes E_{ss}\otimes E_{uu})\Big) \\
&= \mathrm{tr}\Big(\sum_{r,s,t,u=1}^{d} U|irt\rangle\langle jrt|U^\dagger|ksu\rangle\langle lsu|\Big) \\
&= \sum_{r,s,t,u=1}^{d} \langle lsu|U|irt\rangle\langle jrt|U^\dagger|ksu\rangle \\
&= \sum_{r,s,t,u=1}^{d} U_{irt}^{lsu}(U^\dagger)_{ksu}^{jrt} \\
&= \sum_{r,s,t,u=1}^{d} U_{irt}^{lsu}(U^*)_{jrt}^{ksu}. \qquad (3.15)
\end{aligned}$$

Line (A.7) can be transformed in various ways:

$$\begin{aligned}(A.7) &= \sum_{r,s,t,u=1}^{d} (U^{R_{2,4}})^{liu}_{srt} (U^{R_{2,4}*})^{kju}_{srt} \\ &= \sum_{r,s,t,u=1}^{d} (U^{R_{2,4}})^{liu}_{srt} ((U^{R_{2,4}})^{\dagger})^{srt}_{kju} \\ &= \sum_{u=1}^{d} (U^{R_{2,4}} (U^{R_{2,4}})^{\dagger})^{liu}_{kju},\end{aligned}$$

or, analogously,

$$\begin{aligned}(A.7) &= \sum_{s=1}^{d} (U^{R_{3,4}} (U^{R_{3,4}})^{\dagger})^{lsi}_{ksj}, \\ (A.7) &= \sum_{t=1}^{d} (U^{R_{1,5}} (U^{R_{1,5}})^{\dagger})^{ilt}_{jkt}, \\ (A.7) &= \sum_{r=1}^{d} (U^{R_{1,6}} (U^{R_{1,6}})^{\dagger})^{irl}_{jrk}.\end{aligned}$$

With that one gets:

$$\mathrm{Tr}(P_{U\mathcal{L}U^\dagger}P_{\mathcal{L}}^\dagger) = \frac{1}{d^4}\sum_{i,j,k,l=1}^{d} \begin{cases} |\sum_{u=1}^{d}(U^{R_{2,4}}(U^{R_{2,4}})^\dagger)_{kju}^{liu}|^2 \\ |\sum_{s=1}^{d}(U^{R_{3,4}}(U^{R_{3,4}})^\dagger)_{ksj}^{lsi}|^2 \\ |\sum_{t=1}^{d}(U^{R_{1,5}}(U^{R_{1,5}})^\dagger)_{jkt}^{ilt}|^2 \\ |\sum_{r=1}^{d}(U^{R_{1,6}}(U^{R_{1,6}})^\dagger)_{jrk}^{irl}|^2 \end{cases}$$

$$= \frac{1}{d^4}\sum_{i,j,k,l=1}^{d} \begin{cases} \left|\left(\mathrm{tr}_3\left(U^{R_{2,4}}(U^{R_{2,4}})^\dagger\right)\right)_{kj}^{li}\right|^2 \\ \left|\left(\mathrm{tr}_2\left(U^{R_{3,4}}(U^{R_{3,4}})^\dagger\right)\right)_{kj}^{li}\right|^2 \\ \left|\left(\mathrm{tr}_3\left(U^{R_{1,5}}(U^{R_{1,5}})^\dagger\right)\right)_{jk}^{il}\right|^2 \\ \left|\left(\mathrm{tr}_2\left(U^{R_{1,6}}(U^{R_{1,6}})^\dagger\right)\right)_{jk}^{il}\right|^2 \end{cases}$$

$$= \frac{1}{d^2} \begin{cases} \left\|\mathrm{tr}_3\left(U^{R_{2,4}}(U^{R_{2,4}})^\dagger\right)\right\|_2^2 \\ \left\|\mathrm{tr}_2\left(U^{R_{3,4}}(U^{R_{3,4}})^\dagger\right)\right\|_2^2 \\ \left\|\mathrm{tr}_3\left(U^{R_{1,5}}(U^{R_{1,5}})^\dagger\right)\right\|_2^2 \\ \left\|\mathrm{tr}_2\left(U^{R_{1,6}}(U^{R_{1,6}})^\dagger\right)\right\|_2^2 \end{cases}$$

II. Trace condition for $\mathcal{A}_L$ and $\mathcal{R}$

Next, the goal is to compute $\mathrm{Tr}(P_{U\mathcal{L}U^\dagger}P_{\mathcal{R}}^\dagger)$. The calculation proceeds as in the beginning of this proof. Compared to Eq. (A.7), the indices l and k are in the third position, instead of in the first position. One finds:

$$\begin{aligned}
\mathrm{Tr}(P_{U\mathcal{L}U^\dagger}P_{\mathcal{R}}^\dagger) &= \frac{1}{d^4}\sum_{i,j,k,l=1}^{d} |\mathrm{tr}\big((UE_{ij}\otimes \mathbb{I}_{d^2}U^\dagger)(\mathbb{I}_{d^2}\otimes E_{kl})\big)|^2 \\
&= \frac{1}{d^4}\sum_{i,j,k,l=1}^{d} |\mathrm{tr}\big(\sum_{r,s,u,t=1}^{d}(UE_{ij}\otimes E_{rr}\otimes E_{tt}U^\dagger)(E_{ss}\otimes E_{uu}\otimes E_{kl})\big)|^2 \\
&= \frac{1}{d^4}\sum_{i,j,k,l=1}^{d} |\mathrm{tr}\big(\sum_{r,s,u,t=1}^{d} U\,|irt\rangle\,\langle jrt|\,U^\dagger\,|suk\rangle\,\langle sul|\big)|^2 \\
&= \frac{1}{d^4}\sum_{i,j,k,l=1}^{d} |\sum_{r,s,t,u=1}^{d} U_{irt}^{sul}(U^*)_{jrt}^{suk}|^2. \qquad (3.16)
\end{aligned}$$

This expression can be transformed in multiple ways:

$$(A.12) = \frac{1}{d^4}\sum_{i,j,k,l=1}^{d} |\sum_{s=1}^{d}(U^{R_{2,4}}(U^{R_{2,4}})^\dagger)_{sjk}^{sil}|^2,$$

$$(A.12) = \frac{1}{d^4}\sum_{i,j,k,l=1}^{d} |\sum_{u=1}^{d}(U^{\Gamma_{1,4}}(U^{\Gamma_{1,4}})^\dagger)_{juk}^{iul}|^2,$$

$$(A.12) = \frac{1}{d^4}\sum_{i,j,k,l=1}^{d} |\sum_{t=1}^{d}(U^{R_{3,5}}(U^{R_{3,5}})^\dagger)_{jkt}^{ilt}|^2,$$

and

$$(A.12) = \frac{1}{d^4}\sum_{i,j,k,l=1}^{d} |\sum_{r=1}^{d}(U^{\Gamma_{3,6}}(U^{\Gamma_{3,6}})^\dagger)_{jrk}^{irl}|^2.$$

This gives us:

$$\mathrm{Tr}(P_{U\mathcal{L}U^\dagger}P_{\mathcal{R}}^\dagger) = \frac{1}{d^2}\left\{\begin{array}{l} ||\mathrm{tr}_2(U^{\Gamma_{3,6}}(U^{\Gamma_{3,6}})^\dagger)||_2^2 \\ ||\mathrm{tr}_3(U^{R_{3,5}}(U^{R_{3,5}})^\dagger)||^2 \\ ||\mathrm{tr}_2(U^{\Gamma_{1,4}}(U^{\Gamma_{1,4}})^\dagger)||_2^2 \\ ||\mathrm{tr}_1(U^{R_{2,4}}(U^{R_{2,4}})^\dagger)||_2^2 \end{array}\right. .$$

III. Trace condition for $\mathcal{A}_L$ and $\mathcal{M}$

Finally, one has:

$$\begin{aligned}
\mathrm{Tr}(P_{U\mathcal{L}U^\dagger}P_{\mathcal{M}}^\dagger) &= \frac{1}{d^4}\sum_{i,j,k,l=1}^{d} |\mathrm{tr}\big((UE_{ij}\otimes \mathbb{I}_{d^2}U^\dagger)(\mathbb{I}_d\otimes E_{kl}\otimes \mathbb{I}_d)\big)|^2 \\
&= \frac{1}{d^4}\sum_{i,j,k,l=1}^{d} |\mathrm{tr}\big(\sum_{r,s,u,t=1}^{d} (UE_{ij}\otimes E_{rr}\otimes E_{tt}U^\dagger)(E_{ss}\otimes E_{kl}\otimes E_{uu})\big)|^2 \\
&= \frac{1}{d^4}\sum_{i,j,k,l=1}^{d} |\mathrm{tr}\big(\sum_{r,s,u,t=1}^{d} U\,|irt\rangle\,\langle jrt|\,U^\dagger\,|sku\rangle\,\langle slu|\big)|^2 \\
&= \frac{1}{d^4}\sum_{i,j,k,l=1}^{d} |\sum_{r,s,u,t=1}^{d} U_{irt}^{slu}(U^*)_{jrt}^{sku}|^2. \qquad (3.17)
\end{aligned}$$

This expression can again be transformed in multiple ways:

$$(A.9) = \frac{1}{d^4}\sum_{i,j,k,l=1}^{d} |\sum_{r=1}^{d}(U^{R_{2,6}}(U^{R_{2,6}})^\dagger)_{jrk}^{irl}|^2,$$

$$(A.9) = \frac{1}{d^4}\sum_{i,j,k,l=1}^{d} |\sum_{s=1}^{d}(U^{R_{3,4}}(U^{R_{3,4}})^\dagger)_{sli}^{skj}|^2,$$

$$(A.9) = \frac{1}{d^4}\sum_{i,j,k,l=1}^{d} |\sum_{u=1}^{d}(U^{\Gamma_{1,4}}(U^{\Gamma_{1,4}})^\dagger)_{jku}^{ilu}|^2,$$

and

$$(A.9) = \frac{1}{d^4}\sum_{i,j,k,l=1}^{d} |\sum_{t=1}^{d}(U^{\Gamma_{2,5}}(U^{\Gamma_{2,5}})^\dagger)_{ilt}^{jkt}|^2.$$

Hence one is left with:

$$\mathrm{Tr}(P_{U\mathcal{L}U^\dagger}P_{\mathcal{M}}^\dagger) = \frac{1}{d^2}\left\{\begin{array}{l} ||\mathrm{tr}_3(U^{\Gamma_{2,5}}(U^{\Gamma_{2,5}})^\dagger)||_2^2 \\ ||\mathrm{tr}_3(U^{\Gamma_{1,4}}(U^{\Gamma_{1,4}})^\dagger)||_2^2 \\ ||\mathrm{tr}_1(U^{R_{3,4}}(U^{R_{3,4}})^\dagger)||_2^2 \\ ||\mathrm{tr}_2(U^{R_{2,6}}(U^{R_{2,6}})^\dagger)||_2^2 \end{array}\right. .$$

□

Set $\mathcal{A}_M := U\mathcal{M}U^\dagger$ and $\mathcal{A}_R := U\mathcal{R}U^\dagger$. Both subalgebras are isomorphic to $\mathcal{M}_d(\mathbb{C})$ and commute with $\mathcal{A}_L$. One can calculate the trace conditions for these subalgebras in a similar way (see Appendix A). This gives rise to the following table, that displays which quasi-orthogonality condition is linked to which rearrangement of indices:

	$\mathcal{A}_L, \mathcal{L}$	$\mathcal{A}_L, \mathcal{M}$	$\mathcal{A}_L, \mathcal{R}$	$\mathcal{A}_R, \mathcal{L}$	$\mathcal{A}_R, \mathcal{M}$	$\mathcal{A}_R, \mathcal{R}$	$\mathcal{A}_M, \mathcal{L}$	$\mathcal{A}_M, \mathcal{M}$	$\mathcal{A}_M, \mathcal{R}$
$R_{1,5}$	x			x				x	x
$R_{1,6}$	x				x	x	x		
$R_{2,4}$	x		x		x			x	
$R_{2,6}$		x		x		x		x	
$R_{3,4}$	x	x				x			x
$R_{3,5}$			x			x	x	x	
$\Gamma_{1,4}$		x	x	x			x		
$\Gamma_{2,5}$		x			x		x		x
$\Gamma_{3,6}$			x	x	x				x

TABLE 3.1: Relation between the quasi-orthogonality conditions of subalgebras and rearrangements of a unitary U.

Moreover, one can easily show that the following is true:

- $U^{R_{1,5}^T} = U^{T^{R_{2,4}}}$
- $U^{R_{1,6}^T} = U^{T^{R_{3,4}}}$
- $U^{R_{2,4}^T} = U^{T^{R_{1,5}}}$
- $U^{R_{2,6}^T} = U^{T^{R_{3,5}}}$
- $U^{R_{3,4}^T} = U^{T^{R_{1,6}}}$
- $U^{R_{3,5}^T} = U^{T^{R_{2,6}}}$

This means for instance, that, if $U^{R_{1,5}}$ is unitary, then so is $U^{T^{R_{2,4}}}$.

Theorem 3.0.1. *Consider the matrix algebra* $\mathcal{M}_{d^3}(\mathbb{C}) \cong \mathcal{M}_d(\mathbb{C}) \otimes \mathcal{M}_d(\mathbb{C}) \otimes \mathcal{M}_d(\mathbb{C})$ *and let* $\mathcal{L} = \mathcal{M}_d(\mathbb{C}) \otimes \mathbb{I}_{d^2}$, $\mathcal{R} = \mathbb{I}_{d^2} \otimes \mathcal{M}_d(\mathbb{C})$ *and* $\mathcal{M} = \mathbb{I}_d \otimes \mathcal{M}_d(\mathbb{C}) \otimes \mathbb{I}_d$. *Now consider* $U \in U(d^3)$ *and set* $\mathcal{A}_L := U\mathcal{L}U^\dagger$,$\mathcal{A}_M := U\mathcal{M}U^\dagger$ *and* $\mathcal{A}_R := U\mathcal{R}U^\dagger$.

If U *is a multiunitary, in the sense that* $U^{R_{3,4}}$ *and* $U^{R_{3,5}}$ *are unitary, then* $\mathcal{A}_L$,$\mathcal{A}_M$ *and* $\mathcal{A}_R$ *are delocalised.*

Proof. Assume that $U^{R_{3,4}}$ is unitary, one finds that:

$$\begin{aligned}
\mathrm{Tr}(P_{U\mathcal{L}U^\dagger}P_{\mathcal{L}}^\dagger) &= \frac{1}{d^4}\sum_{i,j,k,l=1}^{d} |\sum_{u=1}^{d}(U^{R_{3,4}}(U^{R_{3,4}})^\dagger)_{kju}^{liu}|^2 \\
&= \frac{1}{d^4}\sum_{i,j,k,l=1}^{d} |\sum_{u=1}^{d}(\mathbb{I}_{d^3})_{kju}^{liu}|^2 \\
&= \frac{1}{d^4}\sum_{i,j,k,l=1}^{d} |\mathrm{tr}_3(\mathbb{I}_{d^2}\otimes\mathbb{I}_d)_{kj}^{li}|^2 \\
&= \frac{d^2}{d^4}\sum_{i,j,k,l=1}^{d} |(\mathbb{I}_{d^2})_{kj}^{li}|^2 = \frac{1}{d^2}\cdot d^2 = 1.
\end{aligned}$$

Thus $\mathcal{A}_{\mathcal{L}}$ and $\mathcal{L}$ are quasi-orthogonal. A similar argument shows that $\mathcal{A}_{\mathcal{L}}$ and $\mathcal{M}$, $\mathcal{A}_{\mathcal{R}}$ and $\mathcal{R}$ and $\mathcal{A}_{\mathcal{M}}$ and $\mathcal{R}$ are quasi-orthogonal. Due to cyclicity of the trace, this then implies that $\mathcal{A}_{\mathcal{R}}$ and $\mathcal{M}$ are also quasi-orthogonal.

Similarly, assuming that $U^{R_{3,5}}$ is unitary, one can show that

$$\mathrm{Tr}(P_{U\mathcal{L}U^\dagger}P_{\mathcal{R}}^\dagger) = 1 \tag{3.18}$$

holds and thus $\mathcal{A}_L$ and $\mathcal{R}$, $\mathcal{A}_M$ and $\mathcal{L}$ and $\mathcal{A}_M$ and $\mathcal{M}$ are quasi-orthogonal. Again, because of the cyclicity of the trace, this implies that $\mathcal{A}_{\mathcal{R}}$ and $\mathcal{L}$ are also quasi-orthogonal.

Therefore, if $U^{R_{3,4}}$ and $U^{R_{3,5}}$ are unitary, the subalgebras $\mathcal{A}_L$, $\mathcal{A}_R$ and $\mathcal{A}_M$ are delocalised. □

Of course, one could pick another combination of rearrangements of U to make this construction work as long as they cover all trace conditions.

In particular, the last theorem implies that, if U is 3-unitary, i.e. 9 rearrangements are unitary, then $\mathcal{A}_L$, $\mathcal{A}_R$ and $\mathcal{A}_M$ are delocalised.

Example 2. Consider the matrix algebra $\mathcal{M}_2(\mathbb{C})\otimes\mathcal{M}_2(\mathbb{C})\otimes\mathcal{M}_2(\mathbb{C})$ and consider the following basis for $\mathcal{M}_2(\mathbb{C})$:

$$\{X^iZ^j\}_{i,j=0,1} \text{ with } X = \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} \text{ and } Z = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}. \tag{3.19}$$

Define the three local subalgebras:

$$\begin{aligned}
\mathcal{L} &\cong \mathcal{M}_2(\mathbb{C})\otimes\mathbb{I}_4 = \langle \mathbb{I}_2\otimes\mathbb{I}_4, XZ\otimes\mathbb{I}_4, Z\otimes\mathbb{I}_4, X\otimes\mathbb{I}_4\rangle, \\
\mathcal{R} &\cong \mathbb{I}_4\otimes\mathcal{M}_2(\mathbb{C}) = \langle \mathbb{I}_4\otimes\mathbb{I}_2, \mathbb{I}_4\otimes XZ, \mathbb{I}_4\otimes X, \mathbb{I}_4\otimes Z\rangle, \\
\mathcal{M} &\cong \mathbb{I}_2\otimes\mathcal{M}_2(\mathbb{C})\otimes\mathbb{I}_2 = \langle \mathbb{I}_2\otimes\mathbb{I}_2\otimes\mathbb{I}_2, \mathbb{I}_2\otimes XZ\otimes\mathbb{I}_2, \mathbb{I}_2\otimes Z\otimes\mathbb{I}_2, \mathbb{I}_2\otimes X\otimes\mathbb{I}_2\rangle.
\end{aligned}$$

Now consider the following self-adjoint 3-unitary taken from Ref. [41]:

$$U = \frac{1}{\sqrt{8}} \begin{pmatrix} -1 & -1 & -1 & 1 & -1 & 1 & 1 & 1 \\ -1 & -1 & -1 & 1 & 1 & -1 & -1 & -1 \\ -1 & -1 & 1 & -1 & -1 & 1 & -1 & -1 \\ 1 & 1 & -1 & 1 & -1 & 1 & -1 & -1 \\ -1 & 1 & -1 & -1 & -1 & -1 & 1 & -1 \\ 1 & -1 & 1 & 1 & -1 & -1 & 1 & -1 \\ 1 & -1 & -1 & -1 & 1 & 1 & 1 & -1 \\ 1 & -1 & -1 & -1 & -1 & -1 & -1 & 1 \end{pmatrix}. \tag{3.20}$$

The following subalgebras are delocalised:

$$\mathcal{A}_L = U\mathcal{L}U^\dagger = \langle \mathbb{I}_8, Z \otimes Z \otimes X, XZ \otimes XZ \otimes Z, X \otimes X \otimes XZ \rangle,$$

$$\mathcal{A}_M = U\mathcal{M}U^\dagger = \langle \mathbb{I}_8, XZ \otimes Z \otimes XZ, Z \otimes X \otimes Z, X \otimes XZ \otimes X \rangle,$$

$$\mathcal{A}_R = U\mathcal{R}U^\dagger = \langle \mathbb{I}_8, Z \otimes XZ \otimes XZ, X \otimes Z \otimes Z, XZ \otimes X \otimes X \rangle.$$

The calculations can be found in the Sage notebook on the present author's GitHub repository [35].

The other direction, delocalisation of the three subalgebras implies 3-unitarity, does not hold. The unitary of dimension 27 in the next example provides a counter example.

Example 3. Consider the matrix algebra $\mathcal{M}_3(\mathbb{C}) \otimes \mathcal{M}_3(\mathbb{C}) \otimes \mathcal{M}_3(\mathbb{C})$ and consider the basis $\{X^i Z^j\}_{i,j=0,1,2}$ for $\mathcal{M}_3(\mathbb{C})$ with:

$$X = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \quad \text{and} \quad Z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \omega_3 & 0 \\ 0 & 0 & \omega_3^2 \end{pmatrix}, \text{ where } \omega_3 = \exp(2\pi i/3). \tag{3.21}$$

One can define the three local subalgebras:

$$
\begin{aligned}
\mathcal{L} &\cong \mathcal{M}_3(\mathbb{C}) \otimes \mathbb{I}_9 \\
&= \langle \mathbb{I}_3 \otimes \mathbb{I}_9, X \otimes \mathbb{I}_9, XZ \otimes \mathbb{I}_9, X^2Z^2 \otimes \mathbb{I}_9, XZ^2 \otimes \mathbb{I}_9, X^2 \otimes \mathbb{I}_9, Z \otimes \mathbb{I}_9, \\
&\qquad X^2Z \otimes \mathbb{I}_9, Z^2 \otimes \mathbb{I}_9 \rangle,
\end{aligned}
$$

$$
\begin{aligned}
\mathcal{M} &\cong \mathbb{I}_3 \otimes \mathcal{M}_3(\mathbb{C}) \otimes \mathbb{I}_3 \\
&= \langle \mathbb{I}_3 \otimes \mathbb{I}_3 \otimes \mathbb{I}_3, \mathbb{I}_3 \otimes X \otimes \mathbb{I}_3, \mathbb{I}_3 \otimes XZ \otimes \mathbb{I}_3, \mathbb{I}_3 \otimes X^2Z^2 \otimes \mathbb{I}_3, \mathbb{I}_3 \otimes XZ^2 \otimes \mathbb{I}_3, \\
&\qquad \mathbb{I}_3 \otimes X^2 \otimes \mathbb{I}_3, \mathbb{I}_3 \otimes Z \otimes \mathbb{I}_3, \mathbb{I}_3 \otimes X^2Z \otimes \mathbb{I}_3, \mathbb{I}_3 \otimes Z^2 \otimes \mathbb{I}_3 \rangle,
\end{aligned}
$$

$$
\begin{aligned}
\mathcal{R} &\cong \mathbb{I}_9 \otimes \mathcal{M}_3(\mathbb{C}) \\
&= \langle \mathbb{I}_9 \otimes \mathbb{I}_3, \mathbb{I}_9 \otimes X, \mathbb{I}_9 \otimes XZ, \mathbb{I}_9 \otimes X^2Z^2, \mathbb{I}_9 \otimes XZ^2, \mathbb{I}_9 \otimes X^2, \mathbb{I}_9 \otimes Z, \\
&\qquad \mathbb{I}_9 \otimes X^2Z, \mathbb{I}_9 \otimes Z^2 \rangle.
\end{aligned}
$$

Now consider the following permutation[3], which is *multiunitary* but not 3-unitary, since one rearrangement of U is not unitary:

$$U = \text{Perm}(0, 26, 13, 7, 21, 11, 5, 19, 15, 22, 9, 8, \tag{3.22}$$

$$20, 16, 3, 24, 14, 1, 17, 4, 18, 12, 2, 25, 10, 6, 23). \tag{3.23}$$

Its cycle structure is given by:

$$(0)(1\ 26\ 23\ 25\ 6\ 5\ 11\ 8\ 15\ 24\ 10\ 9\ 22\ 2\ 13\ 16\ 14\ 3\ 7\ 19\ 4\ 21\ 12\ 20\ 18\ 17).$$

The following subalgebras are delocalised:

- $\mathcal{A}_L = U\mathcal{L}U^\dagger$,
- $\mathcal{A}_M = U\mathcal{M}U^\dagger$,
- $\mathcal{A}_R = U\mathcal{R}U^\dagger$.

Again, the calculations can be found in the Sage notebook on the present author's GitHub repository [35].

[3]The notation used here was adopted from Ref. [41] and displays which entry gets mapped to which position through the permutation (in this specific example 0 is fixed, 1 gets mapped to 26, etc.) .

k-Unitaries and Delocalised Subalgebras

In contrast to the bipartite case, for dimensions d^3 only one direction of Prop. 3.0.2 holds. It is natural to ask, if that is also true for arbitrary $k > 3$. For this consider the matrix algebra $\mathcal{M}_{d^k}(\mathbb{C}) \cong \mathcal{M}_d(\mathbb{C}) \otimes \mathcal{M}_d(\mathbb{C}) \otimes ... \otimes \mathcal{M}_d(\mathbb{C})$, where $k > 2$. Now, the following k local subalgebras are both, mutually quasi-orthogonal and commutative: $\mathcal{L} = \mathcal{M}_d(\mathbb{C}) \otimes \mathbb{I}_{d^{k-1}}$, $\mathcal{R} = \mathbb{I}_{d^{k-1}} \otimes \mathcal{M}_d(\mathbb{C})$, $\mathcal{M}_1 = \mathbb{I}_d \otimes \mathcal{M}_d(\mathbb{C}) \otimes \mathbb{I}_{d^{k-2}}$, ..., and $\mathcal{M}_{k-2} = \mathbb{I}_{d^{k-2}} \otimes \mathcal{M}_d(\mathbb{C}) \otimes \mathbb{I}_d$. A subalgebra is called *delocalised*, if it is quasi-orthogonal to all k local subalgebras.

One can now suggest the following:

Proposition 3.0.4. *Consider the matrix algebra $\mathcal{M}_{d^k}(\mathbb{C}) \cong \mathcal{M}_d(\mathbb{C}) \otimes \mathcal{M}_d(\mathbb{C}) \otimes ... \otimes \mathcal{M}_d(\mathbb{C})$ for $k \geq 2$. Let $\mathcal{L} = \mathcal{M}_d(\mathbb{C}) \otimes \mathbb{I}_{d^{k-1}}$, $\mathcal{R} = \mathbb{I}_{d^{k-1}} \otimes \mathcal{M}_d(\mathbb{C})$ and $\mathcal{M}_1 = \mathbb{I}_d \otimes \mathcal{M}_d(\mathbb{C}) \otimes \mathbb{I}_{d^{k-2}}$, ..., $\mathcal{M}_{k-2} = \mathbb{I}_{d^{k-2}} \otimes \mathcal{M}_d(\mathbb{C}) \otimes \mathbb{I}_d$. Now consider $U \in U(d^k)$ and set $\mathcal{A}_L := U\mathcal{L}U^\dagger$, $\mathcal{A}_R := U\mathcal{R}U^\dagger$, $\mathcal{A}_{M_1} := U\mathcal{M}_1U^\dagger$, ..., $\mathcal{A}_{M_{k-2}} := U\mathcal{M}_{k-2}U^\dagger$.*

If U is a multiunitary in the sense that k^2 reorderings of U are unitary, then $\mathcal{A}_L$, $\mathcal{A}_R$, $\mathcal{A}_{M_1}$, ..., $\mathcal{A}_{M_{k-2}}$ are delocalised.

Proof. Let $\sqrt{d}E_{ij} = \sqrt{d}\,|i\rangle\,\langle j|$ be an ONB in $\mathcal{M}_d(\mathbb{C})$. Then

$$P_{\mathcal{L}} = d \sum_{i,j=1}^{d} |E_{ij} \otimes \mathbb{I}_{d^{k-1}}\rangle\,\langle E_{ij} \otimes \mathbb{I}_{d^{k-1}}|$$

is the projection onto the left subalgebra. Similarly, one has

$$P_{U\mathcal{L}U^\dagger} = d \sum_{i,j=1}^{d} |U(E_{ij} \otimes \mathbb{I}_{d^{k-1}})U^\dagger\rangle\,\langle U(E_{ij} \otimes \mathbb{I}_{d^{k-1}})U^\dagger|$$

as projection onto $\mathcal{A}_L$. Compute:

$$\begin{aligned}
\mathrm{Tr}(P_{U\mathcal{L}U^\dagger}P_{\mathcal{L}}^\dagger) &= d^2 \sum_{i,j,m,l=1}^{d} |\langle (UE_{ij}\otimes \mathbb{I}_{d^{k-1}}U^\dagger)|E_{ml}\otimes \mathbb{I}_{d^{k-1}}\rangle|^2 \\
&= d^2 \sum_{i,j,m,l=1}^{d} |\tau\big((UE_{ij}\otimes \mathbb{I}_{d^{k-1}}U^\dagger)(E_{ml}\otimes \mathbb{I}_{d^{k-1}})\big)|^2 \\
&= d^2 \sum_{i,j,m,l=1}^{d} |\frac{1}{d^k}\mathrm{tr}\big((UE_{ij}\otimes \mathbb{I}_{d^{k-1}}U^\dagger)(E_{ml}\otimes \mathbb{I}_{d^{k-1}})\big)|^2 \\
&= \frac{1}{d^{2k-2}} \sum_{i,j,m,l=1}^{d} |\mathrm{tr}\big((UE_{ij}\otimes \mathbb{I}_{d^{k-1}}U^\dagger)(E_{ml}\otimes \mathbb{I}_{d^{k-1}})\big)|^2.
\end{aligned}$$

Further compute:

$$= \mathrm{tr}\left(\sum\nolimits^{d}_{\substack{r_1,..,r_{k-1},\\ s_1,..,s_{k-1}=1}} U\,|ir_1...r_{k-1}\rangle\,\langle jr_1...r_{k-1}|\,U^\dagger\,|ms_1...s_{k-1}\rangle\,\langle ls_1...s_{k-1}|\right)$$
$$= \sum\nolimits^{d}_{\substack{r_1,..,r_{k-1},\\ s_1,..,s_{k-1}=1}} \langle ls_1...s_{k-1}|\,U\,|ir_1...r_{k-1}\rangle\,\langle jr_1...r_{k-1}|\,U^\dagger\,|ms_1...s_{k-1}\rangle$$
$$= \sum\nolimits^{d}_{\substack{r_1,..,r_{k-1},\\ s_1,..,s_{k-1}=1}} U^{ls_1...s_{k-1}}_{ir_1...r_{k-1}}(U^*)^{ms_1...s_{k-1}}_{jr_1...r_{k-1}}.$$

Now the orthogonality condition for $\mathcal{A}_L := U\mathcal{L}U^\dagger$ and $\mathcal{L}$ is given by the following trace equation:

$$\mathrm{Tr}(P_{\mathcal{A}_L}P_{\mathcal{L}}^\dagger) = \frac{1}{d^{2(k-1)}} \sum_{i,j,m,l=1}^{d} |\sum_{\substack{r_1,..,r_{k-1},\\ s_1,..,s_{k-1}=1}}^{d} U^{ls_1...s_{k-1}}_{ir_1...r_{k-1}}(U^*)^{ms_1...s_{k-1}}_{jr_1...r_{k-1}}|^2. \tag{3.24}$$

There are many possible ways to rearrange the indices in these equation in order to simplify them. Apply for example the change $l \leftrightarrow r_1$ in the expression for U and the change $m \leftrightarrow r_1$ in the expression for U^* and denote it as

$U^{R_{1,2}}$. One then gets:

$$\begin{aligned}\mathrm{Tr}(P_{\mathcal{A}_L}P_{\mathcal{L}}^{\dagger}) &= \frac{1}{d^{2(k-1)}}\sum_{i,j,m,l=1}^{d}|\sum_{\substack{r_1,..,r_{k-1},\\ s_1,..,s_{k-1}=1}}^{d}(U^{R_{1,2}})_{il...r_{k-1}}^{r_1s_1...s_{k-1}}(U^{*R_{1,2}})_{jm...r_{k-1}}^{r_1s_1...s_{k-1}}|^2\\ &= \frac{1}{d^{2(k-1)}}\sum_{i,j,m,l=1}^{d}|\sum_{\substack{r_1,..,r_{k-1},\\ s_1,..,s_{k-1}=1}}^{d}(U^{R_{1,2}})_{il...r_{k-1}}^{r_1s_1...s_{k-1}}((U^{R_{1,2}})^{\dagger})_{r_1s_1...s_{k-1}}^{jm...r_{k-1}}|^2\\ &= \frac{1}{d^{2(k-1)}}\sum_{i,j,m,l=1}^{d}|\mathrm{tr}_{3,...,k}\Big((U^{R_{1,2}}(U^{R_{1,2}})^{\dagger})_{il}^{jm}\Big)|^2\end{aligned}$$

where $\mathrm{tr}_{3,...,k}$ denotes the partial trace over the subsystems 3 to k. If $U_{1,2}^{R}$ is unitary then this expressions is equal to one and hence $\mathcal{L}$ and $\mathcal{A}_L$ are quasi-orthogonal in that case. Actually, there are $2\cdot(k-1)$ possible ways to rearrange the indices leading to different rearrangements of U.

A similar calculation shows that the orthogonality condition for $\mathcal{A}_L := U\mathcal{L}U^{\dagger}$ and $\mathcal{R}$ resp. $\mathcal{M}_i$ relies on the following traces:

$$\mathrm{Tr}(P_{\mathcal{A}_L}P_{\mathcal{R}}^{\dagger}) = \frac{1}{d^{2(k-1)}}\sum_{i,j,k,l=1}^{d}|\sum_{\substack{r_1,..,r_{k-1},\\ s_1,..,s_{k-1}=1}}^{d}(U_{js_1...s_{k-1}}^{r_1...r_{k-1}i}(U^*)_{ls_1...s_{k-1}}^{r_1...r_{k-1}m})|^2 \tag{3.25}$$

and

$$\mathrm{Tr}(P_{\mathcal{A}_L}P_{\mathcal{M}_i}^{\dagger}) = \frac{1}{d^{2(k-1)}}\sum_{i,j,k,l=1}^{d}|\sum_{\substack{r_1,..,r_{k-1},\\ s_1,..,s_{k-1}=1}}^{d}(U_{js_1...s_{k-1}}^{r_1...r_{i-1}ir_{i+1}...r_k}(U^*)_{ls_1...s_{k-1}}^{r_1...r_{m-1}mr_{m+1}...r_k})|^2 \tag{3.26}$$

which give $k-2$ trace conditions for the subalgebras $\mathcal{M}_1 = \mathbb{I}_d\otimes\mathcal{M}_d(\mathbb{C})\otimes\mathbb{I}_{d^{k-2}}, ..., \mathcal{M}_{k-2} = \mathbb{I}_{d^{k-2}}\otimes\mathcal{M}_d(\mathbb{C})\otimes\mathbb{I}_d$. Here the first condition leads to k new ways of partitioning the index set (the other $k-2$ are superfluous as they lead to rearrangements of U that already have been covered in the quasi-orthogonality condition of $\mathcal{L}$ and $\mathcal{A}_L$). The remaining $k-2$ conditions give $k-1$ new ways of partitioning the index set. Hence in total one gets: $2(k-1)+k+(k-1)(k-2) = k^2$ ways. So if U is multi-unitary in the sense that k^2 rearrangements are unitary, then $\mathcal{A}_L$ is delocalised. The trace conditions for the other subalgebras can be found in Appendix A. □

In general, far less than k^2 reorderings of U have to be unitary in order for the subalgebras to be delocalised, as Theorem 3.0.3 already suggests. This is because the reorderings of U appear in more than one trace condition. For $k = 4$ for example, four reorderings of U suffice to delocalise all local subalgebras (see Appendix A). This can also be demonstrated in the following example:

Example 4. For $d = 16 = 4^2 = 2^4$ the following permutation matrix of order 2 is 2-unitary. Moreover, it is multiunitary in the sense that 4 rearrangements of U are unitary:

$$U_{16} = \text{Perm}(0, 11, 13, 6, 14, 5, 3, 8, 7, 12, 10, 1, 9, 2, 4, 15). \tag{3.27}$$

Its cycle structure is given by:

$$(0)(1\ 11)(2\ 13)(3\ 6)(4\ 14)(5)(7\ 8)(9\ 12)(10)(15). \tag{3.28}$$

This matrix gives rise to two delocalised subalgebras isomorphic to $\mathcal{M}_4(\mathbb{C})$ and 4 delocalised subalgebras that are isomorphic to $\mathcal{M}_2(\mathbb{C})$ in $\mathcal{M}_{16}(\mathbb{C})$.

How many reorderings of U suffice to delocalise the local subalgebras for general k remains an open question.

In Ref. [88] the author proved that in $\mathcal{M}_{p^k}(\mathbb{C})$, where $p \geq 3$ is a prime, the number of mutually quasi-orthogonal subalgebras isomorphic to $\mathcal{M}_p(\mathbb{C})$ is given by

$$N_k = \frac{p^{2k} - 1}{p^2 - 1}. \tag{3.29}$$

This number is clearly greater than the one derived in Prop. 3.0.4. Consider the case $k = 3$ and $p = 3 = d$ for example. While there have to be 91 mutually quasi-orthogonal subalgebras isomorphic to $\mathcal{M}_3(\mathbb{C})$ in total, the construction via 3-unitaries only gives 9. However, the bound in Ref. [88] only applies to prime numbers, whereas the approach via k-unitaries does not restrict to prime dimensions. The question in which dimensions k-unitaries exist also remains open.

3.2 The Group-Theoretical Perspective

In this section the existence problem of 2-unitaries will be addressed from the group theoretical point of view. This will be done by first formulating

Proposition 3.0.2 in terms of groups and representations and then presenting a search algorithm for the algebra software GAP that aims to find suitable systems of subgroups that give rise to mutually quasi-orthogonal subalgebras via a representation.

3.2.1 Related Work

In Ref. [88] the author gives an example of a quasi-orthogonal decomposition of a matrix algebra, where each subalgebra corresponds to a factor, obtained via a projective representation of subgroups of the group $\mathbb{Z}_p^4$. Although the author himself does not establish the connection, this decomposition also provides an example for Proposition 3.0.2 and hence it is natural to ask if $\mathbb{Z}_p^4$ is the only group that provides such an example or if there also exist other groups. In Ref. [120] the authors go one step further and discuss dual unitarity conditions of a unitary represented via a projective representations of finite groups. They, too, discuss $\mathbb{Z}_p^4$ as a specific example. Interesting to note is, that $\mathbb{Z}_p^4$ with its projective representation happens to be an example of an abstract error group (see [63] for more details), a concept that builds on nice error basis that were introduced by Knill in Ref. [65]. Whether there exist other groups that can be used to construct 2-unitaries will be the central topic of this section.

3.2.2 The Existence of 2-unitaries and the Existence Groups with Factorising Character

Proposition 3.0.2 could be used to find 2-unitaries in arbitrary dimensions d^2 for $d > 2$ but since algebras are in comparison to groups rather complex structures, it might be more fruitful to discuss that matter from a group theoretical perspective. For this, rephrase Prop. 3.0.2 in the language of group theory:

Proposition 3.0.5. *The following is sufficient for the existence of a 2-unitary $U \in U(d^2)$:*

i) There exists a finite group G of order $|G| \geq d^4$ with a d^2-dimensional complex irreducible representation $(\rho, \mathcal{M}_{d^2}(\mathbb{C}))$, which affords a character χ.

ii) There exist subgroups $L, R, A_L, A_R < G$ of order $|L|, |R|, |A_L|, |A_R| \geq d^2$ such that ρ restricted to any of these subgroups is a d-dimensional irrep with multiplicity d.

iii) *For all $l \in L, r \in R$ $l^{-1}r^{-1}lr \in \ker(\chi)$ and $L \cap R = Z(\chi)$. Similarly, for all $a_l \in A_L, a_r \in A_R$ $a_l^{-1}a_r^{-1}a_la_r \in \ker(\chi)$ and $A_L \cap A_R = Z(\chi)$.*

iv) *The character factorises for all pairs of subgroups $L, R, A_L, A_R < G$, i.e. :*

$$d^2\chi(l \cdot r) = \chi(l)\chi(r) \quad \forall \quad l \in L,\ r \in R. \tag{3.30}$$

Proof. According to Prop. 3.0.2, the existence of a 2-unitary is guaranteed by the existence of a delocalised subalgebra of $\mathcal{M}_{d^2}(\mathbb{C})$. In the following the different criteria will be related to their algebraic analogue:

i) This condition fixes the algebra $\mathcal{M}_{d^2}(\mathbb{C})$.

ii) Here the two local subalgebras and the delocalised subalgebra are fixed, as Prop. 2.33.2 implies that $\langle\rho(A)\rangle$, $\langle\rho(R)\rangle$ and $\langle\rho(L)\rangle$ are isomorphic to $\mathcal{M}_d(\mathbb{C})$).

iii) Because of Prop. 2.37.1 , this criterion ensures that the two local subalgebras $\mathcal{L}, \mathcal{R}$ and $\mathcal{A}_L, \mathcal{A}_R$ are each others commutant. Moreover, it implies that the subalgebras satisfy

$$\langle\rho(L)\rangle \cap \langle\rho(R)\rangle = \mathbb{C}\mathbf{1}, \tag{3.31}$$
$$\langle\rho(A_L)\rangle \cap \langle\rho(A_R)\rangle = \mathbb{C}\mathbf{1}, \tag{3.32}$$

and hence are factors.

iv) Following Prop. 2.28.1), this conditions corresponds to all four subalgebras being mutually quasi-orthogonal.

□

What restrictions can one make on the group order? According to Theorem 2.39.1, the order of a group $|G|$ must be divisible by $\chi(e)$. In this case, that means that $d^2 \mid |G|$ and thus there has to exist a number $m \in \mathbb{N}$, such that $|G| = m \cdot d^2$. Since it is also required that $|G| \geq d^4$, one can conclude that $m \geq d^2$. Moreover, according to Theorem 2.39.2, $\chi(e) = d^2$ also has to divide $|G : Z(\chi)|$ and hence there has to exist a number $m' \in \mathbb{N}$ such that $|G : Z(\chi)| = m' \cdot d^2$. Additionally, Theorem 2.38.2 says that $|G : Z(\chi)| \geq d^4$ and hence $m' \geq d^2$. Taking these criteria together, one finds:

$$m'd^2 = |G : Z(\chi)| = \frac{|G|}{|Z(\chi)|} = \frac{md^2}{|Z(\chi)|} \tag{3.33}$$

which is equivalent to

$$|Z(\chi)| = \frac{m}{m'} \quad \text{with} \quad m \geq m' \geq d^2. \tag{3.34}$$

Thus m has to be divisible by m'.

Moreover, one can conclude, that the order of $|G|$ cannot be squarefree. More concretely, the groups one is concerned about have to be of order that is greater or equal to d^4 . Moreover, the order has to be divisible by d^2 and by the order of the index of $Z(\chi)$. For low values of $d \geq 3$ [4] that means:

d	$\lvert G\rvert \geq$	$\lvert G\rvert$ is divisible by
3	$3^4 = 81$	$3^2 = 9$
4	$4^4 = 256$	$4^2 = 16$
5	$5^4 = 625$	$5^2 = 25$
6	$6^4 = 1206$	$6^2 = 36$

What are examples of groups meeting these criteria? Do they come with additional structures/requirements?

Example: Error groups

Recall that a group G is an abstract error group if and only if it is of central type and has cyclic center. Hence, if one assumes that the group G in Prop. 3.0.5 is of central type and has a faithful irreducible representation (this implies that $Z(G)$ is cyclic according to Theorem 2.32 on p. 29 in Ref. [60]), one finds that G is an abstract error group. In particular G is isomorphic to the direct product of an order d^4 index group of a nice error basis and an order d group generated by the factor system (see Definition 2.3.3). This can be seen by considering Theorem 2.38.2, which leads to the following equality:

$$|G| = d^4|Z(G)|. \tag{3.35}$$

The character afforded by ρ has to vanish on $G - Z(G)$, i.e.

$$\chi(g) = \begin{cases} \epsilon\chi(e), & if\ g \in Z(G) \\ 0, & \text{otherwise.} \end{cases} \tag{3.36}$$

[4]For $d = 2$ the construction does not make sense as there are no 2-unitaries in dimension 4.

This means that abstract error groups of order d^5 provide an example to Prop. 3.0.5. If G has trivial center, it corresponds to the Weyl-Heisenberg group in dimension d^4.

Moreover, the subgroups L, R and A also form error groups. To see that, consider an arbitrary element $l \in L$. Because the character is either 0 or $\epsilon\chi(e)$ for every element of G and some $\epsilon \in \mathbb{C}$, l has to fall into one of these classes. If $l \in Z(G)$, then l commutes with every element in G and hence also with every element in L and therefore: $l \in Z(L)$. Per definition, any element of $Z(L)$ cannot have character equal to zero if its degree is unequal to zero, as one has that $Z(L) = \{l \in L \mid |\chi(l)| = \chi(e)\}$. There might be more elements in $Z(L)$ than in $Z(G)$, but per definition these also cannot have vanishing character. Hence χ vanishes on all elements of $L - Z(L)$. According to Theorem 2.38.2, the following equality has to hold:

$$|\chi \restriction_L (e)|^2 = \frac{|L|}{|Z(L)|} \tag{3.37}$$

This can be rewritten into:

$$d^2|Z(L)| = |L|. \tag{3.38}$$

So L is actually also a (smaller) abstract error group corresponding to an error group of order d^2. The factor system has again order d. One can draw similar conclusions for the subgroups R and A.

How can one relate the group order of $|G|, |L|$ and $|R|$? Since ρ is assumed to be faithful, one has: $L \cap R = \{e\}$ and hence

$$|L \cdot R| = |L||R| = d^4|Z(L)||Z(R)|. \tag{3.39}$$

One can thus make the following observation:

$$\frac{|L \cdot R|}{|Z(L)||Z(R)|} = \frac{|G|}{|Z(G)|}. \tag{3.40}$$

In the special case where $G, L,$ and R have trivial center, one can conclude that G is actually a direct product of the subgroups L and R.

In Therorem 3.0.5 it was assumed that the subgroups L, R and A are not Abelian and that their pairwise intersection is not necessarily trivial. This distinguishes the construction from the one given in Ref. [86], where the existence of k subgroups of an index group of a nice error basis was related to the existence of k MASAs. Here the authors assumed that the subgroups have pairwise trivial intersections and are Abelian. Thus, one might say, for some error basis L, R:

> L, R not Abelian, $l^{-1}rlr^{-1} \in \ker(\chi)\ \forall\, l \in L, r \in R$ and $L \cap R = Z(\chi) \to$ factor
>
> L, R Abelian and $L \cap R = \{e\} \to$ MASAs

An explicit example of subgroups of an error group giving rise to quasi-orthogonal factors was given in Ref. [88]:
Let p be a prime number. Consider the Weyl-Heisenberg operators $Z = \mathrm{diag}(1, \omega_p, \omega_p^2, ..., \omega_p^{p-1})$, where $\omega_p = \exp(2\pi i/p)$ and

$$X = \begin{pmatrix} 0 & 0 & ... & 0 & 1 \\ 1 & 0 & ... & 0 & 0 \\ 0 & 1 & ... & 0 & 0 \\ . & . & ... & . & . \\ 0 & 0 & ... & 1 & 0 \end{pmatrix} \tag{3.41}$$

in $\mathcal{M}_p(\mathbb{C})$, defining an orthogonal basis in $\mathcal{M}_p(\mathbb{C})$ via $\{X^i Z^j\}_{i,j \in \mathbb{Z}_p}$.

Let $\pi : \mathbb{Z}_p^4 \to \mathcal{M}_{p^2}(\mathbb{C})$ be a projective homomorphism such that:

$$\pi : u = (k_1, k_2, l_1, l_2) \mapsto X^{k_1} Z^{l_1} \otimes X^{k_2} Z^{l_2}. \tag{3.42}$$

Moreover, let the symplectic product be defined by:

$$[u, u'] = k_1 k_2' - k_2 k_1' + l_1 l_2' - l_2 l_1' \mod p. \tag{3.43}$$

In particular, π is a p^2-dimensional irrep. Let $D \in \mathbb{Z}_p$ be such that $D \neq k^2 \mod p$ for all $k \in \mathbb{Z}_p$. For any $a, a_0, a_1 \in \mathbb{Z}_p$ one can define the following subgroups of $\mathbb{Z}_p^4$:

$$C_{a_0,a_1} = \{b_0(1, a_1, 0, a_0) + b_1(1, a_0, 1, a_1 D) | b_0, b_1 \in \mathbb{Z}_p\} \tag{3.44}$$

$$D_a = \{b_0(1, 1, a, aD) + b_1(1, 2, a, 2aD) | b_0, b_1 \in \mathbb{Z}_p\} \tag{3.45}$$

$$D_\infty = \{b_0(0, 0, 1, 0) + b_1(0, 0, 0, 1) | b_0, b_1 \in \mathbb{Z}_p\}. \tag{3.46}$$

These subgroups give rise to the following subalgebras of $\mathcal{M}_{p^2}(\mathbb{C})$ that are isomorphic to $\mathcal{M}_p(\mathbb{C})$ [88]:

$$\langle \pi(C_{a_0,a_1}) \rangle, \quad \langle \pi(D_a) \rangle \quad \text{and} \quad \langle \pi(D_\infty) \rangle. \tag{3.47}$$

The algebras defined this way are quasi-orthogonal [88]. Now, according to Theorem 3.0.5, this means that π restricted to these subgroups is a p-dimensional irrep with multiplicity p and that the character afforded by π factorises on these subgroups.

The author gives an explicit example for the case $p = 3$:

Example 5. [88] Consider the orthogonal basis in $\mathcal{M}_3(\mathbb{C})$ via $\{X^i Z^j\}_{i,j \in \mathbb{Z}_3}$ in $\mathcal{M}_3(\mathbb{C})$ and the projective representation $\pi : \mathbb{Z}_3^4 \to \mathcal{M}_9(\mathbb{C})$ with:

$$\pi : u = (k_1, k_2, l_1, l_2) \mapsto X^{k_1} Z^{l_1} \otimes X^{k_2} Z^{l_2}. \tag{3.48}$$

Let $D = 2$. The following subgroups of $\mathbb{Z}_3^4$ give rise to 10 quasi-orthogonal factors in $\mathcal{M}_9(\mathbb{C})$ via π:

i) $C_{1,0} = \{b_0(1,0,0,1) + b_1(1,1,1,0) | b_0, b_1 \in \mathbb{Z}_3\}$

ii) $C_{1,1} = \{b_0(1,1,0,1) + b_1(1,1,1,2) | b_0, b_1 \in \mathbb{Z}_3\}$

iii) $C_{1,2} = \{b_0(1,2,0,1) + b_1(1,1,1,1) | b_0, b_1 \in \mathbb{Z}_3\}$

iv) $C_{2,0} = \{b_0(1,0,0,2) + b_1(1,2,1,0) | b_0, b_1 \in \mathbb{Z}_3\}$

v) $C_{2,1} = \{b_0(1,1,0,2) + b_1(1,2,1,2) | b_0, b_1 \in \mathbb{Z}_3\}$

vi) $C_{2,2} = \{b_0(1,2,0,2) + b_1(1,2,1,1) | b_0, b_1 \in \mathbb{Z}_3\}$

vii) $D_0 = \{b_0(1,1,0,0) + b_1(1,2,0,0) | b_0, b_1 \in \mathbb{Z}_3\}$

vii) $D_1 = \{b_0(1,1,-1,2) + b_1(1,2,-1,1) | b_0, b_1 \in \mathbb{Z}_3\}$

viii) $D_2 = \{b_0(1,1,-2,1) + b_1(1,2,-2,2) | b_0, b_1 \in \mathbb{Z}_3\}$

ix) $D_\infty = \{b_0(0,0,1,0) + b_1(0,0,0,1) | b_0, b_1 \in \mathbb{Z}_3\}$

Here the subgroups D_0 and D_∞ give rise to the left and the right subalgebra. By construction, the other eight subgroups then give rise to delocalised subalgebras.

In this example, a 2-unitary U maps an element $W \in H(3^2)$ to another element $W' \in H(3^2)$ under conjugation:

$$UWU^{\dagger} = W'. \tag{3.49}$$

Thus, U is an element of the Clifford group.

Are all 2-unitaries elements of the Clifford group? The following consideration will show that this question must be answered in the negative.

No-go for Clifford 2-unitaries in dimension 36

The following observation can also be found in Ref. [46], co-authored by the present author. Recall that the Chinese remainder theorem gives a possibility to factorise the Weyl-Heisenberg group if the dimension is a product of coprime integers. Let $d = 3 \cdot 2$ and consider the Weyl-Heisenberg operators $Z_6 = \mathrm{diag}(1, \omega_6, \omega_6^2, ..., \omega_6^5)$, where $\omega_6 = \exp(2\pi i/6)$ and

$$X_6 = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}. \tag{3.50}$$

According to the Chinese remainder theorem these operators have to factorise into products of the following form

$$Z_6 \cong Z_2 \otimes Z_3, \quad X_6 \cong X_2 \otimes X_3, \tag{3.51}$$

where $Z_2 = \mathrm{diag}(1, i), Z_3 = \mathrm{diag}(1, \omega_3, \omega_3^2)$ and

$$X_2 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, X_3 = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \tag{3.52}$$

for $w_3 = \exp(2\pi i/3)$. A basis for $\mathcal{M}_6(\mathbb{C})$ is given by $\{X_6^i Z_6^j\}_{i,j \in \mathbb{Z}_6}$ which is isomorphic to

$$\{X_2^{a_1} Z_2^{(3^{-1} \bmod 2) b_1} \otimes X_3^{a_2} Z_3^{(2^{-1} \bmod 3) b_2}\}_{a_1, b_1 \in \mathbb{Z}_2, a_2, b_2 \in \mathbb{Z}_3}. \tag{3.53}$$

This amounts to

$$\{X_2^{a_1} Z_2^{2b_1} \otimes X_3^{a_2} Z_3^{2b_2}\}_{a_1,b_1 \in \mathbb{Z}_2, a_2, b_2 \in \mathbb{Z}_3}. \tag{3.54}$$

This factorisation of the basis extends to all unitaries within the Weyl-Heisenberg group and thus also the Clifford group, implying that one can factorise each 6^2-dimensional unitary U into a tensor product of a 9-dimensional and a 4-dimensional unitary. Since the reshuffle and the partial transpose operations are linear on the tensor factors, 2-unitarity of U would imply that the two sub-matrices are also 2-unitary. But as there do not exist 2-unitaries in dimension 4, one can conclude from this that a 36-dimensional 2-unitary cannot be of this form and thus cannot be an element of the Clifford group. This no-go statement can be generalised to arbitrary dimensions that are congruent to 2 mod 4.

3.2.3 GAP-Search

In light of the last section, where the existence of a Clifford 2-unitary in dimension 36 has been disproven, it is natural to ask, if there exists another example of a group fulfilling the criteria of 3.0.5 that gives rise to a 2-unitary of dimension 36. Moreover, are there any other groups that give rise to non-Clifford 2-unitaries in other dimensions?
Inspired by Ref. [44], where the authors used the computational algebra software GAP [32] to look for *group designs*, i.e. the group-theoretical description of unitary t-designs, by “harvesting“ character tables, one can use the criteria in Prop. 3.0.5 to look for groups that give rise to 2-unitaries within the GAP system.

In trying to answer the above questions, the present author has conducted a search in the SmallGroups-library [13] of the GAP-software. The SmallGroups-library contains groups of order at most 2000 except the ones of order 1024, groups of cubefree order of at most 50000, groups of order p^n for $n \leq 6$ and all primes p, groups of order p^7 for $p = 3, 5, 7, 11$, groups of order $g^n \cdot p$ for $q^n \,|2^8, 3^6, 5^5, 7^4$ and all primes $p \neq q$, groups of squarefree order and groups whose order factorises into at most 3 primes [13].

GAP comes equipped with its own programming language which has control structures (if-statements, while-loops, etc.) that are similar to the language Pascal. Moreover, GAP is equipped with functions that can be used to calculate the most important entities in group theory, representation theory and character theory. Table 3.2 displays some of these functions. For more details the author refers to the GAP-manual [32].

In order to conduct the search the author has written a program that can be run directly in the GAP-software using the command “Read("filename.g")“. In order to reduce the complexity of the search, the algorithm was designed to search for the matrix group arising from the irrep in Proposition 3.0.5, rather than the group itself. This means in particular, that it suffices to check that the subgroups L and R (A_L and A_R) commute with each other in *iii*) of Prop. 3.0.5.

The following criteria have been used to write the algorithm:

- Find group $|G| \geq d^4$ with irrep affording a character χ, that satisfies: $\chi(e_G) = d^2$.
- Find subgroups $|L|, |R|, |A| \geq d^2$, such that $\chi \restriction_A (e) = \chi \restriction_L (e) = \chi \restriction_R (e) = d^2$ and $\langle \frac{1}{d}\chi \restriction_{A_L}, \frac{1}{d}\chi \restriction_{A_L} \rangle = \langle \frac{1}{d}\chi \restriction_R, \frac{1}{d}\chi \restriction_R \rangle = \langle \frac{1}{d}\chi \restriction_L, \frac{1}{d}\chi \restriction_L \rangle = 1$.
- Check that the subgroups $|L|, |R|$ commute
- Check that character factorises for all pairs of subgroups $L, R, A < G$.

Note that the fourth subgroup has been dropped here and the name of the third has been changed to A. This is because the existence of A_L implies the existence of A_R and hence one can reduce the computational complexity by only searching for one subgroup.

In the following, the pseudocode of the program will be presented. The code itself can be found on the present author’s GitHub repository [35]. For better readability, the pseudocode slightly differs from the code there. However, the overall logic stays the same.

The following table displays GAP-functions that were used in the code[5]:

Function	Output
IRR(G):	a list of all irreps of G
SUBGROUPS(G):	a list of all subgroups of G
DEGREEOFCHARACTER(χ):	the degree of χ, i.e. $\chi(e)$
ISSQUAREINT(n):	`true`, if n is a square integer
RESTRICTEDCLASSFUNCTION(χ, H):	χ restricted to H
ISCHARACTER(χ):	`true`, if χ is a character
ISIRREDUCIBLE(χ):	`true`, if χ is irreducible

TABLE 3.2: List of GAP functions used in the code.

[5]Here G refers to a group, H refers to a subgroup of G and χ to a character of G.

At the heart of the program lies the following function that takes as input a group G and outputs a list consisting of a group G, a character degree and a list of subgroup triplets, if this group fulfils the criteria from above. It outputs `fail`, if it does not.

```
function TESTGROUP(G)
    local variables: χ, SubGrps, SubGrps_χ, Triplets, SubGrps_com, SubGrps_noncom
    SUBGROUPS(G) ← SubGrps
    for χ in Irr(G) do
        if ISSQUAREDEG(χ) then
            TESTCHARACTER(G, SubGrps, χ) ← SubGrps_χ
            SORTSUBGROUPS(SubGrps_χ, χ) ← SubGrps_com, SubGrps_noncom
            FINDTRIPLETS(SubGrps_com, SubGrps_noncom) ← Triplets
            return Triplets, G, χ
        end if
    end for
    return fail
end function
```

The function first computes the subgroups of G and stores them in a list SubGrps. Then it loops through the list of irreducible representations of G and checks for each character χ, if it has square dimension. If yes, then the function TESTCHARACTER(G, SubGrps, χ) will be called and ouputs a list of subgroups SubGrps_χ that fulfil the criteria from ii) with respect to χ. In the next step, the function calls SORTSUBGROUPS($\text{SubGrps}_\chi, \chi$) in order to filter out the subgroups that are quasi-orthogonal and to divide these subgroups into two lists: one of commuting and one of non-commuting pairs of subgroups.
In the last step, the function calls FINDTRIPLETS($\text{SubGrps}_{com}, \text{SubGrps}_{noncom}$) to construct triplets of subgroups consisting of two commuting subgroups and one subgroup that does not commute with the other two subgroups. If the construction was successful, the function will output the list of triplets along with the corresponding group and the dimension of the irrep in the last step. If not, it will output `fail`.

The function uses several other functions that will be explained in the following.
The function IsSquareDeg(χ) takes as input a character χ, checks if its degree is a square integer greater than one, using the GAP-functions The function TestCharacter(G, SubGrps, χ) takes as input a group G, a list of subgroups of G, namely SubGrps, and a character χ. It checks for each subgroup, if the restriction of χ onto this subgroup is an irreducible character with multiplicity being the square root of the degree of χ and the degree being equal to the degree of χ. The function returns a list of subgroups of G that fulfil these conditions. If this list is shorter than 4, the function returns `fail` (as one cannot find 4 subgroups in that case).

---

function TestCharacter(G, SubGrps, χ)
  local variables: H, d, $\chi_{restr.}$, Output
  $[\quad] \leftarrow$ Output
  for H in SubGrps **do**
    Sqrt(DegreeOfCharacter(χ)) $\leftarrow d$
    RestrictedClassFunction(χ, H) $\leftarrow d \cdot \chi_{restr.}$
    if DegreeOfCharacter($\chi_{restr.}$) $=$ d and IsCharacter($\chi_{restr.}$) $=$ `true` and IsIrreducible($\chi_{restr.}$) $=$ `true` **then**
      add H to Ouput
    end if
  end for
  if Length(Output) < 4 **then**
    return `false`
  else
    return Output
  end if
end function

The function FactorisingCharacter(χ, $SubGrp1$, $SubGrp2$) takes as input a character χ, two subgroups $SubGrp1$, $SubGrp2$ and outputs `true` if the character factorises and `false` if it does not.

```
function FactorisingCharacter(χ, Subgroup1, Subgroup2)
    local variables: h, k
    for h in Elements(SubGrp1) do
        for k in Elements(SubGrp2) do
            if χ(k)χ(h) ≠ χ(hk)χ(e) then
                return false
            end if
        end for
    end for
    return true
end function
```

The function SortSubgroups(SubGrps, χ) takes as input a list of subgroups and a character χ and checks for which of the subgroups the character factorises, calling the function FactorisingCharacter(χ, $SubGrp1$, $SubGrp2$). Via the function CommutingSubgroups($SubGrp1, SubGrp2$), these groups are then sorted into to two lists - one which contains pairs of subgroups that commute with each other and one which consists of pairs of non-commuting subgroups. If one of the resulting lists has length smaller than 2, the function outputs `fail`, otherwise it will output the two lists.

```
function SortSubgroups(SubGrps, χ)
    local variables: H, K, Output1, Output2
     [  ] ← Output1
    [  ] ← Output2
    for H in SubGrps do
        for K in SubGrps do
            if H ≠ K then
                if FactorisingCharacter(χ, H, K) = true then
                    if CommutingSubgroups(H, K) = true  then
                        Add [H, K] to Output1
                    else
                        Add [H, K] to Output2
                    end if
                end if
            end if
        end for
    end for
    if Length(Output1) < 2 or Length(Output2) < 2 then
        return fail
    else
         return Output1, Output2
    end if
end function
```

The function FINDTRIPLET(List1, List2) takes as input two lists of pairs of objects and creates a new list consisting of triplets, where the first two elements form an element in the first list and the third element is chosen in such a way that both, the first and the third, and the second and the third element, exist as elements in the second list. The function returns `fail`, if the creation was not successful. Otherwise, it will output the list of triplets.

```
function FindTriplet(List1, List2)
    local variables: L, R, B, A, Output
    [  ] ← Output
    for [L, R] in List1 do
        for [B, A] in List2 do
            if (L = B and R ≠ A) or (R = B and L ≠ A) or(L = A and R ≠ B) or (R = A and L ≠ B) then
                add [L,R, A] to Output
            end if
        end for
    end for
    if Length(Output) = 0 then
        return fail
    else
        return Output
    end if
```

The whole search algorithm clearly scales with the order of the group that is tested, since having more group elements implies more and also larger subgroups that have to be tested. Thus, for groups of higher order the calculations become particularly cumbersome and some point max out the memory capacity. This imposes a restriction on the search space within the SmallGroups-library. The main bottleneck of the algorithm is the test if two subgroups commute. This has computational complexity of order $\mathcal{O}(n \cdot m)$, where n and m denote the order of the two subgroups, respectively.

To test, if the code actually does what is desired, each function was individually tested on specific examples within the SmallGroups library, where the outcome was known. More concretely, the whole search algorithm was applied to both an example and a non-example of Prop. 3.0.5, namely the group SmallGroup(243,65) together with the irrep number 65, and the group SmallGroup(32,50) together with the irrep number 83, corresponding to the WH group for $d = 3$ and the WH group for $d = 2$. This was to ensure that the algorithm does not deliver false negatives and false positives.

Since there are restrictions on the order of the groups that should be searched for, clearly, not all of the groups in the library were of interest (e.g. groups of squarefree order). The SmallGroups library is organised in 11 layers, where each layer contains groups of specific orders. The groups of cubefree and squarefree order are located in the 10-th layer, which could thus be left out in the search space. Unfortunately, due to the huge computational complexity for higher order groups, the algorithm maxed out the memory capacity before looping through the whole search space. This already happens for groups having order 1000 leaving the rest of the library unexplored.

The algorithm did not find any example of groups satisfying the criteria other than the WH-group. While this rules out the existence of such a group in GAP's Smallgroups library up to groups of order 1000, it does not rule out the existence of such a group in general. This is not only because the algorithm could loop through the whole library but also because the Smallgroups library only contains groups up to order except 1024, groups of cubefree order at most 50000, groups of order p^n for $n \leq 6$ and all primes p, groups of order p^7 for $p = 3, 5, 7, 11$, groups of order $g^n \cdot p$ for $q^n \; | 2^8, 3^6, 5^5, 7^4$ and all primes $p \neq q$, groups of squarefree order and groups whose order factorises into at most 3 primes [13]. Hence, it is possible that there exist solutions for groups with higher order or other groups that are not part of the library. Of course, it is also possible that the Weyl-Heisenberg group is indeed the only possible solution, which would imply that there are certain 2-unitaries that cannot be described by Prop. 3.0.5, e.g. in dimension $d^2 = 36$.

3.3 Perfect Tensors from Doubly Perfect Sequences

The preceding section established that Clifford 2-unitaries cannot exist in dimension 36, since the Chinese Remainder Theorem would in that case imply that there exists a 2-unitary in dimension 4, which is known to be impossible. However, 2-unitaries are known to exist in dimension 9. This raises the question of whether a 2-unitary in dimension 36 can be obtained from a 2-unitary in dimension 9 combined with an appropriate 4-dimensional matrix. As demonstrated below, such a construction is feasible. Following Rather's Ansatz of constructing a 2-unitary using doubly perfect bi-unimodular sequences, one can use a doubly perfect sequence with period $d = 3$, that gives rise to a 2-unitary in dimension 9, and modify it in such a way that it yields a 2-unitary in dimension 36. This naturally leads to an examination of the relationship between doubly perfect sequences and perfect tensors in arbitrary dimensions, which will be addressed in the following section.

3.3.1 Related Work

Recall that the existence of two orthogonal Latin squares of order $d = 6$ was disproven by Tarry in 1900. With the development of the concept of quantum orthogonal Latin squares, this existence problem got extended to the quantum case. An extensive computer search recently resolved the existence problem for $d = 6$ in the affirmative and additional computer-generated solutions were later reported in Refs. [21, 20, 95]. These solutions are exact in the sense that every matrix entry of the two-unitary can be expressed as an algebraic number. However, while the constructions used symmetries, their deeper structure remained unexplained. This section builds on the results of Rather, who linked the existence of 2-unitaries to the existence of what he called perfectly perfect bi-unimodular sequences (in this work: doubly perfect sequences).

Recall the definition of the Weyl-Heisenberg operators in Sections 2.3. Now consider a bipartite unitary $U \in U(d^2)$ in diagonal decomposition. According to Refs. [113, 95], such a unitary can be decomposed into the maximally entangled basis in the following way:

$$U = \frac{1}{d^n} \sum_{\mathbf{a} \in \mathbb{Z}_d^{2n}} \Lambda(\mathbf{a}) \left|\Phi_{\mathbf{a}}\right\rangle \left\langle\Phi_{\mathbf{a}}\right| \tag{3.55}$$

where $\Lambda(\mathbf{a}) \in \mathbb{C}$ for all $\mathbf{a} = \begin{pmatrix} \mathbf{a}_1 \\ \mathbf{a}_2 \end{pmatrix} \in \mathbb{Z}_d^{2n}$ and

$$|\Phi_{\mathbf{a}}\rangle = (Z^{\mathbf{a}_1} X^{-\mathbf{a}_2} \otimes \mathbb{I}_{d^n}) \sum_{\mathbf{q}\in\mathbb{Z}_d^n} |\mathbf{q}\mathbf{q}\rangle \tag{3.56}$$

with $\{Z^{\mathbf{a}_1} X^{-\mathbf{a}_2}\}_{\mathbf{a}_1,\mathbf{a}_2\in\mathbb{Z}_d^n}$ being the Weyl-Heisenberg basis. Consider the following identity

$$UU^\dagger = \frac{1}{d^{2n}} \sum_{\mathbf{a},\mathbf{b}\in\mathbb{Z}_d^{2n}} \Lambda(\mathbf{a})\overline{\Lambda(\mathbf{b})} \, |\Phi_{\mathbf{a}}\rangle \langle\Phi_{\mathbf{a}} |\Phi_{\mathbf{b}}\rangle \langle\Phi_{\mathbf{b}}| \tag{3.57}$$

$$= \sum_{\mathbf{a}\in\mathbb{Z}_d^{2n}} |\Lambda(\mathbf{a})|^2 \, |\Phi_{\mathbf{a}}\rangle \langle\Phi_{\mathbf{a}}| , \tag{3.58}$$

where it has been used that $\langle\Phi_{\mathbf{a}} |\Phi_{\mathbf{b}}\rangle = \delta_{\mathbf{a},\mathbf{b}} d^{2n}$ in the last step. This expression is equal to the identity matrix in dimensions d^{2n} if and only if $|\Lambda(\mathbf{a})|^2 = 1$ for all $\mathbf{a} \in \mathbb{Z}_d^{2n}$.

That means that one can associate the phases $\Lambda(\mathbf{a})$ with a unimodular sequence. In fact, it has been shown that U is dual unitary if and only if $\Lambda(\mathbf{a})$ is a bi-unimodular sequence [113], i.e. both $\Lambda(\mathbf{a})$ and its Fourier transform are unimodular. One can now make the following assertion, which has already been proven by Rather in Ref. [95]:

Theorem 3.0.2. *A bipartite unitary $U \in U(d^2)$ in diagonal decomposition with coefficients $\{\Lambda(\mathbf{a})\}_{\mathbf{a}\in\mathbb{Z}_d^{2n}}$ is 2-unitary if and only if $\Lambda(\mathbf{a})$ is a doubly perfect bi-unimodular sequence of length d^{2n}.*

Proof. The proof is analogous to the one given in Appendix A of Ref. [95]. The only difference is that the phase space here is given by $\mathbb{Z}_d^{2n}$ rather than $\mathbb{Z}_d^2$.

Let $U \in U(d^2)$ be written as

$$U = \frac{1}{d^n} \sum_{\mathbf{a}\in\mathbb{Z}_d^{2n}} \Lambda(\mathbf{a}) \, |\Phi_{\mathbf{a}}\rangle \langle\Phi_{\mathbf{a}}| = \frac{1}{d^n} \sum_{\mathbf{a}_1,\mathbf{a}_2\in\mathbb{Z}_d^n} \Lambda(\mathbf{a}_1, \mathbf{a}_2) \, |Z^{\mathbf{a}_1} X^{-\mathbf{a}_2}\rangle \langle Z^{\mathbf{a}_1} X^{-\mathbf{a}_2}| . \tag{3.59}$$

Unitarity of U already implies that $|\Lambda(\mathbf{a})| = 1$ and hence unimodularity, as was demonstrated above.

Because $(A \otimes B)^R = |A\rangle\langle B^*|$, U^R can be written as follows

$$U^R = \frac{1}{d^n} \sum_{\mathbf{a}_1, \mathbf{a}_2 \in \mathbb{Z}_d^n} \Lambda(\mathbf{a}_1, \mathbf{a}_2) Z^{\mathbf{a}_1} X^{-\mathbf{a}_2} \otimes (Z^{\mathbf{a}_1} X^{-\mathbf{a}_2})^*. \tag{3.60}$$

One thus finds

$$U^R (U^R)^\dagger = \frac{1}{d^{2n}} \sum_{\mathbf{a}, \mathbf{b} \in \mathbb{Z}_d^{2n}} \Lambda(\mathbf{a}) \overline{\Lambda(\mathbf{b})} Z^{\mathbf{a}_1} X^{-\mathbf{a}_2} (Z^{\mathbf{b}_1} X^{-\mathbf{b}_2})^\dagger \otimes (Z^{\mathbf{a}_1} X^{-\mathbf{a}_2})^* (Z^{\mathbf{b}_1} X^{-\mathbf{b}_2})^T.$$

Using the identities:

$$(X^a Z^b)^T = \omega_d^{-ab} X^{-a} Z^b, \quad (X^a Z^b)^* = X^a Z^{-b} \tag{3.61}$$

and

$$(X^a Z^b)(X^{a'} Z^{b'}) = \omega_d^{a'b} X^{a+a'} Z^{b+b'}, \tag{3.62}$$

this transforms into

$$\begin{aligned}\frac{1}{d^{2n}} \sum_{\mathbf{a}, \mathbf{b} \in \mathbb{Z}_d^{2n}} &\Lambda(\mathbf{a}) \overline{\Lambda(\mathbf{b})} \omega_d^{\mathbf{a}_1(\mathbf{b}_2 - \mathbf{a}_2)} X^{\mathbf{b}_2 - \mathbf{a}_2} Z^{\mathbf{a}_1 - \mathbf{b}_1} \otimes \omega_d^{-\mathbf{a}_1(\mathbf{b}_2 - \mathbf{a}_2)} X^{\mathbf{b}_2 - \mathbf{a}_2} Z^{\mathbf{b}_1 - \mathbf{a}_1} \\ &= \frac{1}{d^{2n}} \sum_{\mathbf{a}, \mathbf{b} \in \mathbb{Z}_d^{2n}} \Lambda(\mathbf{a}) \overline{\Lambda(\mathbf{b})} X^{\mathbf{b}_2 - \mathbf{a}_2} Z^{\mathbf{a}_1 - \mathbf{b}_1} \otimes X^{\mathbf{b}_2 - \mathbf{a}_2} Z^{\mathbf{b}_1 - \mathbf{a}_1}.\end{aligned}$$

This is equal to the identity matrix if and only if the following condition holds:

$$\sum_{\mathbf{a} \in \mathbb{Z}_d^{2n}} \Lambda(\mathbf{a}) \overline{\Lambda(\mathbf{a} + \mathbf{l})} = 0 \quad \text{for} \quad \mathbf{l} \neq (0, .., 0) \tag{3.63}$$

which means that the cross-correlation of Λ vanishes on all off-peak elements. From the condition $|\Lambda(\mathbf{a})| = 1$, one can then derive that the peak element of the cross-correlation of Λ takes the following form:

$$\sum_{\mathbf{a} \in \mathbb{Z}_d^{2n}} |\Lambda(\mathbf{a})|^2 = d^{2n}. \tag{3.64}$$

For the Γ-dual unitarity condition one can make use of the following fact namely that if $(U^R)^\Gamma = U^\Gamma S$, where S denotes the SWAP-gate, is unitary, then so is U^{Γ}. Hence consider:

$$(U^R)^{\Gamma} = \frac{1}{d^n} \sum_{\mathbf{a}_1,\mathbf{a}_2 \in \mathbb{Z}_d^n} \Lambda(\mathbf{a}_1,\mathbf{a}_2) Z^{\mathbf{a}_1} X^{-\mathbf{a}_2} \otimes (Z^{\mathbf{a}_1} X^{-\mathbf{a}_2})^{\dagger}. \tag{3.65}$$

One finds:

$$(U^R)^{\Gamma}((U^R)^{\Gamma})^{\dagger} = \frac{1}{d^{2n}} \sum_{\mathbf{a},\mathbf{b} \in \mathbb{Z}_d^{2n}} \Lambda(\mathbf{a})\overline{\Lambda(\mathbf{b})} Z^{\mathbf{a}_1} X^{-\mathbf{a}_2} (Z^{\mathbf{b}_1} X^{-\mathbf{b}_2})^{\dagger} \otimes (Z^{\mathbf{a}_1} X^{-\mathbf{a}_2})^{\dagger} (Z^{\mathbf{b}_1} X^{-\mathbf{b}_2}).$$

Using the the identities in Eq. 3.61 and Eq. 3.62 again, this transforms into:

$$\frac{1}{d^{2n}} \sum_{\mathbf{a},\mathbf{b} \in \mathbb{Z}_d^{2n}} \Lambda(\mathbf{a})\overline{\Lambda(\mathbf{b})} \omega_d^{\mathbf{a}_1(\mathbf{b}_2-\mathbf{a}_2)} X^{\mathbf{b}_2-\mathbf{a}_2} Z^{\mathbf{a}_1-\mathbf{b}_1} \otimes \omega_d^{-\mathbf{b}_2(\mathbf{b}_1-\mathbf{a}_1)} X^{\mathbf{a}_2-\mathbf{b}_2} Z^{\mathbf{b}_1-\mathbf{a}_1}$$
$$= \frac{1}{d^{2n}} \sum_{\mathbf{a},\mathbf{b} \in \mathbb{Z}_d^{2n}} \Lambda(\mathbf{a})\overline{\Lambda(\mathbf{b})} \omega_d^{\mathbf{a}_1\mathbf{a}_2+\mathbf{b}_1\mathbf{b}_2-2\mathbf{b}_1\mathbf{a}_2} (X^{\mathbf{b}_2-\mathbf{a}_2} Z^{\mathbf{a}_1-\mathbf{b}_1} \otimes X^{\mathbf{a}_2-\mathbf{b}_2} Z^{\mathbf{b}_1-\mathbf{a}_1}).$$

Again this is equal to the identity matrix if and only if $\mathbf{b} = \mathbf{a}$. Set $\mathbf{b} = \mathbf{a} + \mathbf{l}$, where $\mathbf{l} = \begin{pmatrix} \mathbf{l}_1 \\ \mathbf{l}_2 \end{pmatrix} \in \mathbb{Z}_d^{2n}$. Then the prefactor $\omega_d^{\mathbf{a}_1\mathbf{a}_2+\mathbf{b}_1\mathbf{b}_2-2\mathbf{b}_1\mathbf{a}_2}$ turns into:

$$\omega_d^{\mathbf{a}_1\mathbf{l}_2-\mathbf{a}_2\mathbf{l}_1+\mathbf{l}_1\mathbf{l}_2} = \omega_d^{[\mathbf{a},\mathbf{l}]+\mathbf{l}_1\mathbf{l}_2}. \tag{3.66}$$

Thus, $(U^R)^{\Gamma}((U^R)^{\Gamma})^{\dagger}$ is equal to the identity matrix if and only if

$$\sum_{\mathbf{a} \in \mathbb{Z}_d^{2n}} \Lambda(\mathbf{a})\overline{\Lambda(\mathbf{a}+\mathbf{l})} \omega_d^{[\mathbf{a},\mathbf{l}]} = 0 \quad \text{for} \quad \mathbf{l} \neq (0,..,0), \tag{3.67}$$

which means that the twisted cross-correlation of Λ vanishes on all off-peak elements. From the condition $|\Lambda(\mathbf{a})| = 1$, one can then derive again that the peak element of the twisted cross-correlation of Λ takes the following form:

$$\sum_{\mathbf{a} \in \mathbb{Z}_d^{2n}} |\Lambda(\mathbf{a})|^2 = d^{2n}. \tag{3.68}$$

Thus, U is 2-unitary if and only if Λ is doubly perfect and bi-unimodular. □

In Ref. [95] the author has found doubly perfect sequences for $d = 6$ and $d = 3$ that give rise to 2-unitaries in dimension 36 using numerical methods. It is natural to ask, if there is an analytic approach to construct doubly perfect sequences of length 36 and if one can use this framework to construct perfect tensors in arbitrary dimensions using doubly perfect sequences. Both questions will be addressed in the following sections.

3.3.2 Doubly Perfect Sequences in Arbitrary Dimensions

Before discussing an analytic approach to construct a perfect tensor in dimension 36, it is instructive to first consider the more general case, namely that of arbitrary dimensions. In Ref. [95] the author states that bi-unimodular sequences of the form

$$\Lambda = \omega_d^{a^2-b^2+ab} \tag{3.69}$$

are doubly perfect for any odd d that is not a multiple of 5. For odd d that *are* multiples of 5, the following bi-unimodular sequence is perfect [95]:

$$\Lambda = \omega_d^{a^2+b^2+ab} \tag{3.70}$$

Can one find a more general approach that covers all odd d at once and ideally all dimensions? The following theorem will give a generalisation.

Theorem 3.0.3. *Let* a $\in \mathbb{Z}_d^{2n}$ *and* $\tau_d^2 = \omega_d$. *The sequence* $\Lambda(\mathbf{a}) = \tau_d^{\mathbf{a}^T N \mathbf{a}}$, *where* N *is a symmetric* $2n \times 2n$*-matrix, is doubly perfect if and only if* $\ker(N) = \{\mathbf{0}\} = \ker(N + J)$.

Proof. Compute the auto-correlation of Λ:

$$(\Lambda \star \Lambda)(\mathbf{a}) = \sum_{\mathbf{b}\in\mathbb{Z}_d^{2n}} \Lambda(\mathbf{a}+\mathbf{b})\overline{\Lambda(\mathbf{b})} = \sum_{\mathbf{b}\in\mathbb{Z}_d^{2n}} \tau_d^{(\mathbf{a}+\mathbf{b})^T N(\mathbf{a}+\mathbf{b})}\tau_d^{-\mathbf{b}^T N\mathbf{b}} \tag{3.71}$$

$$= \tau_d^{\mathbf{a}^T N\mathbf{a}} \sum_{\mathbf{b}\in\mathbb{Z}_d^{2n}} \tau_d^{2\mathbf{a}^T N\mathbf{b}} = \tau_d^{\mathbf{a}^T N\mathbf{a}} \sum_{\mathbf{b}\in\mathbb{Z}_d^{2n}} \omega_d^{\mathbf{a}^T N\mathbf{b}}, \tag{3.72}$$

where it was used that $\mathbf{b}^T N\mathbf{a} = \mathbf{b}^T N^T\mathbf{a} = (N\mathbf{b})^T\mathbf{a} = (\mathbf{a}^T N\mathbf{b})^T = \mathbf{a}^T N\mathbf{b}$.

Since the sum over all roots of unity vanishes, this expression is equal to $\delta(\mathbf{a})$ if and only if $\ker(N) = \{\mathbf{0}\}$.

Similarly, compute the twisted auto-correlation of Λ:

$$(\Lambda \tilde{\star} \Lambda)(\mathbf{a}) = \sum_{\mathbf{b}\in\mathbb{Z}_d^{2n}} \Lambda(\mathbf{a}+\mathbf{b})\overline{\Lambda(\mathbf{b})}\omega_d^{\mathbf{a}^T J\mathbf{b}} = \tau_d^{\mathbf{a}^T N\mathbf{a}} \sum_{\mathbf{b}\in\mathbb{Z}_d^{2n}} \omega_d^{\mathbf{a}^T (J+N)\mathbf{b}}. \quad (3.73)$$

This expression is equal to $\delta(\mathbf{a})$ if and only if $\ker(J+N) = \{\mathbf{0}\}$. □

The condition $\ker(J+N) = \{\mathbf{0}\} = \ker(N)$ for the matrices N and $N+J$ is equivalent to requiring that both N and $N+J$ have non-zero determinant, i.e. that they are invertible.

What are examples of matrices satisfying this condition? One obvious choice would be the identity matrix: $N = \mathbb{I}_{2n}$. However, this only works for odd d as the following observation will demonstrate. For odd d the $2n \times 2n$-matrix generating the symplectic product is defined by:

$$J = \begin{pmatrix} 0 & \mathbb{I}_n \\ -\mathbb{I}_n & 0 \end{pmatrix}. \quad (3.74)$$

With that one gets:

$$\det(N+J) = \det\begin{pmatrix} \mathbb{I}_n & \mathbb{I}_n \\ -\mathbb{I}_n & \mathbb{I}_n \end{pmatrix} = \det(\mathbb{I}_n + \mathbb{I}_n) = 2\det(\mathbb{I}_n) = 2 \neq 0. \quad (3.75)$$

However, for even d the matrix J turns into:

$$J = \begin{pmatrix} \mathbb{I}_n & \mathbb{I}_n \\ \mathbb{I}_n & \mathbb{I}_n \end{pmatrix}, \quad (3.76)$$

and thus one gets

$$\det(N+J) = 0. \quad (3.77)$$

This leads to the following statement:

Proposition 3.0.6. *Let $\tau_d = \exp(\pi i/d)$. If d is odd, the bi-unimodular sequence $\Lambda(\mathbf{a}) = \tau_d^{\mathbf{a}^T \mathbb{I}_{2n}\mathbf{a}} = \tau_d^{\sum_{i=0}^{2n} a_i^2}$ is doubly perfect and has length d^{2n}.*

Example 6. Let $d = 3$ and $N = \mathbb{I}_2$. Then the sequence $\Lambda(\mathbf{a}) = \tau_3^{\mathbf{a}^T N\mathbf{a}} = \omega_3^{2(a_1^2+a_2^2)}$ is doubly perfect. The diagonal matrix constructed with this sequence is a 2-unitary in dimension $3^2 = 9$:

$$U_{\Lambda,3} = \frac{1}{3}\begin{pmatrix} \omega_3^2-\omega_3 & 0 & 0 & 0 & \omega_3+2 & 0 & 0 & 0 & \omega_3+2 \\ 0 & \omega_3-1 & 0 & 0 & 0 & \omega_3^2-\omega_3 & \omega_3^2-\omega_3 & 0 & 0 \\ 0 & 0 & \omega_3-1 & \omega_3^2-\omega_3 & 0 & 0 & 0 & \omega_3^2-\omega_3 & 0 \\ 0 & 0 & \omega_3^2-\omega_3 & \omega_3-1 & 0 & 0 & 0 & \omega_3^2-\omega_3 & 0 \\ \omega_3+2 & 0 & 0 & 0 & \omega_3^2-\omega_3 & 0 & 0 & 0 & \omega_3+2 \\ 0 & \omega_3^2-\omega_3 & 0 & 0 & 0 & \omega_3-1 & \omega_3^2-\omega_3 & 0 & 0 \\ 0 & \omega_3^2-\omega_3 & 0 & 0 & 0 & \omega_3^2-\omega_3 & \omega_3-1 & 0 & 0 \\ 0 & 0 & \omega_3^2-\omega_3 & \omega_3^2-\omega_3 & 0 & 0 & 0 & \omega_3-1 & 0 \\ \omega_3+2 & 0 & 0 & 0 & \omega_3+2 & 0 & 0 & 0 & \omega_3^2-\omega_3 \end{pmatrix}.$$

The construction in Prop. 3.0.6 gives rise to 2-unitaries in dimensions d^{2n} where d is odd. However, even dimensions are not covered by this. What happens if one changes the index space to be $\mathbb{Z}_2^{2n}$? As it turns out the following statement is true:

Proposition 3.0.7. *For every $n > 1$ there exist doubly perfect sequences of the form $\Lambda(\mathbf{a}) = i^{\mathbf{a}^T N \mathbf{a}}$ for $\mathbf{a} \in \mathbb{Z}_2^{2n}$.*

Before proving this theorem, it is instructive to consider the following example of $2n \times 2n$-matrices N over $\mathbb{Z}_2$ that fulfil $\ker(J+N) = \{\mathbf{0}\} = \ker(N)$:

$$N = \begin{pmatrix} A_n & \mathbb{I}_n \\ \mathbb{I}_n & A_n \end{pmatrix}, \quad \text{where} \quad A_n^T = A_n. \tag{3.78}$$

What are the requirements for the matrix A_n that guarantee that N and $N+J$ have non-zero determinant? The matrix N has determinant given by

$$\det(N) = \det(A_n^2 - \mathbb{I}_n) = \det(A_n - \mathbb{I}_n)\det(A_n + \mathbb{I}_n) = \det(A_n + \mathbb{I}_n)^2. \tag{3.79}$$

Over $\mathbb{Z}_2$, this expression is only equal to 0 if $\det(A_n + \mathbb{I}_n) = 0$ and hence if N generates a doubly perfect sequence the following has to hold:

$$\det(A_n + \mathbb{I}_n) \neq 0. \tag{3.80}$$

Denoting the characteristic polynomial by $P_{A_n}(\lambda)$, this is equivalent to

$$\det(A_n + \mathbb{I}_n) = P_{A_n}(-1) = P_{A_n}(1) \neq 0 \tag{3.81}$$

which means that 1 cannot be an eigenvalue of A_n.

Now consider the matrix

$$N + J = \begin{pmatrix} A_n & 0 \\ 0 & A_n \end{pmatrix}. \tag{3.82}$$

Its determinant is given by

$$\det(N + J) = \det(A_n^2) = \det(A_n)^2 = P_{A_n}(0)^2 \neq 0 \tag{3.83}$$

This expression is only non zero, if A_n is invertible. Using this construction, one can now prove Proposition 3.0.7:

Proof. It is sufficient to prove that there exist some matrices $N \in \mathbb{Z}_2^{2n} \times \mathbb{Z}_2^{2n}$ that satisfy: $\ker(J + N) = \{\mathbf{0}\} = \ker(N)$. Consider the matrix

$$N = \begin{pmatrix} A & \mathbb{I}_n \\ \mathbb{I}_n & A \end{pmatrix}, \quad \text{where} \quad A^T = A. \tag{3.84}$$

One has to construct A in such a way that it does not have 1 and 0 as eigenvalues. In the following, it will be referred to $\mathbb{F}_{2^n}$ instead of $\mathbb{Z}_2^n$.

Using Theorem 2 from Ref. [71], there exists a self-dual orthonormal basis $\{\alpha, \alpha^2, ..., \alpha^{2^n}\} \subset \mathbb{F}_{2^n}$ for the trace form $(a, b)_{\text{tr}} = \text{tr}_{\mathbb{F}_{2^n}/\mathbb{F}_2}(ab)$, where $a, b \in \mathbb{F}_{2^n}$. Now, let $0, 1 \neq \beta = \sum_{i=0}^{n-1} b_i \alpha^{2^i} \in \mathbb{F}_{2^n}$. The action by multiplication with β on a basis element can be represented by: $\beta \cdot \alpha^{2^j} = \sum_{k=0}^{n-1} A_{kj} \alpha^{2^k}$[6]. Now using the linearity of the trace and the fact that the basis is self-dual, one obtains $\text{tr}_{\mathbb{F}_{2^n}/\mathbb{F}_2}(\alpha^{2^i}, \beta \cdot \alpha^{2^j}) = A_{ij}$, i. e. the matrix coefficients of the matrix A representing the action of multiplication by β. Therefore, the matrices

$$N = \begin{pmatrix} A & \mathbb{I}_n \\ \mathbb{I}_n & A \end{pmatrix} \quad \text{and} \quad N + J = \begin{pmatrix} A & 0 \\ 0 & A \end{pmatrix} \tag{3.85}$$

are matrix representations of the following matrices:

$$\begin{pmatrix} \beta & 1 \\ 1 & \beta \end{pmatrix}, \quad \begin{pmatrix} \beta & 0 \\ 0 & \beta \end{pmatrix}. \tag{3.86}$$

Now, because $0, 1 \neq \beta$ and thus $\beta^2 \neq 0$ and $\beta^2 - 1 \neq 0$, it follows that

$$\det(N) = \beta^2 - 1 \neq 0 \quad \text{and} \quad \det(N + J) = \beta^2 \neq 0.$$

□

[6]Here the trace function is given by: $\text{tr}_{\mathbb{F}_{2^m}/\mathbb{F}_2}(\beta) = \sum_{i=0}^{m-1} \beta^{2^i}$

What are concrete examples of these instances?

Example 7. Consider the matrices

$$N = \begin{pmatrix} A & \mathbb{I}_n \\ \mathbb{I}_n & A \end{pmatrix} \quad \text{and} \quad N + J = \begin{pmatrix} A & 0 \\ 0 & A \end{pmatrix}. \tag{3.87}$$

For $n = 2$ choosing the matrix to be

$$C = \begin{pmatrix} 0 & 1 \\ 1 & 1 \end{pmatrix} \tag{3.88}$$

leads to

$$N = \begin{pmatrix} 0 & 1 & 1 & 0 \\ 1 & 1 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 1 \end{pmatrix} \quad \text{and} \quad N + J = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 1 \end{pmatrix}. \tag{3.89}$$

Both matrices have non-zero determinant and thus generate a doubly perfect sequence of length 16 and period 2.

For $n = 3$, choosing

$$C = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix} \tag{3.90}$$

gives a doubly perfect sequence of length 64.

In general, the existence of these types of matrices in dimension m relies on the existence of a self-complementary orthonormal basis (SCN basis) of $\mathbb{F}_{2^m}$ over $\mathbb{F}_2$. In Ref. [71], the author proves that one can construct such a basis for every odd m using a normal basis in $\mathbb{F}_{2^m}$. The corresponding algorithm looks as follows:

1. Find a normal basis generator $\alpha_0 \in \mathbb{F}_{2^m}$ and construct a *normal* basis $\{\alpha_0, \alpha_0^2, \alpha_0^{2^2}, ..., \alpha_0^{2^m}\}$ of $\mathbb{F}_{2^m}$ over $\mathbb{F}_2$.

2. Compute the matrix $A = \mathrm{tr}(\alpha\alpha')$, where $\alpha' = S \cdot (\alpha_0, \alpha_0^2, \alpha_0^{2^2}, ..., \alpha_0^{2^m})^T$ with S being a $m \times m$ cyclic permutation matrix with entries $S_{ij} = \delta_{i,j-1}$ for all $i, j \in [m]$.

3. Compute A^{-1} and $\omega = (\sum_{i=0}^{m-1} \alpha_0^{2^i} S^i)_{00}$

4. Compute $\gamma = \Omega \cdot A^{-1}$ where $\Omega_i = \omega^{2^{-iM}}$ with $0 \leq i < m$ and $M = (1/2)(m+1)$. Now γ is a SCN basis of $\mathbb{F}_{2^m}$ over $\mathbb{F}_2$.

This basis can now be extended to a SCN basis of $\mathbb{F}_{2^{2m}}$ over $\mathbb{F}_2$ following the subsequent procedure:

1. Pick a random element $\kappa \in \mathbb{F}_{2^2}$ with $\mathrm{tr}_{\mathbb{F}_{2^2}/\mathbb{F}_2}(\kappa) = 1$.

2. Compute the product of $\{\kappa, \kappa^2\}$ and the SCN basis γ of $\mathbb{F}_{2^m}$ over $\mathbb{F}_2$. This gives a SCN basis γ' of $\mathbb{F}_{2^{2m}}$ over $\mathbb{F}_2$.

Now, following the proof of Prop. 3.0.7, picking an arbitrary element $\beta \in \mathbb{F}_{2^m}$ with $\beta \neq 0, 1$, the $m \times m$ matrix $\mathrm{tr}_{\mathbb{F}_{2^m}/\mathbb{F}_2}(\gamma^{2^i}, \beta \cdot \gamma^{2^j}) = c_{ij}$ is invertible and thus the matrices

$$N = \begin{pmatrix} C & \mathbb{I}_m \\ \mathbb{I}_m & C \end{pmatrix} \quad \text{and} \quad N + J_{2m} = \begin{pmatrix} C & 0 \\ 0 & C \end{pmatrix} \tag{3.91}$$

are also invertible. Similarly, the $2m \times 2m$ matrix $\mathrm{tr}_{\mathbb{F}_{2^{2m}}/\mathbb{F}_2}(\gamma'^{2^i}, \beta \cdot \gamma'^{2^j}) = c'_{ij}$ is invertible and thus the matrices

$$N' = \begin{pmatrix} C' & \mathbb{I}_{2m} \\ \mathbb{I}_{2m} & C' \end{pmatrix} \quad \text{and} \quad N' + J_{4m} = \begin{pmatrix} C' & 0 \\ 0 & C' \end{pmatrix} \tag{3.92}$$

are also invertible. Therefore, one can construct examples for all (even and odd) powers of 2. A SageMath-implementation of this procedure has been realised by the present author in I., Appendix B.1.

There are also other examples of matrices over $\mathbb{Z}_2$ generating doubly perfect sequences, that do not fall into the category above. These will be discussed in the following.

Example 8. Consider matrices of the form

$$N = \begin{pmatrix} A_n & B_n \\ B_n^T & A_n \end{pmatrix}, \quad \text{where} \quad A_n^T = A_n. \tag{3.93}$$

Let $n = 2$ and let

$$A_2 = \begin{pmatrix} 0 & 1 \\ 1 & 1 \end{pmatrix} \quad \text{and} \quad B_2 = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}. \tag{3.94}$$

The following matrix generates a doubly perfect sequence of length 16:

$$N = \begin{pmatrix} 0 & 1 & 0 & 1 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 1 & 1 \end{pmatrix}. \tag{3.95}$$

For $n = 3$ one can use the matrices

$$A_3 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix} \quad \text{and} \quad B_2 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{3.96}$$

to build a matrix

$$N = \begin{pmatrix} A_3 & B_3 \\ B_3^T & A_3 \end{pmatrix} \tag{3.97}$$

that gives rise to a doubly perfect sequence of length 64.

Another, less straightforward example that leads to doubly perfect sequences over $\mathbb{Z}_2^{2n}$ is given by "kite-shaped" matrices:

Example 9. Consider $2n \times 2n$-matrices of the form:

$$N_{ij} = \begin{cases} 1 & \text{for} \quad i + j \leq 2n - 1, \\ 0 & \text{otherwise.} \end{cases} \tag{3.98}$$

A computer search showed that these types of matrices generate doubly perfect sequences, if n is not congruent to 1 mod 3, for all $n \in [500]$. This can be found in a SageMath notebook in II., Appendix B.1.

Lacking a rigorous proof that "kite-shaped" matrices generate doubly perfect sequences for all dimensions, one can make the following conjecture:

Conjecture: For all n not congruent to 1 mod 3, the kite-shaped $2n \times 2n$-matrices over $\mathbb{Z}_2$ generate doubly perfect sequences of length d^{2n}.

Complex Hadamard matrices (CHMs) were introduced in Section 2.1. In Ref. [95] the author constructed CHM in dimension 36 using bi-unimodular doubly perfect sequences. Other construction schemes for 2-unitary CHMs in square dimensions were presented in Ref. [20] using permutations and Hadamard matrices. The next theorem generalises these findings by showing that it is possible to construct 2-unitary CHMs in dimensions d^{2n} using doubly perfect sequences.

Theorem 3.0.4. *Let $\Lambda : \mathbb{Z}_d^{2n} \to \mathbb{C}$ be a sequence and G and H be matrices with entries given by $G_{\mathbf{a},\mathbf{b}} = \omega_d^{\mathbf{a}_1^T\mathbf{a}_2}\Lambda(\mathbf{a}-\mathbf{b})\omega_d^{-\mathbf{b}_1^T\mathbf{b}_2}$ and $H_{\mathbf{a},\mathbf{b}} = \Lambda(\mathbf{a}-\mathbf{b})\omega_d^{[\mathbf{a},\mathbf{b}]}$ for $\mathbf{a},\mathbf{b} \in \mathbb{Z}_d^{2n}$ and $\omega_d = \exp(2\pi i/d)$. Then G and H are proportional to a two-unitary if and only if Λ is bi-unimodular and doubly perfect.*

Proof. The proof can be done by showing that the matrix with entries $G_{\mathbf{a},\mathbf{b}} = \omega_d^{\mathbf{a}_1^T\mathbf{a}_2}\Lambda(\mathbf{a}-\mathbf{b})\omega_d^{-\mathbf{b}_1^T\mathbf{b}_2}$ is locally equivalent to a diagonal matrix with the entries being the Fourier transform of the sequence Λ.

Let $\Lambda(\mathbf{a})$ be a sequence. Consider the circulant matrix $(\Lambda(\mathbf{a}-\mathbf{b}))_{\mathbf{a},\mathbf{b}\in\mathbb{Z}_d^{2n}}$. Since circulant matrices are diagonalised by the Fourier matrix, one has:

$$(\Lambda(\mathbf{a}-\mathbf{b}))_{\mathbf{a},\mathbf{b}\in\mathbb{Z}_d^{2n}} = (F_d \otimes F_d) \sum_{\mathbf{a}\in\mathbb{Z}_d^{2n}} \mathcal{F}(\Lambda)(\mathbf{a}) \left|\mathbf{a}\right\rangle \left\langle\mathbf{a}\right| (F_d^\dagger \otimes F_d^\dagger). \tag{3.99}$$

The phase factors are implemented by the controlled-Z-gate

$$\mathrm{CZ} = \bigotimes_{i=0}^{n} \sum_{m_i\in\mathbb{Z}_d} Z^{m_i} \otimes \left|m_i\right\rangle \left\langle m_i\right|. \tag{3.100}$$

This means one can write $G = \mathrm{CZ}(\Lambda(\mathbf{a}-\mathbf{b}))_{\mathbf{a},\mathbf{b}\in\mathbb{Z}_d^{2n}}\mathrm{CZ}^T$. and hence

$$\begin{aligned} G &= \mathrm{CZ}(\Lambda(\mathbf{a}-\mathbf{b}))_{\mathbf{a},\mathbf{b}\in\mathbb{Z}_d^{2n}}\mathrm{CZ}^T & (3.101)\\ &= \mathrm{CZ}(F_d \otimes F_d) \sum_{\mathbf{a}\in\mathbb{Z}_d^{2n}} \mathcal{F}(\Lambda)(\mathbf{a}) \left|\mathbf{a}\right\rangle \left\langle\mathbf{a}\right| (F_d^\dagger \otimes F_d^\dagger)\mathrm{CZ}^T. & (3.102)\end{aligned}$$

Using the fact that:

$$F_d X_d F_d^\dagger = Z_d, \tag{3.103}$$

one can show that the following holds:

$$\mathrm{CZ}(F_d \otimes F_d) = \bigotimes_{i=0}^{n} \sum_{m_i \in \mathbb{Z}_d} Z^{m_i} F_d \otimes |m_i\rangle \langle m_i| F_d \tag{3.104}$$

$$= \bigotimes_{i=0}^{n} \sum_{m_i \in \mathbb{Z}_d} F_d X^{m_i} \otimes |m_i\rangle \langle m_i| F_d \tag{3.105}$$

$$= (F_d \otimes \mathbb{I}_d)\mathrm{C}X(\mathbb{I}_d \otimes F_d). \tag{3.106}$$

Here $\mathrm{C}X = \bigotimes_{i=0}^{n} \sum_{m_i \in \mathbb{Z}_d} X^{m_i} \otimes |m_i\rangle \langle m_i|$ is the controlled-X-gate. Using this, one finds:

$$G = (F_d \otimes \mathbb{I}_d)\mathrm{C}X(\mathbb{I}_d \otimes F_d) \sum_{\mathbf{a} \in \mathbb{Z}_d^{2n}} \mathcal{F}(\Lambda)(\mathbf{a}) |\mathbf{a}\rangle \langle \mathbf{a}| (\mathbb{I}_d \otimes F_d^\dagger)\mathrm{C}X^T(F_d^\dagger \otimes \mathbb{I}_d)$$

$$= (F_d \otimes \mathbb{I}_d) \sum_{\mathbf{a} \in \mathbb{Z}_d^{2n}} \mathcal{F}(\Lambda)(\mathbf{a}) |\Phi_{\mathbf{a}}\rangle \langle \Phi_{\mathbf{a}}| (F_d^\dagger \otimes \mathbb{I}_d).$$

According to Theorem 3.0.2, the matrix:

$$U_{\mathcal{F}(\Lambda)} = \sum_{\mathbf{a} \in \mathbb{Z}_d^{2n}} \mathcal{F}(\Lambda)(\mathbf{a}) |\Phi_{\mathbf{a}}\rangle \langle \Phi_{\mathbf{a}}| \tag{3.107}$$

is 2-unitary if and only if $\mathcal{F}(\Lambda)(\mathbf{a})$ is a doubly perfect bi-unimodular sequence and due to Theorem 2.26.1 this is the case if and only if $\Lambda(\mathbf{a})$ is a doubly perfect bi-unimodular sequence. Now G, being locally equivalent to $U_{\mathcal{F}(\Lambda)}$, is 2-unitary if and only if $\Lambda(\mathbf{a})$ is a doubly perfect bi-unimodular sequence.

Now if G is 2-unitary, then G^Γ is also 2-unitary according to Prop. 2.17.1. But the partial transpose of G is given by:

$$(G_{\mathbf{a},\mathbf{b}})^\Gamma = (G_{\mathbf{a}_1\mathbf{a}_2}^{\mathbf{b}_1\mathbf{b}_2})^\Gamma = G_{\mathbf{a}_1\mathbf{b}_2}^{\mathbf{b}_1\mathbf{a}_2} = \omega^{\mathbf{a}_1\mathbf{b}_2 - \mathbf{a}_2\mathbf{b}_1}\Gamma(\Lambda(\mathbf{a}_1 - \mathbf{b}_1, \mathbf{b}_2 - \mathbf{a}_2)), \tag{3.108}$$

which leads to

$$(G_{\mathbf{a},\mathbf{b}})^\Gamma = \omega^{[\mathbf{a},\mathbf{b}]}\Gamma(\Lambda(\mathbf{a} - \mathbf{b})) \tag{3.109}$$

From this one can conclude that

$$\omega^{[\mathbf{a},\mathbf{b}]}\Gamma(\Lambda(\mathbf{a} - \mathbf{b})) \tag{3.110}$$

is a doubly perfect sequence. The sequence $\Gamma(\Lambda(\mathbf{a}))$ gives rise to the following matrix:

$$\sum_{\mathbf{a}\in\mathbb{Z}_d^n} \Gamma(\Lambda(\mathbf{a}))\,|\Phi_{\mathbf{a}}\rangle\langle\Phi_{\mathbf{a}}| = \sum_{\mathbf{a}\in\mathbb{Z}_d^n} \Lambda(\mathbf{a})\,|(Z^{\mathbf{a}_1}X^{-\mathbf{a}_2})^T\rangle\langle(Z^{\mathbf{a}_1}X^{-\mathbf{a}_2})^T| \tag{3.111}$$

$$= \sum_{\mathbf{a}\in\mathbb{Z}_d^n} \Lambda(\mathbf{a})S\,|Z^{\mathbf{a}_1}X^{-\mathbf{a}_2}\rangle\langle Z^{\mathbf{a}_1}X^{-\mathbf{a}_2}|\,S \tag{3.112}$$

$$= SU_\Lambda S \tag{3.113}$$

Here S denotes the swap operator. Since the swap operator preserves 2-unitarity, the above matrix is 2-unitary if and only if $\Gamma(\Lambda(\mathbf{a}))$ is doubly perfect. Thus one can conclude that

$$\omega^{[\mathbf{a},\mathbf{b}]}\Lambda(\mathbf{a}-\mathbf{b}) = H_{\mathbf{a},\mathbf{b}} \tag{3.114}$$

is doubly perfect and hence H is 2-unitary if and only if G is 2-unitary. □

The resulting matrices are Hadamard as each entry fulfils $|G_{\mathbf{a},\mathbf{b}}| = |\Lambda(\mathbf{a}-\mathbf{b})| = 1$ for $\mathbf{a},\mathbf{b}\in\mathbb{Z}_d^{2n}$ due to bi-unimodularity of $\Lambda(\mathbf{a}-\mathbf{b})$.

Example 10. The following matrix with entries $G_{\mathbf{a},\mathbf{b}} = \omega_3^{\mathbf{a}_1^T\mathbf{a}_2}\Lambda(\mathbf{a}-\mathbf{b})\omega_3^{-\mathbf{b}_1^T\mathbf{b}_2}$, where $\mathbf{a},\mathbf{b}\in\mathbb{Z}_3^2$, can be obtained from the doubly perfect bi-unimodular sequence $\Lambda(\mathbf{a}) = \omega_3^{2\mathbf{a}^T\mathbb{I}_2\mathbf{a}} = \omega_3^{2(a_1^2+a_2^2)}$:

$$U_{\Lambda_{CHM},3} = \frac{1}{3}\begin{pmatrix}
1 & \omega_3 & \omega_3 & \omega_3 & \omega_3 & 1 & \omega_3 & 1 & \omega_3 \\
\omega_3 & 1 & \omega_3 & \omega_3^2 & 1 & 1 & \omega_3^2 & \omega_3^2 & \omega_3 \\
\omega_3 & \omega_3 & 1 & \omega_3^2 & \omega_3 & \omega_3^2 & \omega_3^2 & 1 & 1 \\
\omega_3 & \omega_3^2 & \omega_3^2 & 1 & 1 & \omega_3^2 & \omega_3 & 1 & \omega_3 \\
1 & \omega_3^2 & 1 & \omega_3^2 & 1 & 1 & 1 & 1 & \omega_3^2 \\
\omega_3 & \omega_3 & 1 & 1 & \omega_3^2 & 1 & \omega_3 & \omega_3^2 & \omega_3^2 \\
\omega_3 & \omega_3^2 & \omega_3^2 & \omega_3 & \omega_3 & 1 & 1 & \omega_3^2 & 1 \\
\omega_3 & 1 & \omega_3 & \omega_3 & \omega_3^2 & \omega_3^2 & 1 & 1 & \omega_3^2 \\
1 & 1 & \omega_3^2 & 1 & \omega_3^2 & 1 & \omega_3^2 & 1 & 1
\end{pmatrix}. \tag{3.115}$$

To sum up, this section introduced construction schemes of doubly perfect bi-unimodular sequences for all dimensions that are of the form 2^m, 2^{2m} or d^n, where m and d are odd integers greater than 1 and n is an arbitrary integer, which lead to 2-unitaries in dimension 2^{2m}, 2^{4m} and d^{2n}, respectively.

However, these construction schemes do not encompass the case 36, which will be discussed separately in the next section.

The present author has constructed a SageMath notebook, which produces doubly perfect sequences and their corresponding 2-unitary matrices in all dimensions mentioned above. As an input only the dimension and the matrix N that characterises the sequence are needed. This notebook can be found in II., Appendix B.1.

3.3.3 An Artisanal 2-Unitary in dimension 36

In the previous section, a doubly perfect sequence of period 3 and length 9 has been derived. Can one use this matrix to construct a doubly perfect sequence of length 36 and period 3? In other words, is it possible to construct a 36-dimensional 2-unitary "by hand"?

Theorem 3.0.5. *Consider the quadratic form $f : \mathbb{Z}_3^2 \to \mathbb{Z}_3$, $f(a_1, a_2) = a_1^2 + a_2^2$. The sequences $\Lambda : \mathbb{Z}_3^2 \times \mathbb{Z}_2^2 \to \mathbb{C}$ defined by*

$$\Lambda_{sym}(\mathbf{a}, \mathbf{x}) = \omega_3^{f(a_1,a_2)-g(a_1,a_2,x_1-x_2)} \tag{3.116}$$

and

$$\Lambda_{sparse}(\mathbf{a}, \mathbf{x}) = \omega_3^{f(a_1,a_2)+g(0,a_2,x_1-x_2)}, \tag{3.117}$$

where

$$g : \mathbb{Z}_3^3 \to \mathbb{Z}_3 \tag{3.118}$$

$$g(a_1, a_2, x_1 - x_2) = \begin{cases} 0, & \text{for } (x_1, x_2) = (1, 1) \\ (a_1 + a_2 + (x_1 - x_2))^2, & \text{for } (x_1, x_2) \neq (1, 1) \end{cases} \tag{3.119}$$

are doubly perfect corresponding to a symmetric and a sparse 2-unitary in dimension 36.

Proof. The proof makes us of quadratic Gauß sums. More concretely, the following relations will be used:

$$\sum_{x \in \mathbb{Z}_3} \omega_3^{ax^2+bx+c} = i\sqrt{3}a\omega_3^{-ab^2+c}, \quad a \neq 0 \tag{3.120}$$

$$\sum_{x \in \mathbb{Z}_3} \omega_3^{bx+c} = 3\omega_3^c \delta(b). \tag{3.121}$$

Let $\Lambda_{sparse}(k,l,x_1,x_2) = \omega_3^{f(k,l)+g(l,x_1-x_2)}$ where $g(l,x_1-x_2)$ equals to $(l+(x_1-x_2)^2$, if $(x_1,x_2) \neq (1,1)$ and 0 else. Setting $\mathbf{x} = (x_1,x_2)$, the cross-correlation of Λ is then given by:

$$
\begin{aligned}
(\Lambda \star \Lambda)(k,l,\mathbf{x}) &= \sum_{k',l' \in \mathbb{Z}_3} \sum_{\mathbf{x}' \in \mathbb{Z}_2^2} \omega_3^{(k+k')^2+(l+l')^2+g(l+l',x_1+x_1',x_2+x_2')-k'^2-l'^2-g(l',x_1',x_2')} \\
&= \sum_{k',l' \in \mathbb{Z}_3} \sum_{\mathbf{x}' \in \mathbb{Z}_2^2} \omega_3^{k^2+l^2+2kk'+2ll'+g(l+l',x_1+x_1',x_2+x_2')-g(l',x_1',x_2')}
\end{aligned}
$$

Set $\Delta g := g(l+l',x_1+x_1',x_2+x_2') - g(l',x_1',x_2')$ and consider that $2 \cong -1 \bmod 3$. Then:

$$
(\Lambda \star \Lambda)(k,l,x_1,x_2) = \omega_3^{k^2+l^2} \sum_{k' \in \mathbb{Z}_3} \omega_3^{-kk'} \sum_{x_1',x_2' \in \mathbb{Z}_2, l' \in \mathbb{Z}_3} \omega_3^{-ll'+\Delta g} \tag{3.122}
$$

$$
= \omega_3^{k^2+l^2} 3\delta_k \sum_{x_1',x_2' \in \mathbb{Z}_2, l' \in \mathbb{Z}_3} \omega_3^{-ll'+\Delta g} \tag{3.123}
$$

where it has been used that the sum over all $n-th$-roots of unity vanishes in the last step.

One now has to show that

$$
\sum_{x_1',x_2' \in \mathbb{Z}_2, l' \in \mathbb{Z}_3} \omega_3^{-ll'+\Delta g} \propto \delta_l \delta_{x_1} \delta_{x_2} \tag{3.124}
$$

So the only case where this sum should not vanish is when $(x_1,x_2) = (0,0)$. In this case one finds:

x_1'	x_2'	$-ll' + g(l+l',x_1',x_2') - g(l',x_1',x_2')$
0	0	$2l^2 + ll' + 2l$
0	1	$2l^2 + ll' - 2l$
1	0	$2l^2 + ll'$
1	1	0

This leads to

$$
(\Lambda \star \Lambda)(k,l,0,0) = \omega_3^{k^2+l^2} 9\delta_k(\delta_l(\omega_3^{-l} + \omega_3^{l} + 1) + 1) \tag{3.125}
$$

which gives:

$$(\Lambda \star \Lambda)(0,0,0,0) = 36. \tag{3.126}$$

It is now left to prove that

$$\sum_{x_1',x_2' \in \mathbb{Z}_2, l' \in \mathbb{Z}_3} \omega_3^{-ll'+\Delta g} = 0 \tag{3.127}$$

for $(x_1, x_2) \neq (0,0)$. Unfortunately, this can only be done by going through each possible combination of the variables x_1, x_2, x_1', x_2' step by step which is a rather cumbersome thing to do analytically.

Start with $(x_1, x_2) = (1,1)$. In this case, one finds:

x_1'	x_2'	$-ll' + g(l+l', 1+x_1', 1+x_2') - g(l', x_1', x_2')$
0	0	$-ll' - l'^2$
0	1	$l^2 - l + ll' + l'$
1	0	$l^2 + l + ll' - l'$
1	1	$l^2 + ll' + l'^2$

This leads to

$$(\Lambda \star \Lambda)(k,l,1,1) = \omega_3^{k^2} 9\delta_k \sum_{l' \in \mathbb{Z}_3} (\omega_3^{l^2 - ll' - l'^2} + \omega_3^{-l^2 + l + l'(l-1)} + \omega_3^{-l^2 - l + l'(l+1)} + \omega_3^{-l^2 + ll' + l'^2}),$$

which using Eqs. 3.120, leads to:

$$(\Lambda \star \Lambda)(k,l,1,1) = \omega_3^{k^2} 9\delta_k (-\sqrt{3} i \omega_3^{-l^2} + 3\delta(l-1)\omega_3^{-l^2+l} + 3\delta(l+1)\omega_3^{-l^2-l} + \sqrt{3} i \omega_3^{l^2}).$$

For $l = 0$, this vanishes trivially. For $l = 1$ one finds:

$$\begin{aligned}(\Lambda \star \Lambda)(k,1,1,1) &= \omega_3^{k^2} 9\delta_k (-\sqrt{3} i \omega_3^{-1} + 3 + \sqrt{3} i \omega_3^{1}) \\ &= \omega_3^{k^2} 9\delta_k (-2\sqrt{3}\sin(2\pi/3) + 3) = \omega_3^{k^2} 9\delta_k (-2\sqrt{3}\frac{\sqrt{3}}{2} + 3) = 0.\end{aligned}$$

A similar argument can be made for $l = -1$. Hence $(\Lambda \star \Lambda)(k, l, 1, 1)$ vanishes for all values of l and k.

Next, consider $(x_1, x_2) = (0, 1)$. One finds:

x_1'	x_2'	$-ll' + g(l + l', x_1', 1 + x_2') - g(l', x_1', x_2')$
0	0	$ll' + l' + l + l^2 + 1$
0	1	$l^2 - l' + ll' - 1$
1	0	$-l'^2 - ll' + l' - 1$
1	1	$l^2 + l'^2 - l - l' + ll' + 1$

This leads to

$$(\Lambda \star \Lambda)(k, l, 0, 1) = \omega_3^{k^2} 9\delta_k \sum_{l' \in \mathbb{Z}_3} (\omega_3^{l'(1+l) - l^2 + l + 1} + \omega_3^{l'(l-1) - l^2 - 1} + \omega_3^{-l'^2 + l'(1-l) + l^2 - 1} + \omega_3^{l'^2 + l'(l-1) - l^2 - l + 1}),$$

which using Eqs. 3.120, leads to:

$$(\Lambda \star \Lambda)(k, l, 0, 1) = \omega_3^{k^2} 9\delta_k (3\delta(l+1)\omega_3^{-l^2 + l + 1} + 3\delta(l-1)\omega_3^{-l^2 - l} - \sqrt{3} i \omega_3^{-l^2 + l} + \sqrt{3} i \omega_3^{l^2 + l}).$$

For $l = 0$, this expression again vanishes trivially. For $l = 1$ one finds:

$$\begin{aligned}(\Lambda \star \Lambda)(k, 1, 0, 1) &= \omega_3^{k^2} 9\delta_k (0 + 3\omega_3^1 - \sqrt{3} i \omega_3^0 + \sqrt{3} i \omega_3^2) \\ &= \omega_3^{k^2} 9\delta_k \left(\frac{3}{2}\left(-1 + i\sqrt{3}\right) - i\sqrt{3} - \frac{i\sqrt{3}}{2}\left(1 + i\sqrt{3}\right) \right) \\ &= \omega_3^{k^2} 9\delta_k (-\frac{3}{2} + \frac{i3\sqrt{3}}{2} - i\sqrt{3} - \frac{i\sqrt{3}}{2} + \frac{3}{2} \Big) = 0.\end{aligned}$$

A similar argument can be made for $l = -1$. Hence $(\Lambda \star \Lambda)(k, l, 0, 1)$ vanishes for all values of l and k.

Finally, consider $(x_1, x_2) = (1, 0)$. One finds:

x_1'	x_2'	$-ll' + g(l + l', 1 + x_1', x_2') - g(l', x_1', x_2')$
0	0	$ll' - l' - l + l^2 + 1$
0	1	$-l'^2 - l' - ll' - 1$
1	0	$l^2 - ll' + l' - 1$
1	1	$l^2 + l'^2 + l + l' + ll' + 1$

This leads to

$$(\Lambda \star \Lambda)(k,l,1,0) = \omega_3^{k^2} 9\delta_k \sum_{l' \in \mathbb{Z}_3} (\omega_3^{l'(l-1)-l^2-l+1} + \omega_3^{-l'^2-l'(l+1)+l^2-1} + \omega_3^{l'(1+l)-l^2-1} + \omega_3^{l'^2+l'(l+1)-l^2+l+1})$$

which using Eqs. 3.120, leads to:

$$(\Lambda \star \Lambda)(k,l,1,0) = \omega_3^{k^2} 9\delta_k (3\delta(l-1)\omega_3^{-l^2-l+1} - \sqrt{3}i\omega_3^{-l^2-l} + 3\delta(l+1)\omega_3^{-l^2-l} + \sqrt{3}i\omega_3^{l^2-l}).$$

For $l = 0$, this expression again vanishes trivially. For $l = 1$, one finds:

$$\begin{aligned}(\Lambda \star \Lambda)(k,1,0,1) &= \omega_3^{k^2} 9\delta_k (3\omega_3^2 - \sqrt{3}i\omega_3^1 + \sqrt{3}i\omega_3^0) \\ &= \omega_3^{k^2} 9\delta_k \left(\frac{-3}{2}\left(1+i\sqrt{3}\right) - \frac{i\sqrt{3}}{2}\left(-1+i\sqrt{3}\right) + i\sqrt{3} \right) \\ &= \omega_3^{k^2} 9\delta_k \left(-\frac{3}{2} - \frac{i3\sqrt{3}}{2} + \frac{i\sqrt{3}}{2} + \frac{3}{2} + \frac{i2\sqrt{3}}{2} \right) = 0.\end{aligned}$$

A similar argument can be made for $l = -1$. Hence $(\Lambda \star \Lambda)(k,l,1,0)$ vanishes for all values of l and k. One can thus conclude that Eq. 3.127 indeed holds, if $(x_1, x_2) \neq (0,0)$.

In order to compute the twisted cross-correlation it is necessary to first discuss what the Chinese remainder isomorphism does to the twisted cross-correlation. For $d = 6$ the twisted cross correlation is defined with $\omega_6 = \exp(2\pi i/6)$. This can be factorised into:

$$\omega_6 = (-1)^{3^1 \bmod 2} \omega_3^{2^1 \bmod 3} = (-1) \cdot \omega_3^2. \tag{3.128}$$

Therefore, one finds:

$$\omega_6^{[\mathbf{a},\mathbf{a}']} = \omega_3^{2[(k,l),(k',l')]} (-1)^{[(x_1,x_2),(x_1',x_2')]}. \tag{3.129}$$

One then finds:

$$\begin{aligned}(\Lambda\tilde{\star}\Lambda)(k,l,\mathbf{x}) &= \sum_{\substack{k',l'\in\mathbb{Z}_3,\\ \mathbf{x}'\in\mathbb{Z}_2^2}} \omega_3^{(k+k')^2+(l+l')^2+g(l+l',\mathbf{x}+\mathbf{x}')-k'^2-l'^2-g(l',\mathbf{x}')+kl'-k'l}(-1)^{[\mathbf{x},\mathbf{x}']} \\ &= \sum_{k',l'\in\mathbb{Z}_3}\sum_{\mathbf{x}'\in\mathbb{Z}_2^2} \omega_3^{k^2+l^2+(2k-l)k'+(2l+k)l'+\Delta g}(-1)^{x_1x_2'-x_2x_1'}\end{aligned}$$

Set $\Delta g := g(l+l',\mathbf{x}+\mathbf{x}') - g(l',\mathbf{x}')$ again and consider that $2 \cong -1 \bmod 3$. Then:

$$\begin{aligned}(\Lambda\tilde{\star}\Lambda)(k,l,\mathbf{x}) &= \omega_3^{k^2+l^2}\sum_{k'\in\mathbb{Z}_3}\omega_3^{-(k+l)k'}\sum_{x_1',x_2'\in\mathbb{Z}_2,l'\in\mathbb{Z}_3}\omega_3^{(k-l)l'+\Delta g}(-1)^{x_1x_2'-x_2x_1'} \\ &= \omega_3^{k^2+l^2}3\delta_{-l,k}\sum_{x_1',x_2'\in\mathbb{Z}_2,l'\in\mathbb{Z}_3}\omega_3^{(k-l)l'+\Delta g}(-1)^{x_1x_2'-x_2x_1'} \\ &= \omega_3^{k^2+l^2}3\sum_{x_1',x_2'\in\mathbb{Z}_2,l'\in\mathbb{Z}_3}\omega_3^{ll'+\Delta g}(-1)^{x_1x_2'-x_2x_1'}.\end{aligned}$$

Similarly to the previous case, one now has to show that

$$\sum_{x_1',x_2'\in\mathbb{Z}_2,l'\in\mathbb{Z}_3}\omega_3^{ll'+\Delta g}(-1)^{x_1x_2'-x_2x_1'} \propto \delta_l\delta_{x_1}\delta_{x_2} \tag{3.130}$$

Consider the case $(x_1,x_2) = (0,0)$:

x_1'	x_2'	$ll' + g(l+l',x_1',x_2') - g(l',x_1',x_2')$	$x_1x_2' - x_2x_1'$
0	0	l^2	0
0	1	l^2+l	0
1	0	l^2-l'	0
1	1	ll'	0

This leads to

$$(\Lambda\tilde{\star}\Lambda)(k,l,0,0) = \omega_3^{k^2+l^2}9\delta_k(\delta_l+1+1+\omega_3^{-l}) = 36 \tag{3.131}$$

and thus in particular:

$$(\Lambda\tilde{\star}\Lambda)(0,0,0,0) = 36. \tag{3.132}$$

It is now left to prove that

$$\sum_{x_1',x_2' \in \mathbb{Z}_2, l' \in \mathbb{Z}_3} \omega_3^{ll'+\Delta g}(-1)^{x_1x_2'-x_2x_1'} = 0 \tag{3.133}$$

for $(x_1,x_2) \neq (0,0)$.

For $(x_1,x_2) = (1,1)$ one has:

x_1'	x_2'	$ll' + g(l+l',1+x_1',1+x_2') - g(l',x_1',x_2')$	$x_2' - x_1'$
0	0	$-l'^2 + ll'$	0
0	1	$l' + l^2 - l - 1$	-1
1	0	$-l' + l^2 + l'$	1
1	1	$l'^2 + l^2$	0

For $(x_1',x_2') = (1,0)$ and $(x_1',x_2') = (0,1)$ it is easy to see that the sum over l' vanishes. Thus one is left with:

$$(\Lambda \tilde{\star} \Lambda)(k,l,1,1) = \omega_3^{k^2+l^2} 9\delta_k(-i\sqrt{3}\omega_3^{-l^2} + i\sqrt{3}\omega_3^{-l^2}) = 0. \tag{3.134}$$

So $(\Lambda \tilde{\star} \Lambda)(k,l,1,1)$ vanishes for all choices of k and l.

For $(x_1,x_2) = (0,1)$ one finds:

x_1'	x_2'	$ll' + g(l+l',x_1',1+x_2') - g(l',x_1',x_2')$	$-x_1'$
0	0	$l' + l^2 + l + 1$	0
0	1	$-l' + l^2 - 1$	0
1	0	$-l'^2 + ll' + l' - 1$	-1
1	1	$l'^2 - l' + l^2 - l + 1$	-1

For $(x_1',x_2') = (0,0)$ and $(x_1',x_2') = (0,1)$ it is again easy to see that the sum over l' vanishes. Thus one is left with:

$$(\Lambda \tilde{\star} \Lambda)(k,l,0,1) = \omega_3^{k^2+l^2} 9\delta_k(-i\sqrt{3}\omega_3^{-l^2-l} + i\sqrt{3}\omega_3^{-l^2-l}) = 0. \tag{3.135}$$

So $(\Lambda \tilde{\star} \Lambda)(k,l,0,1)$ vanishes for all choices of k and l.

Lastly, consider the case $(x_1,x_2) = (1,0)$:

x_1'	x_2'	$ll' + g(l+l',1+x_1',x_2') - g(l',x_1',x_2')$	x_2'
0	0	$-l' + l^2 - l + 1$	0
0	1	$-l'^2 + ll' - l' - 1$	1
1	0	$l' + l^2 - 1$	0
1	1	$l'^2 + l' + l^2 + l + 1$	1

For $(x'_1, x'_2) = (0,0)$ and $(x'_1, x'_2) = (1,0)$ it is again easy to see that the sum over l' vanishes. Thus one is left with:

$$(\Lambda \tilde{\star} \Lambda)(k,l,1,0) = \omega_3^{k^2+l^2} 9\delta_k(-i\sqrt{3}\omega_3^{-l^2+l} + i\sqrt{3}\omega_3^{-l^2+l}) = 0. \tag{3.136}$$

So $(\Lambda \tilde{\star} \Lambda)(k,l,1,0)$ vanishes for all choices of k and l. From this one can conclude that Eq. 3.133 is satisfied if $(x_1, x_2) \neq (0,0)$.

Hence the sequence Λ_{sparse} is doubly perfect and according to Theorem 3.0.2, Λ_{sparse} gives rise to a 2-unitary in dimension 36.

The proof that Λ_{symm} is doubly perfect can be done analogously. The author refers to the SageMath notebook in Appendix B.1 for a numerical proof of this theorem. □

How does the 2-unitary in dimension 36 look like? Does it have any special properties? Writing the sequences from Theorem 3.0.5 out, one finds:

$$\Lambda_{sparse} = \exp\left(\frac{2\pi i}{3}[0,2,0,1,0,0,0,1,1,2,2,1,2,1,2,0,2,2,1,2,2,0,0,2,2,1,2,0,\right.$$
$$\left. 2,2,0,1,1,2,2,1]\right),$$

$$\Lambda_{sym} = \exp\left(\frac{2\pi i}{3}[0,2,0,1,0,0,0,1,2,2,1,1,0,2,2,0,1,1,1,2,2,0,0,2,0,2,1,2,\right.$$
$$\left. 2,2,2,1,2,2,2,1]\right).$$

These arrays can be reshaped into:

$$\Lambda_{sparse} = \begin{pmatrix} 1 & \omega_3^2 & \omega_3 & \omega_3^2 & \omega_3 & \omega_3 \\ \omega_3 & \omega_3 & \omega_3 & \omega_3^2 & 1 & \omega_3 \\ \omega_3^2 & \omega_3 & 1 & \omega_3 & 1 & 1 \\ \omega_3^2 & \omega_3^2 & \omega_3^2 & 1 & \omega_3 & \omega_3^2 \\ \omega_3^2 & \omega_3 & 1 & \omega_3 & 1 & 1 \\ \omega_3 & \omega_3 & \omega_3 & \omega_3^2 & 1 & \omega_3 \end{pmatrix}, \tag{3.137}$$

and

$$\Lambda_{sym} = \begin{pmatrix} 1 & \omega_3^2 & 1 & \omega_3 & 1 & 1 \\ 1 & \omega_3 & \omega_3^2 & \omega_3^2 & \omega_3 & \omega_3 \\ 1 & \omega_3^2 & \omega_3^2 & 1 & \omega_3 & \omega_3 \\ \omega_3 & \omega_3^2 & \omega_3^2 & 1 & 1 & \omega_3^2 \\ 1 & \omega_3^2 & \omega_3 & \omega_3^2 & \omega_3^2 & \omega_3^2 \\ \omega_3^2 & \omega_3 & \omega_3^2 & \omega_3^2 & \omega_3^2 & \omega_3 \end{pmatrix}. \tag{3.138}$$

Inserting these into

$$U_\Lambda = \frac{1}{36} \sum_{\mathbf{a} \in \mathbb{Z}_6^2} \Lambda_{a_1,a_2} |\Phi_{\mathbf{a}}\rangle \langle \Phi_{\mathbf{a}}|, \tag{3.139}$$

where

$$\mathbf{a} = \begin{pmatrix} a_1 \\ a_2 \end{pmatrix} \quad \text{and} \quad |\Phi_{\mathbf{a}}\rangle = \frac{1}{6}(Z_6^{a_1} X_6^{-a_2} \otimes \mathbb{I}_6) \sum_{n \in \mathbb{Z}_6} |nn\rangle,$$

one obtains two 2-unitaries in dimension 36, namely U_{sparse} and $U_{symmetric}$. A computer calculation shows that their traces do not coincide and hence these unitaries are not unitarily equivalent. Moreover, the absolute value of each entry is equal to 1. The quadratic form $f(a_1, a_2) = a_1^2 + a_2^2$ can be rewritten as $f(\mathbf{a}) = \mathbf{a}^T \mathbb{I}_2 \mathbf{a}$ and hence, the sequence in the previous theorem is essentially a modified solution for the case $d = 3$ and $n = 1$ and $N = \mathbb{I}_2$ in Theorem 3.0.3, which corresponds to a 2-unitary in dimension 9. More concretely, if one interprets the $\mathbf{x}$-values of the sequences in Theorem 3.0.5 as indices, one can construct four 9-dimensional matrices, three of which are dual unitary (corresponding to $(x_1, x_2) \in \{(1,0), (0,1), (0,0)\}$) and one which is 2-unitary (corresponding to $(x_1, x_2) = (1,1)$). The details of the calculations can be found in the SageMath notebook in Appendix B.1.

For the sparse solution one finds the following perfect subsequences that give rise to dual-unitaries in dimensions 9:

i) $(x_1, x_2) = (0, 0)$

$$\rightsquigarrow \Lambda_{sparse}(a_1, a_2, 0, 0) = \omega_3^{2a_1^2 + a_2^2}. \tag{3.140}$$

$$M_{00} = \frac{1}{3}\begin{pmatrix}
\omega_3-\omega_3^2 & 0 & 0 & 0 & \omega_3^2+2 & 0 & 0 & 0 & \omega_3^2+2 \\
0 & \omega_3^2+2 & 0 & 0 & 0 & \omega_3^2-1 & \omega_3^2-1 & 0 & 0 \\
0 & 0 & \omega_3^2+2 & \omega_3^2-1 & 0 & 0 & 0 & \omega_3^2-1 & 0 \\
0 & 0 & \omega_3^2-1 & \omega_3^2+2 & 0 & 0 & 0 & \omega_3^2-1 & 0 \\
\omega_3^2+2 & 0 & 0 & 0 & \omega_3-\omega_3^2 & 0 & 0 & 0 & \omega_3^2+2 \\
0 & \omega_3^2-1 & 0 & 0 & 0 & \omega_3^2+2 & \omega_3^2-1 & 0 & 0 \\
0 & \omega_3^2-1 & 0 & 0 & 0 & \omega_3^2-1 & \omega_3^2+2 & 0 & 0 \\
0 & 0 & \omega_3^2-1 & \omega_3^2-1 & 0 & 0 & 0 & \omega_3^2+2 & 0 \\
\omega_3^2+2 & 0 & 0 & 0 & \omega_3^2+2 & 0 & 0 & 0 & \omega_3-\omega_3^2
\end{pmatrix}$$

ii) $(x_1, x_2) = (0, 1)$

$$\rightsquigarrow \Lambda_{sparse}(a_1, a_2, 0, 1) = \omega_3^{2a_1^2+a_2^2-a_2+1} \tag{3.141}$$

$$M_{01} = \frac{1}{3}\begin{pmatrix}
\omega_3^2-1 & 0 & 0 & 0 & \omega_3^2+2 & 0 & 0 & 0 & \omega_3^2-1 \\
0 & \omega_3-\omega_3^2 & 0 & 0 & 0 & \omega_3^2-1 & \omega_3-\omega_3^2 & 0 & 0 \\
0 & 0 & \omega_3-\omega_3^2 & \omega_3^2-1 & 0 & 0 & 0 & \omega_3-\omega_3^2 & 0 \\
0 & 0 & \omega_3-\omega_3^2 & \omega_3-\omega_3^2 & 0 & 0 & 0 & \omega_3^2-1 & 0 \\
\omega_3^2-1 & 0 & 0 & 0 & \omega_3^2-1 & 0 & 0 & 0 & \omega_3^2+2 \\
0 & \omega_3-\omega_3^2 & 0 & 0 & 0 & \omega_3-\omega_3^2 & \omega_3^2-1 & 0 & 0 \\
0 & \omega_3^2-1 & 0 & 0 & 0 & \omega_3-\omega_3^2 & \omega_3-\omega_3^2 & 0 & 0 \\
0 & 0 & \omega_3^2-1 & \omega_3-\omega_3^2 & 0 & 0 & 0 & \omega_3-\omega_3^2 & 0 \\
\omega_3^2+2 & 0 & 0 & 0 & \omega_3^2-1 & 0 & 0 & 0 & \omega_3^2-1
\end{pmatrix}$$

iii) $(x_1, x_2) = (1, 0)$

$$\rightsquigarrow \Lambda_{sparse}(a_1, a_2, 1, 0) = \omega_3^{2a_1^2+a_2^2+a_2+1} \tag{3.142}$$

$$M_{10} = \frac{1}{3}\begin{pmatrix}
\omega_3^2-1 & 0 & 0 & 0 & \omega_3^2-1 & 0 & 0 & 0 & \omega_3^2+2 \\
0 & \omega_3-\omega_3^2 & 0 & 0 & 0 & \omega_3-\omega_3^2 & \omega_3^2-1 & 0 & 0 \\
0 & 0 & \omega_3-\omega_3^2 & \omega_3-\omega_3^2 & 0 & 0 & 0 & \omega_3^2-1 & 0 \\
0 & 0 & \omega_3^2-1 & \omega_3-\omega_3^2 & 0 & 0 & 0 & \omega_3-\omega_3^2 & 0 \\
\omega_3^2+2 & 0 & 0 & 0 & \omega_3^2-1 & 0 & 0 & 0 & \omega_3^2-1 \\
0 & \omega_3^2-1 & 0 & 0 & 0 & \omega_3-\omega_3^2 & \omega_3-\omega_3^2 & 0 & 0 \\
0 & \omega_3-\omega_3^2 & 0 & 0 & 0 & \omega_3^2-1 & \omega_3-\omega_3^2 & 0 & 0 \\
0 & 0 & \omega_3-\omega_3^2 & \omega_3^2-1 & 0 & 0 & 0 & \omega_3-\omega_3^2 & 0 \\
\omega_3^2-1 & 0 & 0 & 0 & \omega_3^2+2 & 0 & 0 & 0 & \omega_3^2-1
\end{pmatrix}$$

Similarly, for the symmetric solution one also finds three perfect subsequences that give rise to dual-unitaries in dimensions 9:
$i)(x_1, x_2) = (0, 0)$

$$\rightsquigarrow \Lambda_{sym}(a_1, a_2, 0, 0) = \omega_3^{a_1^2 + a_2^2 + a_1 a_2} \tag{3.143}$$

$$N_{00} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

$ii) \quad (x_1, x_2) = (0, 1)$

$$\rightsquigarrow \Lambda_{sym}(a_1, a_2, 0, 1) = \omega_3^{a_1^2 + a_2^2 - a_1 - a_2 + a_1 a_2 + 2} \tag{3.144}$$

$$N_{01} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \omega_3 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & \omega_3^2 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \omega_3^2 & 0 & 0 & 0 & 0 & 0 \\ \omega_3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \omega_3^2 & 0 \\ 0 & 0 & 0 & 0 & \omega_3 & 0 & 0 & 0 & 0 \end{pmatrix}$$

$iii) \quad (x_1, x_2) = (1, 0)$

$$\rightsquigarrow \Lambda_{sym}(a_1, a_2, 1, 0) = \omega_3^{a_1^2 + a_2^2 + a_1 + a_2 + a_1 a_2 + 2} \tag{3.145}$$

$$N_{10} = \begin{pmatrix} 0 & 0 & 0 & 0 & \omega_3 & 0 & 0 & 0 & 0 \\ 0 & \omega_3^2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \omega_3 \\ 0 & 0 & 0 & 0 & 0 & \omega_3^2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \omega_3^2 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ \omega_3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

Now consider the case $(x_1, x_2) = (1, 1)$. Here one has that the subsequences for the sparse and the symmetric solution coincide:

$$\Lambda_{sym}(a_1, a_2, 1, 1) = \omega_3^{2(a_1^2 + a_2^2)} = \Lambda_{sparse}(a_1, a_2, 1, 1) \tag{3.146}$$

This is the sequence from Example 6, which is doubly perfect and gives rise to the following 2-unitary matrix of order 3:

$$U_{\Lambda,3} = \frac{1}{3} \begin{pmatrix} \omega_3^2 - \omega_3 & 0 & 0 & 0 & \omega_3 + 2 & 0 & 0 & 0 & \omega_3 + 2 \\ 0 & \omega_3 - 1 & 0 & 0 & 0 & \omega_3^2 - \omega_3 & \omega_3^2 - \omega_3 & 0 & 0 \\ 0 & 0 & \omega_3 - 1 & \omega_3^2 - \omega_3 & 0 & 0 & 0 & \omega_3^2 - \omega_3 & 0 \\ 0 & 0 & \omega_3^2 - \omega_3 & \omega_3 - 1 & 0 & 0 & 0 & \omega_3^2 - \omega_3 & 0 \\ \omega_3 + 2 & 0 & 0 & 0 & \omega_3^2 - \omega_3 & 0 & 0 & 0 & \omega_3 + 2 \\ 0 & \omega_3^2 - \omega_3 & 0 & 0 & 0 & \omega_3 - 1 & \omega_3^2 - \omega_3 & 0 & 0 \\ 0 & \omega_3^2 - \omega_3 & 0 & 0 & 0 & \omega_3^2 - \omega_3 & \omega_3 - 1 & 0 & 0 \\ 0 & 0 & \omega_3^2 - \omega_3 & \omega_3^2 - \omega_3 & 0 & 0 & 0 & \omega_3 - 1 & 0 \\ \omega_3 + 2 & 0 & 0 & 0 & \omega_3 + 2 & 0 & 0 & 0 & \omega_3^2 - \omega_3 \end{pmatrix}.$$

Now it is natural to ask, if there is a way to decompose U_{sparse} and $U_{symmetric}$ into a 9-dimensional 2-unitary and some other unitary matrix. A direct approach would be to just build the direct sum of all of the submatrices. This would clearly lead to a unitary, as every submatrix is unitary. However, this approach does not result in a 2-unitary. In order to obtain a 2-unitary out of these submatrices, one has to combine them in another way. This will be discussed in the following.

For this, divide the sequence Λ_{sparse} again into sub-sequences, but this time only separate the $(x, y) = (1, 1)$ sub-sequence from the rest. This gives rise to two matrices: $U_{\Lambda,3}$, which is 9-dimensional, and a 27-dimensional unitary that can be obtained by taking the direct sum of the matrices M_{00}, M_{01}

and M_{10}. This unitary will be denoted by $U_{\Lambda_{sparse},27}$. Now consider the bell basis:

$$|\Phi_{00}\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle), \tag{3.147}$$

$$|\Phi_{01}\rangle = \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle), \tag{3.148}$$

$$|\Phi_{10}\rangle = \frac{1}{\sqrt{2}}(|00\rangle - |11\rangle), \tag{3.149}$$

$$|\Phi_{11}\rangle = \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle). \tag{3.150}$$

Here the indexation already indicates the association to one of the submatrices M_{00}, M_{01}, M_{10} and $U_{\Lambda,3} = M_{11}$. One can now define the following map, which projects a state in $\mathbb{C}^3$ onto one of the three bell states $\{|\Phi_{00}\rangle, |\Phi_{01}\rangle, |\Phi_{10}\rangle\}$:

$$B = \sum_{(x,y)\in\{(0,0),(0,1),(1,0)\}} |\Phi_{xy}\rangle \langle \hat{x} - \hat{y}| \,. \tag{3.151}$$

The hat above the x and y indicates that x and y are elements of $\mathbb{Z}_3$ rather than $\mathbb{Z}_2$, meaning in particular, that -1 corresponds to 2.

Now, the following matrix is 2-unitary (and equal to U_{sparse}):

$$U_\Lambda = U_{\Lambda,3} \otimes |\Phi_{11}\rangle \langle \Phi_{11}| + (\mathbb{I}_9 \otimes B) U_{\Lambda_{sparse},27} (\mathbb{I}_9 \otimes B^\dagger). \tag{3.152}$$

A similar decomposition can be made for the symmetric solution, using the matrices N_{00}, N_{01} and N_{10}.

In the algebraic picture, one can construct two delocalised subalgebras of $\mathcal{M}_{36}(\mathbb{C})$ isomorphic to $\mathcal{M}_6(\mathbb{C})$ by conjugating the two local subalgebras $\mathcal{L} = \mathcal{M}_6(\mathbb{C}) \otimes \mathbb{I}$ and $\mathcal{R} = \mathbb{I} \otimes \mathcal{M}_6(\mathbb{C})$ with U_Λ:

$$\mathcal{A}_L := U_\Lambda \mathcal{L} U_\Lambda^\dagger, \tag{3.153}$$

$$\mathcal{A}_R := U_\Lambda \mathcal{R} U_\Lambda^\dagger. \tag{3.154}$$

The exact form of these subalgebras can be found in the SageMath notebook on the present author's GitHub repository [35]. It is noteworthy that, while $\mathcal{L}$ and $\mathcal{R}$ can be expressed as the spans of the WH-basis, $\mathcal{A}_L$ and $\mathcal{A}_R$ cannot. In particular, comparing this to the case $d^2 = 9$, where a 2-unitary in dimension 9 maps basis operators to basis operators up to a phase, this is not the case for $d^2 = 36$.

3.4 Further Discussions

This section discusses further observations that were made while conducting the research presented in this chapter. Starting with exploring the minimal orders of the 2-unitaries that have been considered in this chapter, the section ends with a discussion on the relation between different 2-unitaries of dimension 9 and a quasi-orthogonal decomposition of $\mathcal{M}_9(\mathbb{C})$.

3.4.1 Order of 2-Unitaries

Recall that Prop. 3.0.5 relates the existence problem of a 2-unitary in dimension d^2 to the existence of a finite group of order greater than d^4 with d^2-dimensional irreducible representation and a quadruple of subgroups of order greater than d^2 that meet certain criteria. If the 2-unitary itself can be described through this representation, it naturally has to have a finite order. Hence one can ask what the minimal order of a 2-unitary is. In the algebraic picture, this boils down to the following question: given a factor of a finite-dimensional algebra $\mathcal{A}$ which has the form $U\mathcal{A}U^\dagger$, where U is a unitary, what is the minimal order of U such that $U\mathcal{A}U^\dagger$ is delocalised, i.e. U is 2-unitary?

i) $d^2 = 9$: So far, the lowest known order of a 2-unitary permutation is 4. For example, the 2-unitary obtained from an OLS(3) in normal form in Example 1 is of order 4. It has the following cycle structure:

$$(0)(1\,8\,2\,4)(3\,5\,6\,7). \tag{3.155}$$

The existence of 2-unitary permutation matrices with order 2 can be ruled out as it is impossible to construct an OLS(3) whose entries only make up 2-cycles. To see that, assume that the OLS(3) is in normal form, i.e.:

$$\begin{matrix} 11 & 2\cdot & 3\cdot \\ 2\cdot & \cdot & \cdot \\ 3\cdot & \cdot & \cdot \end{matrix}$$

The only possible completion of the first row without creating a cycle that is greater than 2 is given by:

11	23	32
2 ·	·	·
3 ·	·	·

If one assumes that the OLS(3) is made of 2-cycles, this leads to:

11	23	32
2 ·	·	12
3 ·	13	·

This clearly cannot be an OLS(3).

The 2-unitary from Example 6, which is not a permutation, has order 3. So far, this is the lowest known order of a 2-unitary in dimension 9. However, there might exist 2-unitaries of order 2, which have not been found so far.

ii) $d^2 = 16$: The following permutation matrix has order 2:

$$U_{16} = \text{Perm}(0, 11, 13, 6, 14, 5, 3, 8, 7, 12, 10, 1, 9, 2, 4, 15). \tag{3.156}$$

Its cycle structure is given by:

$$(0)(1\ 11)(2\ 13)(3\ 6)(4\ 14)(5)(7\ 8)(9\ 12)(10)(15). \tag{3.157}$$

iii) $d^2 = 25$: The following permutation matrix obtained from an OLS(5) in normal form has order 2:

$$U_{25} = \text{Perm}(0, 23, 19, 7, 11, 22, 6, 3, 14, 15, 16, 4, 12, 20, 8, 9, 10, 21, 18, 2, 13, 17, 5, 1, 24).$$

Its cycle structure is given by:

$$(0)(1\ 23)(2\ 19)(3\ 7)(4\ 11)(5\ 22)(6)(8\ 14)(4\ 11)(5\ 22)(6)(8\ 14)(9\ 15)(10\ 16)(12)(13\ 20)(17\ 21)(18)(24).$$

iv) $d^2 = 36$: Due to the non-existence of an OLS(6), there does not exist a 2-unitary permutation matrix. The 2-unitaries from Theorem 3.0.5 have order 3. There might exist 2-unitaries with order 2 which have not been found so far.

The following table summarises these findings:

d^2	9	16	25	36
min order	3	2	2	3

(3.158)

3.4.2 The Number of MOLS and the Number of Quasi-Orthogonal Factors of $\mathcal{M}_{p^2}(\mathbb{C})$

Let p be a prime unequal to two. From Proposition 3.0.2 it becomes clear that any 2-unitary permutation matrix of order p^2 gives rise to two quasi-orthogonal factors isomorphic to $\mathcal{M}_p(\mathbb{C})$. Since any p^2-dimensional 2-unitary permutation matrix is equivalent to a pair of orthogonal Latin squares of order p, this instance leads to the following statement:

Proposition 3.0.8. *Every pair of OLS(p) gives rise two quasi-orthogonal factors of $\mathcal{M}_{p^2}(\mathbb{C})$.*

Proof. This follows immediately from Theorem 3.0.5. □

Is there a way to generalise that to a set of k MOLS(p)? By simple counting arguments one can prove the following:

Proposition 3.0.9. *A set of k MOLS(p) gives rise to $k(k-1)/2$ pairs of quasi-orthogonal factors of $\mathcal{M}_{p^2}(\mathbb{C})$.*

Proof. Let $K^1, ..., K^k$ be mutually orthogonal Latin squares of order p. According to Prop. 2.19.1 each pair of orthogonal Latin squares gives rise to a 2-unitary in dimension p^2. Now a simple counting argument yields that there are

$$\sum_{i=1}^{k-1} i = \frac{k(k-1)}{2} \tag{3.159}$$

different pairs. According to 3.0.8 each pair gives rise to a pair of quasi-orthogonal factors of $\mathcal{M}_{p^2}(\mathbb{C})$. □

The question now arises, if these subalgebras are actually distinct from each other. As it turns out, this is in general not the case.

Consider the following 3 MOLS(4) (a complete set of MOLS of order 4):

$$K^1 = \begin{matrix} 1 & 2 & 3 & 4 \\ 2 & 1 & 4 & 3 \\ 3 & 4 & 1 & 2 \\ 4 & 3 & 2 & 1 \end{matrix} \qquad K^2 = \begin{matrix} 1 & 2 & 3 & 4 \\ 4 & 3 & 2 & 1 \\ 2 & 1 & 4 & 3 \\ 3 & 4 & 1 & 2 \end{matrix} \qquad K^3 = \begin{matrix} 1 & 2 & 3 & 4 \\ 3 & 4 & 1 & 2 \\ 4 & 3 & 2 & 1 \\ 2 & 1 & 4 & 3 \end{matrix}$$

There are three possibilities to form distinct pairs:

I. (K^1, K^2)

II. (K^1, K^3)

III. (K^2, K^3)

According to 2.19.1 each of these pairs gives rise to a 2-unitary in dimension 16. Write the elements of $\mathcal{L} = \mathcal{M}_4(\mathbb{C}) \otimes \mathbb{I}_4$ and $\mathcal{R} = \mathbb{I}_4 \otimes \mathcal{M}_4(\mathbb{C})$ in terms of the Weyl-Heisenberg basis: $\{X^i Z^j\}_{i,j \in [3]}$ where

$$X = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix} \qquad Z = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & i & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -i \end{pmatrix}.$$

Now apply each of these 2-unitaries to $\mathcal{L}$ and $\mathcal{R}$. This results in three pairs of quasi-orthogonal factors:

I. (A_{L_1}, A_{R_1})

II. (A_{L_2}, A_{R_2})

III. (A_{L_3}, A_{R_3})

But $A_{R_3} = A_{R_1}$ (the calculation can be found in a Sage notebook on the present author's GitHub repository [35]) and hence these pairs are not distinct.

3.4.3 Quasi-Orthogonal Decomposition of $\mathcal{M}_3(\mathbb{C}) \otimes \mathcal{M}_3(\mathbb{C})$

In this section the following question will be addressed: given a maximal set of mutually quasi-orthogonal distinct factors, what can be said about the

2-unitaries are needed to generate these factors by conjugating the local subalgebras? This will be done for local dimension $p = 3$, in which case the maximal number of orthogonal Latin squares is two. This OLS(3) gives rise to one pair of quasi-orthogonal factors of $\mathcal{M}_9(\mathbb{C})$ according to Prop. 3.0.8. However, in Ref. [88] the author shows that the following ten factors of $\mathcal{M}_9(\mathbb{C})$ are distinct and hence form a quasi-orthogonal decomposition of $\mathcal{M}_9(\mathbb{C})$ [88]:

$\mathcal{A}_1 = \mathrm{span}(\mathbb{I}_9, X \otimes Z, X^2 \otimes Z^2, Z \otimes X^2, XZ \otimes X^2Z, X^2Z \otimes X^2Z^2, Z^2 \otimes X, XZ^2 \otimes XZ, X^2Z^2 \otimes XZ^2)$

$\mathcal{A}_2 = \mathrm{span}(\mathbb{I}_9, XZ \otimes Z, X^2Z^2 \otimes Z^2, Z \otimes X^2Z^2, XZ^2 \otimes X^2, X^2 \otimes X^2Z, Z^2 \otimes XZ, X \otimes XZ^2, X^2Z \otimes X^2)$

$\mathcal{A}_3 = \mathrm{span}(\mathbb{I}_9, XZ^2 \otimes Z, X^2Z \otimes Z^2, Z \otimes X^2Z, X \otimes X^2Z^2, X^2Z^2 \otimes X^2, Z^2 \otimes XZ^2, XZ \otimes X, X^2 \otimes XZ)$

$\mathcal{A}_4 = \mathrm{span}(\mathbb{I}_9, X \otimes Z^2, X^2 \otimes Z, Z^2 \otimes X^2, XZ^2 \otimes X^2Z^2, X^2Z^2 \otimes X^2Z, Z \otimes X, XZ \otimes XZ^2, X^2Z \otimes XZ)$

$\mathcal{A}_5 = \mathrm{span}(\mathbb{I}_9, XZ \otimes Z^2, X^2Z^2 \otimes Z, Z^2 \otimes X^2Z^2, X \otimes X^2Z, X^2Z \otimes X^2, Z \otimes XZ, XZ^2 \otimes X, X^2 \otimes XZ^2)$

$\mathcal{A}_6 = \mathrm{span}(\mathbb{I}_9, XZ^2 \otimes Z^2, X^2Z \otimes Z, Z^2 \otimes X^2Z, XZ \otimes X^2, X^2 \otimes X^2Z^2, Z \otimes XZ^2, X \otimes XZ, X^2Z^2 \otimes X)$

$\mathcal{A}_7 = \mathrm{span}(\mathbb{I}_9, XZ \otimes X^2Z^2, X^2Z^2 \otimes XZ, XZ^2 \otimes X^2Z, X^2 \otimes X, Z \otimes Z^2, X^2Z \otimes XZ^2, Z^2 \otimes Z, X \otimes X^2)$

$\mathcal{A}_8 = \mathrm{span}(\mathbb{I}_9, XZ \otimes XZ, X^2Z^2 \otimes X^2Z^2, XZ^2 \otimes XZ^2, X^2 \otimes X^2, Z \otimes Z, X^2Z \otimes X^2Z, Z^2 \otimes Z^2, X \otimes X)$

$\mathcal{L} = \mathrm{span}(\mathbb{I}_9, XZ \otimes \mathbb{I}_3, X^2Z^2 \otimes \mathbb{I}_3, XZ^2 \otimes \mathbb{I}_3, X^2 \otimes \mathbb{I}_3, Z \otimes \mathbb{I}_3, X^2Z \otimes \mathbb{I}_3, Z^2 \otimes \mathbb{I}_3, X \otimes \mathbb{I}_3)$

$\mathcal{R} = \mathrm{span}(\mathbb{I}_9, \mathbb{I}_3 \otimes XZ, \mathbb{I}_3 \otimes X^2Z^2, \mathbb{I}_3 \otimes XZ^2, \mathbb{I}_3 \otimes X^2, \mathbb{I}_3 \otimes Z, \mathbb{I}_3 \otimes X^2Z, \mathbb{I}_3 \otimes Z^2, \mathbb{I}_3 \otimes X)$

Combinatorially, this can be regarded as dividing the $d^2 \times d^2 = 9 \times 9 = 81$ basis operators of $\mathcal{M}_9(\mathbb{C})$ into $d^2 + 1 = 10$ different sets of cardinality $d^2 = 9$ that only intersect in one element, namely the identity matrix. This is the same combinatorial structure as an affine plane of order 9 or equivalently a complete set of MOLS(9). The corresponding quantum design is affine with parameters $v = 81,\ b = 90,\ r = 10,\ k = 0, 9$ and $\lambda = 0, 9$.

In light of Theorem 3.0.5, the following question arises: what are the 2-unitaries that map the two local subalgebras $\mathcal{L}$ and $\mathcal{R}$ to the remaining eight subalgebras? Do they have special features? As it turns out one can use the following four 2-unitaries to generate the decomposition:

I.

$$U_{CHM,3} = \frac{1}{3}\begin{pmatrix} 1 & 1 & 1 & 1 & \omega_3 & \omega_3^2 & 1 & \omega_3^2 & \omega_3 \\ 1 & 1 & 1 & \omega_3^2 & 1 & \omega_3 & \omega_3 & 1 & \omega_3^2 \\ 1 & 1 & 1 & \omega_3 & \omega_3^2 & 1 & \omega_3^2 & \omega_3 & 1 \\ 1 & \omega_3 & \omega_3^2 & 1 & \omega_3^2 & \omega_3 & 1 & 1 & 1 \\ \omega_3 & \omega_3^2 & 1 & 1 & \omega_3^2 & \omega_3 & \omega_3^2 & \omega_3^2 & \omega_3^2 \\ \omega_3^2 & 1 & \omega_3 & 1 & \omega_3^2 & \omega_3 & \omega_3 & \omega_3 & \omega_3 \\ 1 & \omega_3^2 & \omega_3 & 1 & 1 & 1 & 1 & \omega_3 & \omega_3^2 \\ \omega_3^2 & \omega_3 & 1 & \omega_3 & \omega_3 & \omega_3 & 1 & \omega_3 & \omega_3^2 \\ \omega_3 & 1 & \omega_3^2 & \omega_3^2 & \omega_3^2 & \omega_3^2 & 1 & \omega_3 & \omega_3^2 \end{pmatrix} \tag{3.160}$$

This 2-unitary was taken from Ref. [41].

II.

The following 2-unitary was taken from Ex. 6 and corresponds to the doubly perfect sequence $\Lambda(a_1, a_2) = \omega_3^{2(a_1^2+a_2^2)}$:

$$U_{\Lambda,3} = \frac{1}{3}\begin{pmatrix} \omega_3^2-\omega_3 & 0 & 0 & 0 & \omega_3+2 & 0 & 0 & 0 & \omega_3+2 \\ 0 & \omega_3-1 & 0 & 0 & 0 & \omega_3^2-\omega_3 & \omega_3^2-\omega_3 & 0 & 0 \\ 0 & 0 & \omega_3-1 & \omega_3^2-\omega_3 & 0 & 0 & 0 & \omega_3^2-\omega_3 & 0 \\ 0 & 0 & \omega_3^2-\omega_3 & \omega_3-1 & 0 & 0 & 0 & \omega_3^2-\omega_3 & 0 \\ \omega_3+2 & 0 & 0 & 0 & \omega_3^2-\omega_3 & 0 & 0 & 0 & \omega_3+2 \\ 0 & \omega_3^2-\omega_3 & 0 & 0 & 0 & \omega_3-1 & \omega_3^2-\omega_3 & 0 & 0 \\ 0 & \omega_3^2-\omega_3 & 0 & 0 & 0 & \omega_3^2-\omega_3 & \omega_3-1 & 0 & 0 \\ 0 & 0 & \omega_3^2-\omega_3 & \omega_3^2-\omega_3 & 0 & 0 & 0 & \omega_3-1 & 0 \\ \omega_3+2 & 0 & 0 & 0 & \omega_3+2 & 0 & 0 & 0 & \omega_3^2-\omega_3 \end{pmatrix}.$$

III.

$$U_{\Lambda_{CHM},3} = \frac{1}{3}\begin{pmatrix}
1 & \omega_3 & \omega_3 & \omega_3 & \omega_3 & 1 & \omega_3 & 1 & \omega_3 \\
\omega_3 & 1 & \omega_3 & \omega_3^2 & 1 & 1 & \omega_3^2 & \omega_3^2 & \omega_3 \\
\omega_3 & \omega_3 & 1 & \omega_3^2 & \omega_3 & \omega_3^2 & \omega_3^2 & 1 & 1 \\
\omega_3 & \omega_3^2 & \omega_3^2 & 1 & 1 & \omega_3^2 & \omega_3 & 1 & \omega_3 \\
1 & \omega_3^2 & 1 & \omega_3^2 & 1 & 1 & 1 & 1 & \omega_3^2 \\
\omega_3 & \omega_3 & 1 & 1 & \omega_3^2 & 1 & \omega_3 & \omega_3^2 & \omega_3^2 \\
\omega_3 & \omega_3^2 & \omega_3^2 & \omega_3 & \omega_3 & 1 & 1 & \omega_3^2 & 1 \\
\omega_3 & 1 & \omega_3 & \omega_3 & \omega_3^2 & \omega_3^2 & 1 & 1 & \omega_3^2 \\
1 & 1 & \omega_3^2 & 1 & \omega_3^2 & 1 & \omega_3^2 & 1 & 1
\end{pmatrix}. \tag{3.161}$$

This 2-unitary Hadamard matrix of order 6 was taken from Example 10 (obtained from Theorem 3.0.4). According to Theorem 3.0.4, the partial transpose of $U_{\Lambda_{CHM,3}}$ is also 2-unitary and has order 4.

IV.

$$U_{OLS,3} = \begin{pmatrix}
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix} \tag{3.162}$$

This unitary corresponds to the 2-unitary permutation matrix obtained from an OLS in normal form that was introduced in Section 3.1 in Example 1.

The following table displays commutative pairs of delocalised subalgebras, their underlying groups (see Ex. 5), the 2-unitary mapping the two local subalgebras $\mathcal{L}$ and $\mathcal{R}$ to the pair, its order and its trace[7]:

[7] More detailed calculations can be found on the present author's GitHub repository [35].

Pair of subalgebras	Underlying groups	U	ord(U)	tr(U)
$\mathcal{A}_1, \mathcal{A}_4$	$C_{1,0}, C_{2,0}$	$U_{CHM,3}$	8	1
$\mathcal{A}_2, \mathcal{A}_5$	$C_{1,1}, C_{2,1}$	$U_{\Lambda,3}$	3	-3
$\mathcal{A}_3, \mathcal{A}_6$	$C_{1,2}, C_{2,2}$	$U_{\Lambda_{CHM},3}$	6	3
$\mathcal{A}_7, \mathcal{A}_8$	D_1, D_2	$U_{OLS,3}$	4	1

Here $U_{CHM,3}$ and $U_{OLS,3}$ are equivalent under local unitary transformations[8] [41].

In Ref. [98] it was shown that there is only one equivalence class of 2-unitary permutation matrices of dimension 9 under local unitary transformations. In fact, it was conjectured that *all* 2-unitaries in dimension 9 are LU-equivalent [96]. If this is true, all of the 2-unitaries above should be LU-equivalent.

[8]This means that for each 9-dimensional 2-unitary, there exist unitary operators U_1, U_2, U_3, U_4 such that: $U = (U_1 \otimes U_2) U_{OLS} (U_3 \otimes U_4)$.

4 (Quantum) Combinatorial Structures in Category Theory

In Section 2.1 the concepts of block designs and quantum designs were introduced. Based on Def. 2.4 and Def. 2.10, a category-theoretic model for both classical and quantum designs will be developed in this chapter, using arrow categories and the categories $\mathbf{Mat}(\mathbb{N})$ and $\mathbf{CP}[\mathbf{FHilb}]$. This framework transfers the essential properties of block designs into a pointed monoidal dagger category leading to the more abstract notion of *categorical block designs*. This approach not only generalises the description of classical and quantum designs using completely positive maps, but also establishes a connection between them via a functor. Furthermore, based on these techniques, a category of MUBs will be defined, and the concept of combinatorial quantum channels will be derived.

This chapter is based on the present author's publication Ref. [37] (c.f. *Teilpublikationen* on page iii) which is joint work with Jamie Vicary. All results in this chapter have been derived by the present author. The statements of technical definitions, lemmas, theorems, and their proofs have largely been carried over verbatim from the publication. All those texts were written by the present author. Section 4.4 has not previously appeared.

4.0.1 Related Work

The previous chapter illustrated the rich range of applications that design theory has in quantum theory. It is therefore natural to ask how these findings can be translated into the language of category-theoretical quantum theory. A categorical approach to hypergraphs was proposed by Dörfler and Waller (see [27]). Since every block design can be represented as a uniform and regular hypergraph, their construction already provides a category-theoretical description of block designs. Nevertheless, because their approach relies on the power-set functor, this notion is rather complicated and thus in this work a category of block designs will be defined in a slightly different way, namely via the category of matrices and natural numbers $\mathbf{Mat}(\mathbb{N})$. This formulation not only generalises the framework of Dörfler and Waller, which appears as a subcategory, but also has the advantage that it does not make use of the power-set functor.

First attempts to find a category-theoretical description of quantum and classical designs have been developed in the present author's master's thesis [36] by using the arrow category of the category of finite-dimensional Hilbert spaces and completely positive maps, $\mathbf{CP}[\mathbf{FHilb}]$ and the arrow categories of the category of matrices and natural numbers, $\mathbf{Mat}(\mathbb{N})$. Category-theoretical formulations of certain combinatorial structures, such as Latin squares (LS) and quantum Latin squares (QLS), already exist (see [81, 84]). However, these are not embedded within framework developed in Ref. [36]. The following chapter aims to generalise these notions and embed them into a broader category-theoretical framework.

Before diving into the more general framework, recall the definitions of block designs and homomorphisms between them (Def. 2.4 and Def. 2.5). One straightforward way to define a category of block designs is given by the following:

Definition 4.1. [37] The category **Design** has designs as objects, and design homomorphisms as morphisms. The category **Block** is the full subcategory on the block designs.

This definition could equivalently be formulated in terms of points and blocks. However, the more abstract formulation is adopted here to align more closely with the categorical framework developed in the following sections. For quantum designs the situation is less obvious as it is not clear how to define quantum designs as objects. However, the abstract notion developed in the next section will turn out to be elucidating.

4.1 The Design Construction

In this section the so-called *design construction*, that gives an abstract notion of the uniformity-, regularity- and λ-balanced condition from Section 2.1 in an arbitrary rigid monoidal category, will be developed.

Definition 4.2 (Design construction)**.** [37] Let $F : \mathcal{D} \hookrightarrow \mathcal{C}$ be a faithful monoidal functor between pointed monoidal dagger categories. The category $\mathbf{Design}[\mathcal{C}, \mathcal{D}]$ is the subcategory of $\mathbf{Arr}[\mathcal{C}]$ where the morphisms are given by pairs of morphisms of $\mathcal{C}$ which are in the image of the functor F; omit F from the notation, ensuring it is clear from the context. Where $F = \mathrm{id}$, simply write $\mathbf{Design}[\mathcal{C}]$.

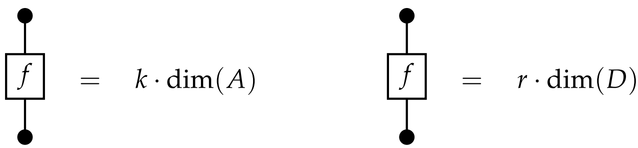
Definition 4.3. [37] The category $\mathbf{RUDesign}[\mathcal{C}, \mathcal{D}]$ is the subcategory of $\mathbf{Design}[\mathcal{C}, \mathcal{D}]$ where objects $f : A \to D$ are r-regular and k-uniform, for scalars $r, k \in \mathrm{Hom}(\mathbb{I}_{\mathcal{C}}, \mathbb{I}_{\mathcal{C}})$, with the pointed structure and its dagger represented by a black dot:

Lemma 4.3.1. *[37] In $\mathbf{RUDesign}[\mathcal{C}, \mathcal{D}]$ for any k-uniform, r-regular object $f : A \to D$, the following equations hold:*

$$k \cdot \dim(A) = r \cdot \dim(D) \tag{4.1}$$

where $\dim(A) = p_A^\dagger \circ p_A$ for $A \in \mathrm{obj}(\mathcal{C})$. Here $p_A : 1 \to A$ is the pointed structure of $\mathcal{C}$.

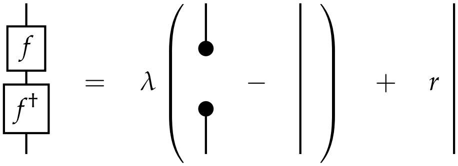
Proof. Via composition with $p_D^\dagger$ and p_A respectively, the regularity and uniformity condition become:



Hence Eq. 4.1 holds. □

Definition 4.4. [37] The category $\mathbf{BDesign}[\mathcal{C}, \mathcal{D}]$ is the subcategory of $\mathbf{RUDesign}[\mathcal{C}, \mathcal{D}]$ where all k-uniform and r-regular objects $f : A \to D$ are

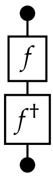
λ-balanced for scalars $\lambda \in \mathrm{Hom}(\mathbb{I}_{\mathcal{C}}, \mathbb{I}_{\mathcal{C}})$:



Lemma 4.4.1. *[37] In* **BDesign**$[\mathcal{C}, \mathcal{D}]$ *for any k-uniform, r-regular object $f : A \to D$, the following equation holds, where* $\dim(D) = p_D^\dagger \circ p_D$ *for $D \in$* $\mathrm{obj}(\mathcal{C})$*:*

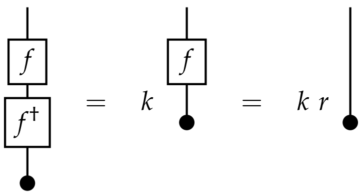
$$\lambda \cdot (\dim(D) - 1) = r \cdot (k - 1) \tag{4.2}$$

Proof. To prove Eq. 4.2, concatenate the λ-condition with both p_A and $p_A^\dagger$ which gives:

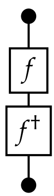


$$= \quad \lambda(\dim(D)^2 - \dim(D)) + r \dim(D)$$

On the other hand one has:



If one now concatenates with $p_D^\dagger$, one gets:



$$= \quad k\ r\ \dim(D)$$

From this one can easily deduce Eq. 4.2. □

4.2 The Category of Block Designs

In this section the design-constructions from Section 4.1 will be applied to the categories **Mat**($\mathbb{N}$) and **CP**[**FHilb**] that have been discussed in Section 2.4 and it will be shown that this yields a categorical model of both classical quantum designs.

Consider the category of finite sets and functions **FSet**. There exists a faithful functor **FSet** $\hookrightarrow$ **Mat**($\mathbb{N}$) which takes every set to the natural number coinciding with its cardinality. Furthermore, following Theorem 2.57.1, it holds that **FSet** $\hookrightarrow$ **Mat**($\mathbb{N}$) $\cong$ $\mathbf{CP_c}$[**FHilb**].

In the following, it will be demonstrated that there exists a functor from the category **BDesign**[**Mat**($\mathbb{N}$), **FSet**] to the category **Block**. Additionally, it will be proved that **BDesign**[**Mat**($\mathbb{N}$), **FSet**] is equivalent to the category **BDesign**[$\mathbf{CP_c}$[**FHilb**], **FSet**].

Theorem 4.4.1. *[37] There exists a functor G :* **BDesign**[**Mat**($\mathbb{N}$), **FSet**] $\longrightarrow$ **Block**.

Proof. First note that the morphisms in **BDesign**[**Mat**($\mathbb{N}$), **FSet**] are given by pairs of functions. The functor sends each object in **BDesign**[**Mat**($\mathbb{N}$), **FSet**] to an incidence matrix in **Block** by sending each matrix entry greater than 0 to 1. The uniformity, regularity and λ-conditions of the design construction ensure that the incidence matrix one obtains that way, represents a uniform, regular and λ-balanced design. On morphisms the functor acts as the identity. □

Similarly, one can argue that the following holds.

Theorem 4.4.2. *[37] There exists a functor G :* **Design**[**Mat**($\mathbb{N}$), **FSet**] $\longrightarrow$ **Design**.

This indicates that the categories **Design**[**Mat**($\mathbb{N}$), **FSet**] and **BDesign**[**Mat**($\mathbb{N}$), **FSet**] actually define a more general concept of (block)designs, which will be referred to as *categorical (block)designs* [37].

Lemma 4.4.2. *[37] The category* **BDesign**[**Mat**($\mathbb{N}$), **FSet**] *is equivalent to the category* **BDesign**[$\mathbf{CP_c}$[**FHilb**], **FSet**].

Proof. According to Proposition 2.57.1 the categories $\mathbf{CP_c}$[**FHilb**] and **Mat**($\mathbb{N}$) are equivalent. Using Theorem 2.58.1 from Section 2.4, this gives rise to an equivalence between their arrow categories. □

There already exists a category-theoretical characterisation of LS (see Ref. [81]). However, these objects do not fit into the framework here.

4.3 The Category of Quantum Designs

Having retrieved the category of block designs by applying the design construction to the categories $\mathbf{Mat}(\mathbb{N})$ and $\mathbf{CP_c}[\mathbf{FHilb}]$, in this section, the design construction will be applied to the category $\mathbf{CP}[\mathbf{FHilb}]$. As it turns out, this will give a notion of a category of quantum designs that contains a category $\mathbf{QDesign}_\mathrm{B}$, which has objects that are uniform and regular quantum designs of degree 1, as a subcategory. Another important subcategory is given by the category $\mathbf{QDesign}_\mathrm{RU}$ which has uniform and regular quantum designs as objects. This subcategory also contains a subcategory **MUB**, with objects that are sets of mutually unbiased bases.

Recall from Section 2.4 that $\mathbf{CP}[\mathbf{FHilb}]$ is comprised of finite dimensional H^*-algebras and completely positive maps. Applying the design construction to this category, one then gets a category $\mathbf{Design}[\mathbf{CP}[\mathbf{FHilb}]]$, with objects that are CP-maps between finite dimensional H^*-algebras, and morphisms that are pairs of CP-maps:

Definition 4.5. [37] The category **QDesign** is defined to be the category $\mathbf{Design}[\mathbf{CP}[\mathbf{FHilb}]]$.

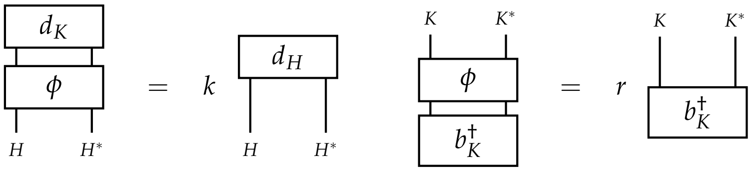
This category will be referred to as the category of quantum designs, where quantum designs are here a more abstract thing than what was defined by Zauner (see Def. 2.10).

Definition 4.6. [37] The subcategory $\mathbf{RUDesign}[\mathbf{CP}[\mathbf{FHilb}]]$ of **QDesign** is called $\mathbf{QDesign}_\mathrm{RU}$. Its objects are uniform and regular quantum designs.

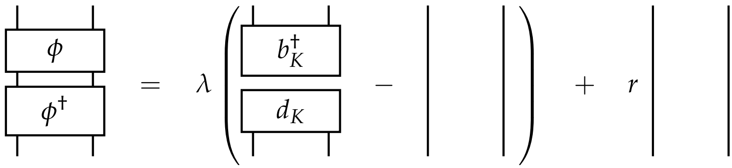
Definition 4.7. [37] The subcategory $\mathbf{BDesign}[\mathbf{CP}[\mathbf{FHilb}]]$ of $\mathbf{QDesign}_\mathrm{RU}$ is called $\mathbf{QDesign}_\mathrm{B}$. Its objects are uniform and regular quantum designs with degree 1.

Example 1. [37]
Consider the subcategory of $\mathbf{QDesign}_\mathrm{B}$ where all objects are CP-maps between matrix algebras: $\phi : H \otimes H^* \to K \otimes K^*$ where $\dim(H) = b$ and $\dim(K) = v$. Because H is a special Frobenius algebra, one gets $\dim(H) =$

$\mathrm{tr}(\mathrm{id}_H)$. One then has the following uniformity and regularity conditions:



The λ-condition is given by:



Let $H = \mathbb{C}^2 = K$ and consider the CP-map $\varphi : \mathbb{C}^2 \otimes \mathbb{C}^2 \to \mathbb{C}^2 \otimes \mathbb{C}^2$ with matrix representation:

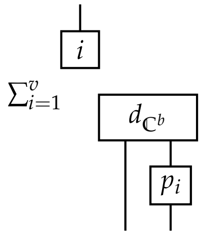
$$\begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & \frac{1}{2} & \frac{1}{2} & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix}$$

This map represents a quantum design with parameters $\lambda = k = r = 2 = v = b$.

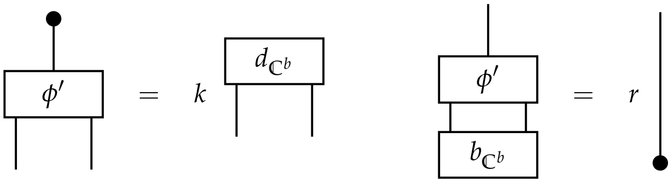
Having considered completely positive maps from a non-commutative algebra to a non-commutative algebra in **FHilb** in Ex. 1, it is natural to ask what happens if one considers CP-maps from a commutative algebra to a non-commutative algebra, i.e. maps of the form: $\varphi : H \to K^* \otimes K$. In fact, it will turn out that one can encode uniform and regular quantum designs of degree 1 according to Zauner's notion via these maps. The next theorem can be found in similar spirit in the present author's master's thesis [36] but is also part of Ref. [37].

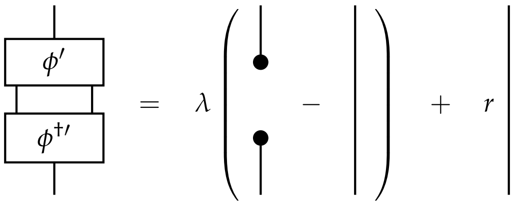
Theorem 4.7.1. *[37] There exists a subcategory of* $\mathbf{QDesign}_{\mathrm{B}}$ *that has objects that represent uniform and regular quantum designs of degree 1 according to Zauner's notion.*

Proof. Consider a uniform, regular and λ-balanced quantum design $D = \{p_1, ..., p_v\}$, where each p_i is a $b \times b$ projection matrix in a Hilbert space $\mathbb{C}^b$. Following Example 1, these projections $p_i : \mathbb{C}^b \to \mathbb{C}^b$ then give rise to a completely positive map $\phi : \mathbb{C}^v \to \mathbb{C}^b \otimes \mathbb{C}^b$ in **FHilb**. This is valid because imposing the uniformity-, regularity- and λ-condition on the projector has no impact on the CP-condition. Now take $\phi' = \phi^\dagger : \mathbb{C}^b \otimes \mathbb{C}^b \to \mathbb{C}^v$, i.e.:



Then one finds:





These coincide with the conditions given by the design construction applied to **FHilb**. Moreover, one can recover Eq. 2.4 and Eq. 2.5 from Lemma 2.12.1, as $\dim(\mathbb{C}^v) = v$ and $\dim(\mathbb{C}^b) = b$ and Eq. 4.1 and Eq. 4.2 hold. □

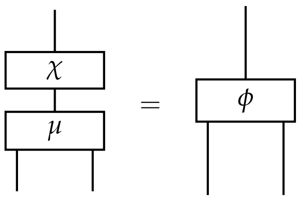
4.3.1 A Functor Between Categorical Block Designs and Categorical Quantum Designs

In this section a functor between **BDesign**[**Mat**($\mathbb{N}$), **FSet**] and **QDesign**$_B$ will be constructed that relates classical block designs to quantum designs.

Since these results already have been published in the present author's Master's thesis [36], they will only be included for the sake of completeness.

Proposition 4.7.1. *[36, 37] There exists a functor* $Q : \mathbf{BDesign}[\mathbf{Mat}(\mathbb{N}), \mathbf{FSet}] \to \mathbf{QDesign}_B$ *that relates a generalised balanced incomplete block designs to uniform, regular and* λ*-balanced quantum designs.*

Proof. According to Lemma 4.4.2 the categories $\mathbf{BDesign}[\mathbf{Mat}(\mathbb{N}), \mathbf{FSet}]$ and $\mathbf{BDesign}[\mathbf{CP}_c[\mathbf{FHilb}], \mathbf{FSet}]$ are equivalent. So one can actually represent an arbitrary object $\chi : b \to v$ in $\mathbf{BDesign}[\mathbf{Mat}(\mathbb{N}), \mathbf{FSet}]$ via a uniform, regular and λ-balanced CP-map $\chi : \mathbb{C}^b \to \mathbb{C}^v$. The functor Q acts on objects by sending each object $\chi : \mathbb{C}^b \to \mathbb{C}^v$ in $\mathbf{BDesign}[\mathbf{Mat}(\mathbb{N}), \mathbf{FSet}]$ with parameters k, r and λ to the map $\phi = \chi \circ L : \mathbb{C}^b \otimes \mathbb{C}^b \to \mathbb{C}^b \to \mathbb{C}^v$, where the map $L : \mathbb{C}^b \otimes \mathbb{C}^b \to \mathbb{C}^b$ is the so-called Cayley embedding, which in the present case simply becomes the multiplication $\mu : \mathbb{C}^b \otimes \mathbb{C}^b \to \mathbb{C}^b$ as one has that $A = \mathbb{C}^b \cong (\mathbb{C}^b)^* = A^*$. Its conjugate $L^\dagger$ is just the comultiplication $\Delta : \mathbb{C}^b \to \mathbb{C}^b \otimes \mathbb{C}^b$. The resulting map ϕ is as concatenation of completely positive maps also completely positive. Depict this via the following string diagram:



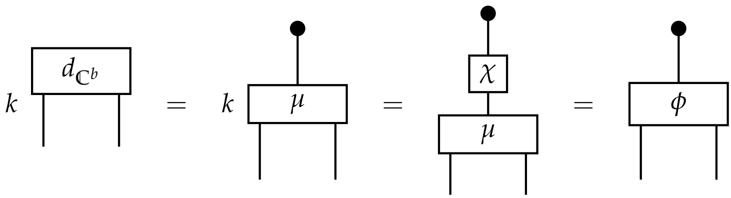
Via concatenation, each morphism in $\mathbf{BDesign}[\mathbf{Mat}(\mathbb{N}), \mathbf{FSet}]$

$$\begin{array}{ccc} \mathbb{C}^b & \xrightarrow{\xi'} & \mathbb{C}^{b'} \\ \downarrow{\scriptstyle \chi} & & \downarrow{\scriptstyle \chi'} \\ \mathbb{C}^v & \xrightarrow{\xi} & \mathbb{C}^{v'} \end{array}$$

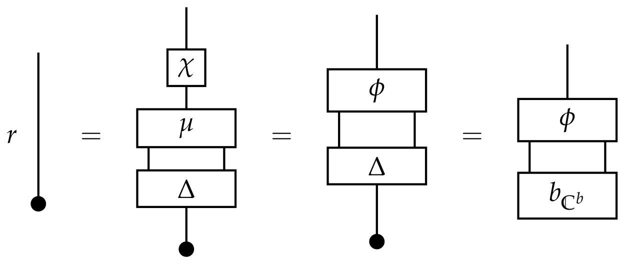
gets mapped to a morphism in $\mathbf{QDesign}_B$, as follows:

$$
\begin{array}{ccc}
\mathbb{C}^b \otimes \mathbb{C}^b & \xrightarrow{\xi' \otimes \xi'} & \mathbb{C}^{b'} \otimes \mathbb{C}^{b'} \\
\downarrow \mu & & \downarrow \mu \\
\mathbb{C}^b & \xrightarrow{\quad \xi' \quad} & \mathbb{C}^{b'} \\
\downarrow \chi & & \downarrow \chi' \\
\mathbb{C}^v & \xrightarrow{\quad \xi \quad} & \mathbb{C}^{v'}
\end{array}
$$

This diagram commutes, because ξ' can be extended to a morphism of monoids as ξ' is a function. It is easy to verify that this functor respects composition and sends the identity morphism in $\mathbf{BDesign}[\mathbf{Mat}(\mathbb{N}), \mathbf{FSet}]$, i.e. $\mathrm{id}_\psi = (\mathrm{id}, \mathrm{id})$, to the identity morphism $\mathrm{id}_{Q(\psi)} = (\mathrm{id} \otimes \mathrm{id}, \mathrm{id} \otimes \mathrm{id})$ in $\mathbf{QDesign}_\mathrm{B}$. The regularity-condition then becomes:



which is exactly the regularity-condition in $\mathbf{QDesign}_\mathrm{B}$. Here the fact that $\mathbb{C}^b$ is a special Frobenius algebra has been used in the first step. For uniformity one finds:



which is precisely the uniformity condition in $\mathbf{QDesign}_\mathrm{B}$. In a similar way one can verify that the λ-condition in $\mathbf{BDesign}[\mathbf{Mat}(\mathbb{N}), \mathbf{FSet}]$ gets mapped to the λ-condition in $\mathbf{QDesign}_\mathrm{B}$. □

In this construction, every classical design gives rise to a uniform and regular quantum design of degree 1, analogously to Theorem 2.13.1. However, it is straightforward to verify that the functor Q does not yield an equivalence of categories, as it is not essentially surjective.

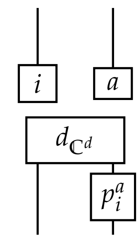
4.3.2 The Category of MUB's

How do MUB's fit into this picture? Recall that MUB's are quantum designs of degree 2 and hence they cannot be in the category $\mathbf{QDesign}_{\mathrm{B}}$. But what about the category $\mathbf{QDesign}_{\mathrm{RU}}$? In the present author's Master's thesis a notion of a "MUB-quantum design" in a category-theoretical setting has already been discussed. Another category-theoretical description can be found in Ref. [81]. However, in these pictures, MUBs were only considered as objects in a category rather than as a class of objects that form a category themselves. In this section, a category of MUBs, namely **MUB**, will be defined as a subcategory of $\mathbf{QDesign}_{\mathrm{RU}}$, that has objects that are collections of MUBs. This not only provides a more general framework for MUBs in a category-theoretical setting, but also highlights the strong connections between MUBs and design theory in general.

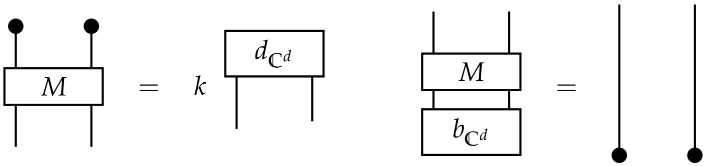
Theorem 4.7.2. *[37] There exists a subcategory* **MUB** *of* $\mathbf{QDesign}_{\mathrm{RU}}$ *with objects that are collections of MUBs and morphisms that are pairs of functions.*

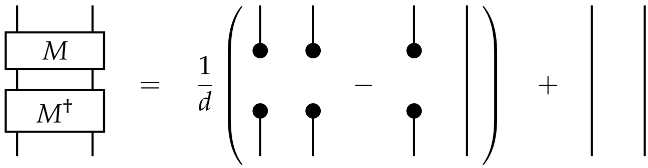
Proof. Let $A_1 = \{p_1^1, ...p_d^1\}, ..., A_k = \{p_1^k, ..., p_d^k\}$ be a set of k MUBs is $\mathbb{C}^d$ and consider the CP-map $M : \mathbb{C}^{k\cdot d} \cong \mathbb{C}^d \otimes \mathbb{C}^k \to \mathbb{C}^d \otimes \mathbb{C}^d$:

$$M = \sum_{a=1}^{k} \sum_{i=1}^{d}$$



This map satisfies the following equations:





Here the last equation can be understood as a modified λ-equation[1]. Restricting $\mathbf{QDesign}_{RU}$ to objects of this form, one gets a category that has objects that are 1-uniform and k-regular quantum designs of degree 2 where $\Lambda = \{\frac{1}{d}, 0\}$, i.e. k MUBs in dimension d. □

This theorem can also be formulated in terms of collections of MASAs. However, to the present author's knowledge, these objects have not yet been established in the language of category theory.

A widely-discussed topic is the existence of MUBs in non-primepower dimensions. One can ask, if it is possible to extend the functor Q to a functor $\widetilde{Q} : \mathbf{BDesign}[\mathbf{Mat}(\mathbb{N}), \mathbf{FSet}] \to \mathbf{MUB}$ that maps a classical design to a set of MUBs. Since the domain of the functor is given by the category of BIBDs, this would be mean that $\widetilde{Q}$ needs to map the λ-condition in $\mathbf{BDesign}[\mathbf{Mat}(\mathbb{N}), \mathbf{FSet}]$ to the modified λ-condition in $\mathbf{MUB}$. It is unclear, if and how that works. A more promising approach would be to define $\widetilde{Q}$ on a category of *resolvable* BIBDs, as the incidence structure underlying a set of k MUBs is also a resolvable BIBD. However, such a category remains to be established.

4.3.3 Combinatorial Quantum Channels

Quantum channels are modelled by completely positive trace-preserving maps ([10], p. 246). In light of the previous discussions, the question arises, how the CP-maps representing quantum designs relate to quantum channels.

[1] In fact, this is because the design has degree 2 and hence there are two parameters for λ.

Theorem 4.7.3. *[37] Every 1-uniform and r-regular quantum design in* $\mathbf{QDesign_{RU}}$, *which has the form* $S : H \otimes H^* \to K \otimes K^*$, *defines a quantum channel.*

Proof. By definition, S is completely positive. Applying the uniformity condition to $S(\rho)$, where ρ is an arbitrary state in $H \otimes H^*$, shows that S is also trace-preserving. □

This motivates the following definition:

Definition 4.8. A *combinatorial quantum channel* is a 1-uniform, r-regular quantum design in $\mathbf{QDesign_{RU}}$ having the form $S : H \otimes H^* \to K \otimes K^*$.

It is easy to verify that the following equation holds:

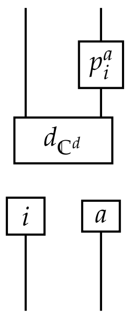
$$\dim(H) = r \cdot \dim(K). \tag{4.3}$$

Example 1. Consider the Pauli channel $\Lambda : \mathcal{M}_2(\mathbb{C}) \to \mathcal{M}_2(\mathbb{C})$, $\Lambda(\rho) = \sum_{i=0}^{3} p_i \sigma_i \rho \sigma_i$, where $\sum_{i=0}^{3} p_i = 1$ and ρ is an arbitrary density matrix in $\mathcal{M}_2(\mathbb{C})$. This is a combinatorial quantum channel with parameters $v = 2 = b$ and $k = 1 = r$.

Another example can actually be constructed from the category-theoretical description of MUB's:

Example 2. Let $A_1 = \{p_1^1, ...p_d^1\}, ..., A_k = \{p_1^k, ..., p_d^k\}$ be a set of k MUBs is $\mathbb{C}^d$ and consider the CP-map $\widetilde{M} := M^\dagger : \mathbb{C}^d \otimes \mathbb{C}^d \to \mathbb{C}^{k \cdot d} \cong \mathbb{C}^d \otimes \mathbb{C}^k$:

$$\widetilde{M} = \sum_{a=1}^{k} \sum_{i=1}^{d}$$



This map is trace preserving and completely positive and hence defines a combinatorial superoperator with parameters $d, d \cdot k, k$.

4.4 Further Discussions

This section aims to put the category theoretical notion of quantum designs into an algebraic picture and thus links this chapter to Chapter 3, ultimately discussing 2-unitaries in a design-theoretic context.

4.4.1 Combinatorial Superoperators

The CP-maps representing quantum designs can be taken out of the category-theoretical context and can be discussed in an algebraic way. In fact, every CP-map describes a superoperator satisfying certain symmetries. Dropping the requirement for the superoperator to be completely positive, one gets a more generalised description:

Definition 4.9. An operator $S \in \mathcal{L}(B) \otimes \mathcal{L}(V)^*$ (or equivalently a map $S : \mathcal{L}(B) \to \mathcal{L}(V)$), where V and B are Hilbert spaces of dimension v and b respectively, is called a *combinatorial superoperator* with parameters $v, b, k, r, \lambda \in \mathbb{R}$, if there exist bases $\{|\beta_i\rangle_B\}_{\beta_i \in [b]} \in B$ and $\{|\nu_j\rangle\}_{\nu_j \in [v]} \in V$, such that for $|\Phi_b\rangle = \sum_{i=0}^{b-1} |ii\rangle$ and $|\Phi_v\rangle = \sum_{j=0}^{v-1} |jj\rangle$[2] the following holds:

- uniformity:

$$S |\Phi_b\rangle = r \cdot |\Phi_v\rangle \tag{4.4}$$

- regularity:

$$\langle \Phi_v | S = k \cdot \langle \Phi_b | \tag{4.5}$$

- λ-condition:

$$S \cdot S^\dagger = \lambda \sum_{\substack{i,j=0, \\ i \neq j}}^{v-1} |ii\rangle \langle jj| + r \cdot \mathbb{I}_v. \tag{4.6}$$

This generalises the concept of block designs.

Proposition 4.9.1. *The parameters of a combinatorial superoperator relate via the following equations:*

$$v \cdot r = b \cdot k \tag{4.7}$$

$$\lambda \cdot (v-1) = r \cdot (k-1) \tag{4.8}$$

[2] These are vectorizations of the trace operators.

Proof. In order to prove the first equation, apply $\langle\Phi_v|$ from the left to the uniformity condition and $|\Phi_b\rangle$ from the right to the regularity condition. One then gets on the one hand

$$\langle\Phi_v| \, S \, |\Phi_b\rangle = r \cdot \langle\Phi_v|\Phi_v\rangle = r \cdot v$$

and on the other:

$$\langle\Phi_v| \, S \, |\Phi_b\rangle = k \cdot \langle\Phi_b|\Phi_b\rangle = k \cdot b.$$

But then:

$$k \cdot b = r \cdot v.$$

The second equation can be proven as follows:

$$\begin{aligned}\langle\Phi_v| \, S \cdot S^\dagger \, |\Phi_v\rangle &= \lambda \sum_{m,n=0}^{v-1} \sum_{i,j=0, i\neq j}^{v-1} \langle nn|ii\rangle\langle jj|mm\rangle + r \cdot v \\ &= \lambda \cdot v(v-1) + r \cdot v.\end{aligned}$$

On the other hand one has:

$$\langle\Phi_v| \, S \cdot S^\dagger \, |\Phi_v\rangle = k \, \langle\Phi_v| \, S \, |\Phi_b\rangle = k \cdot r\langle\Phi_v|\Phi_v\rangle = k \cdot r \cdot v.$$

It follows:

$$\lambda \cdot v(v-1) + r \cdot v = r \cdot k \cdot v \Longleftrightarrow \lambda \cdot (v-1) = r \cdot (k-1).$$

□

From Proposition 4.9.1 it is immediate that a combinatorial superoperator with $v = b$ automatically fulfils $r = k$.

In terms of matrix algebras, a combinatorial superoperator can be described as a map $S : \mathcal{M}_b(\mathbb{C}) \to \mathcal{M}_v(\mathbb{C})$, i.e. as an element of $\mathcal{M}_b(\mathbb{C}) \otimes \mathcal{M}_v(\mathbb{C})^*$. The following example shows that there exist superoperators that encode quantum designs according to Zauner's notion with parameters $v, b, k, r, \lambda \in \mathbb{R}$. This coincides with Theorem 4.7.1.

Example 1. Consider the combinatorial superoperator $S = \sum_{i=1}^{v} |ii\rangle \otimes \langle p_i| \in \mathcal{M}_b(\mathbb{C}) \otimes \mathcal{M}_v(\mathbb{C})^*$ with parameters $v, b, k, r, \lambda \in \mathbb{R}$, where $p_i = p_i^2 = p_i^\dagger \in \mathcal{M}_b(\mathbb{C})$. Now the following holds:

i) $S|\Phi_b\rangle = r|\Phi_v\rangle \Leftrightarrow \mathrm{tr}(p_i) = r$

ii) $\langle\Phi_v| S = k\langle\Phi_b| \Leftrightarrow \sum_{i=1}^{v} p_i = k\mathbb{I}_b$

iii) $S \cdot S^\dagger = \lambda \sum_{i,j=1,i\neq j}^{v} |ii\rangle\langle jj| + r\mathbb{I}_v \Leftrightarrow \mathrm{tr}(p_i p_j) = \lambda$ for $i \neq j$.

The following example coincides with Theorem 4.7.2:

Example 2. Consider the combinatorial superoperator $M : \mathcal{M}_d(\mathbb{C}) \to \mathcal{M}_{d\cdot k}(\mathbb{C})$, $M = \sum_{a=1}^{k}\sum_{i=1}^{d} |ia\rangle \otimes \langle p_i^a|$ with parameters $v = d, b = d\cdot k, k, r = 1, \lambda = 1/d$, where the operators $p_i = p_i^2 = p_i^\dagger \in \mathcal{M}_d(\mathbb{C})$ correspond to a set of k MUBs. If $k = d+1$, this gives a complete set of MUB's. One finds:

i) $M|\Phi_d\rangle = |\Phi_{k\cdot d}\rangle$

ii) $\langle\Phi_{k\cdot d}| M = k\langle\Phi_d|$

iii) $M \cdot M^\dagger = \frac{1}{d}\sum_{a,b=1,a\neq b}^{k}\sum_{i,j=1}^{d} |ia\rangle\langle jb| + \mathbb{I}_{k\cdot d}$

4.4.2 Perfect Tensors as Combinatorial Superoperators

A question that arises immediately is, if this framework also encompasses 2-unitaries. This question will be addressed in the following.

Proposition 4.9.2. *A 2-unitary $U = \sum_{i,j=0}^{d-1} |L_{ij}K_{ij}\rangle\langle ij| \in U(d^2)$, where the $|L_{ij}K_{ij}\rangle$ forms an idempotent*[3] *OLS(d) is a combinatorial superoperator with values $v = d^2 = b$, $k = 1 = r$ and $\lambda = 0$.*

Proof. Let $U = \sum_{i,j=0}^{d-1} |L_{ij}K_{ij}\rangle\langle ij| \in U(d^2)$ be a 2-unitary, where $L_{ij}K_{ij}$ forms an OLS(d). Denote $|\Phi\rangle = \sum_{m=0}^{d-1}|mm\rangle$ and assume that the OLS is idempotent. Then the following holds:

i) $U|\Phi\rangle = \sum_{m=0}^{d-1}|L_{mm}K_{mm}\rangle = |\Phi\rangle$

ii) $U^\dagger|\Phi\rangle = \sum_{i,j,m=0}^{d-1}\langle L_{ij}K_{ij}|mm\rangle|ij\rangle = \sum_{i,j,m=0}^{d-1}\delta_{L_{ij},m}\delta_{K_{ij},m}|ij\rangle = |\Phi\rangle$

iii) $UU^\dagger = \mathbb{I}_{d^2}$.

□

[3] That means that the main diagonal of the OLS is given by $(00, 11, ..., dd)$.

Example 3. The 2-unitary permutation from Example 4, which can be obtained from an idempotent OLS(4), is combinatorial superoperator with values $v = 16 = b$, $k = 1 = r$ and $\lambda = 0$.

In the more general case, where one assumes that the OLS is not necessarily idempotent, the following holds:

i) $U\left|\Phi\right\rangle = \sum_{m=0}^{d-1}\left|L_{mm}K_{mm}\right\rangle = \sum_{l\in \mathrm{diag}(L),k\in \mathrm{diag}(K)}\left|lk\right\rangle$

ii) $U^{\dagger}\left|\Phi\right\rangle = \sum_{i,j,m=0}^{d-1}\langle L_{ij}K_{ij}|mm\rangle\left|ij\right\rangle = \sum_{i,j,m=0}^{d-1}\delta_{L_{ij},m}\delta_{K_{ij},m}\left|ij\right\rangle$

iii) $UU^{\dagger} = \mathbb{I}_{d^2}$.

Thus, one can reproduce the state $\left|\Phi\right\rangle = \sum_{m=0}^{d-1}\left|mm\right\rangle$ only up to a permutation.

How does the situation change if one assumes that U corresponds to a QOLS(d) that is not isomorphic to a permutation? In this case, the construction might fail, as the following example shows:

Example 4. The 36-dimensional 2-unitary corresponding to the sparse solution of Theorem 3.0.5 does not correspond to a combinatorial superoperator. Indeed, applying $U_{\Lambda_{sparse}}$ to $\left|\Phi\right\rangle = \sum_{m=0}^{6}\left|mm\right\rangle$ gives:

$$\begin{aligned} U_{\Lambda_{sparse}}\left|\Phi\right\rangle = \frac{1}{6}\Big(&\omega_3^2, 3\omega_3, -\omega_3+2, -3\omega_3+3, -\omega_3+2, 3\omega_3, 3\omega_3-3, \omega_3^2, 3, \\ &\omega_3^2, 3\omega_3-3, 2\omega_3-1, \omega_3^2, -3, \omega_3^2, -3\omega_3+3, 2\omega_3-1, \\ &-3\omega_3+3, 3\omega_3-3, -\omega_3+2, -3\omega_3, \omega_3^2, -3\omega_3, -\omega_3+2, \omega_3^2, \\ &-3\omega_3+3, 2\omega_3-1, -3\omega_3+3, \omega_3^2, -3, 3\omega_3-3, 2\omega_3-1, \\ &3\omega_3-3, \omega_3^2, 3, \omega_3^2\Big). \end{aligned}$$

This expression cannot be transformed into $\left|\Phi\right\rangle = \sum_{m=0}^{6}\left|mm\right\rangle$.

5 Conclusion

This chapter gives a brief summary of the main results that were attained in the course of the thesis. Moreover, it addresses some questions that remain open and might be interesting for future work. While the central focus of this thesis laid on perfect tensors and finding possible construction schemes, a significant part of the thesis was also devoted to study general combinatorial notions in the language of category theory. In doing that, the aim was to gain a better understanding of quantum combinatorial objects and their relation to each other.

One question, posed in the beginning of this thesis, was, if the combinatorial aspects of quasi-orthogonal systems of subalgebras of matrix algebras that have been widely discussed in the works of Ohno, Weiner and Petz in Refs. [88, 114, 93, 92] can be extended to perfect tensors. This question was addressed in Chapter 3. Here perfect tensors were discussed from multiple angles, beginning with a matrix-algebraic perspective on perfect tensors in Section 3.1. It was shown that the existence of a perfect tensor is equivalent to the existence of four mutually quasi-orthogonal factors of $\mathcal{M}_{d^2}(\mathbb{C})$ isomorphic to $\mathcal{M}_d(\mathbb{C})$. Furthermore, it was shown that this equivalence does not hold for k-unitaries and k quasi-orthogonal subalgebras of $\mathcal{M}_{d^k}(\mathbb{C})$ isomorphic to $\mathcal{M}_d(\mathbb{C})$: While the existence of a k-unitary implies the existence of k quasi-orthogonal subalgebras, the other direction does not hold. Here a specific counterexample was given for the case $d^3 = 27$. This answered the question how perfect tensors are related to systems of quasi-orthogonal subalgebras of matrix algebras, namely via four mutually quasi-orthogonal factors of $\mathcal{M}_{d^2}(\mathbb{C})$. These results somehow contrast with the algebraic k-nets defined by Nietert et al. that are related to mutually quasi-orthogonal MASAs of $\mathcal{M}_{d^2}(\mathbb{C})$ [86]. If and how these two concepts are related, remains an open question, that could reveal more insights on the problem of constructing MUBs and which role perfect tensors play in that matter. Moreover, one could ask how k-unitaries are related to MOQLS and hence how MOQLS are related to quasi-orthogonal systems of matrix algebras.

Building on this, this equivalence was put in the more abstract framework of groups and representations in Section 3.2 in trying to answer the question how perfect tensors can be described group-theoretically. Here the existence of a 2-unitary was related to the existence of a group G with a d^2-dimensional irreducible representation and four subgroups on which the representation is also irreducible with multiplicity d and on which the respective character factorises (see Prop. 3.0.5). As an explicit example of such a group nice error bases were discussed, and it was shown that 2-unitaries can only be elements of the Clifford group for dimensions that are not congruent to 2 mod 4, ruling out the existence of 36-dimensional Clifford 2-unitaries. Moreover, a search algorithm implemented in the algebra software GAP was presented that was used to look for groups that satisfy the criteria from Prop. 3.0.5. While this algorithm could reproduce the already known example, it could not find any other example within the GAP's SmallGroups library for groups up to order 1000. This left out a part of the library that remains to be explored. This could either be done by trying to improve the computational complexity of the search algorithm or by using more computational power. Moreover, as the library is limited to certain groups, there also might be other groups that satisfy the criteria that are not in the library. Hence the problem of finding groups that satisfy criteria from Prop. 3.0.5 other than WH-group, or ruling out their existence remains open.

The objective of making existence statements about perfect tensors in arbitrary dimension was discussed in the third part of the chapter, Section 3.3. Here construction schemes for perfect tensors from doubly perfect sequences for all dimensions that are of the form 2^m, 2^{2m} or d^n, where m and d are odd integers greater than 1 and n is an arbitrary integer greater than 1, were presented. These lead to 2-unitaries in dimension 2^{2m}, 2^{4m} and d^{2n}, respectively, providing an entire new way to construct perfect tensors in these dimensions. Moreover, an analytic solution for $d^2 = 36$ was constructed, using Rather's bi-unimodular doubly perfect sequence ansatz and the Chinese remainder theorem, yielding two 2-unitaries in dimension $d^2 = 36$: a sparse and a symmetric 2-unitary. These 2-unitaries can not only be obtained without using any numerical tools, they also have some interesting aspects to them that distinguish them from the computer found solution in Ref. [99], e.g. both 2-unitaries have order 3 and the absolute value of all entries is equal to 1. Moreover, it was shown that these 2-unitaries can be decomposed into a direct sum of one 9-dimensional 2-unitary and three 9-dimensional dual unitaries.

In the final section of Chapter 3, the minimal order of 2-unitaries in dimensions $d^2 = 9, 16, 25, 36$ was discussed. Here it was observed that in dimensions 16 and 25, the minimal order of 2-unitaries equals 2, whereas in dimensions 9 and 36, the smallest order identified so far is 3. It would be interesting to know, if there are 2-unitaries in dimension 9 and 36 that have order 2. Moreover, the relation between a quasi-orthogonal decomposition of $\mathcal{M}_9(\mathbb{C})$ into factors and different 2-unitaries in dimension 9 was discussed, showing that four 2-unitaries, of which 2 are unitarily equivalent, can be used to generate such a decomposition by conjugating the local algebras $\mathcal{L}$ and $\mathcal{R}$. Given that the decomposition consists of 10 factors, where two of them correspond to the two local algebras, one could ask how many (inequivalent) 2-unitaries are needed in general to generate such a decomposition.

Another question that was posed in the introduction was, if one can generalise the category theoretical description of classical and quantum block designs derived in Ref. [36] to a more general construction scheme that can be applied to any monoidal pointed category. Answering this question was the central objective of chapter 4. Here a category-theoretical framework based on arrow categories, called the design construction, that generalises both quantum and classical block designs by transferring the essential properties of block designs into a pointed monoidal dagger category was introduced. It was shown that applying this framework to the categories $\mathbf{Mat}(\mathbb{N})$ and $\mathbf{CP}[\mathbf{FHilb}]$ yields a categorical representation of block designs and quantum designs, respectively, which can be connected via a functor. Furthermore, the more abstract notion of categorical block designs was derived, which gave a new way to look at quantum designs. In fact, this construction generalises the notion of quantum designs given by Zauner to a notion of quantum designs that could also be understood as combinatorial superoperators. Furthermore, it was shown, that one can define a category of MUBs and a category of so-called combinatorial quantum channels, using these techniques. In the last section of the chapter, these findings were then reformulated in the language of matrix algebras and it was discussed how perfect tensors can be put into this framework. This, however, did not yield particularly significant results. There are several open questions that could be worth further exploration. For example, given that SIC-POVMs can also be described in a design-theoretic way, it would be interesting to know, if one can define a category of SIC-POVMs similarly to the category of MUBs. This could give new structural insights on SIC-POVMs and their relation to other combinatorial structures. Another open problem is given by defining a category of *resolvable* BIBDs, which would encompass a broader class of block designs, and checking if this category can be mapped to the category of MUBs via a functor. This could lead to new insights on the existence problem of MUBs and would make the category-theoretical framework of classical designs more complete. In this context, it would also be worth exploring, if and how the already existing categorical notions of (quantum) Latin squares can be embedded into the design construction. Finally, finding interesting examples of combinatorial superoperators/quantum channels (if there are any) and investigating how the design construction relates to classical channels also remains to be done.

Overall, the results of this thesis contribute partial but meaningful answers to the questions that were raised in the introduction. By discussing well known combinatorial structures in the language of matrix algebras, group theory and category theory, the thesis gave some new insights on the diverse connections between classical combinatorics and quantum combinatorial objects and even providing a more generalised view on them in the language of category theory. These findings could be interesting in the quest of establishing a unified framework of classical and quantum combinatorics that not only encompass quantum designs but also QLS, perfect tensors, k-unitaries and QOA and from which classical combinatorics would emerge as a special (commutative) case.

List of Abbreviations

AME	**A**bsolutely **M**aximally **E**ntangled
BIBD	**B**alanced **I**ncomplete **B**lock **D**esign
MOLS	**M**utually **O**rthogonal **L**atin **S**quares
LS	**L**atin **S**quare
OLS	**O**rthogonal **L**atin **S**quare
OA	**O**rthogonal **A**rray
MUB	**M**utually **U**nbiased **B**asis
POVM	**P**ositive **O**perator **V**alued **M**easure
SIC-POVM	**S**ymmetric **I**nformationally **C**omplete POVM
MASA	**M**aximal **A**belian **S**ub **A**lgebra
QOA	**Q**uantum **O**rthogonal **A**rray
QLS	**Q**uantum **L**atin **S**quare
QOLS	**Q**uantum **O**rthogonal **L**atin **S**quare
†-SCFA	**D**agger **S**pecial **C**ommutative **F**robenius **A**lgebras

List of Symbols

H	Hilbert space
H^*	Dual Hilbert space
$L(H)$	Hilbert space of bounded linear operators
$U(H), U(n)$	Unitary group over a Hilbert space H of dimension n
$GL(V)$	General linear group over a vector space V
ω	Root of unity
$\mathcal{A}, \mathcal{L}, \mathcal{R}, \mathcal{M}$	(Sub)algebras
$\mathbf{1}$	Identity element of an algebra
$\mathcal{M}_d(\mathbb{C})$	Matrix algebra over complex numbers
$\mathbb{C}\mathbf{1}$	Subalgebra generated by all diagonal matrices
$\mathcal{C}, \mathcal{D}$	Categories
$\mathcal{F}, \mathcal{G}$	Functors
id	Identity morphism
η	Natural transformation or unit of a monoid
μ	Multiplication of a monoid
ϵ	Counit of a comonoid or root of unity
Δ	Comultiplication of a comonoid
$\mathcal{F}(\cdot)$	Fourier transform
$\mathbb{F}, \mathbb{K}$	Fields
X	Incidence matrix
$\mathbb{I}$	Identity matrix or tensor unit (in a monoidal category)
J	Matrix generating the symplectic product
E	All-one-matrix
$\mathrm{diag}(\cdot)$	Diagonal matrix
S	SWAP gate
CX	Controlled X-gate
CZ	Controlled Z-gate
F	Fourier gate
$\mathrm{Tr}(\cdot), \mathrm{tr}(\cdot)$	Trace

$\tau(\cdot)$	Normalised trace
$\langle\cdot,\cdot\rangle, (\cdot,\cdot)$	Inner product
$\|\|\cdot\|\|_p$	p-norm
δ_{ij}	Kronecker delta
$\langle\cdot\rangle$	Span of elements of an algebra/a vector space
$\mathbf{a}, \mathbf{b}$	Vectors
$\mathbb{Z}_d$	Cyclic group of order d
$[G : K]$	Index of the subgroup K in a group G
χ	Character afforded by a representation
ρ, π	Representations
v, b, k, r, λ	Parameters of a BIBD
Λ	Bi-unimodular sequence
$\otimes, \boxtimes$	Tensor product (in a category)
$\times$	Cartesian product
$\star$	Convolution product
$[d]$	All numbers from 0 to $d-1$

A Additional Material for Section 3.1, Chapter 3

In the following some additional material to Chapter 3, Section 3.1 will be provided.

A.1 Alternative proof for Theorem 3.0.2:

Consider two arbitrary operators $p_{\mathcal{L}} = \sqrt{d}\sum_{i,j=0}^{d} e_{ij} \otimes \mathbb{I} \in \mathcal{L}$ and $p_{\mathcal{A}} = \sqrt{d}\sum_{i,j=0}^{d} U(e_{ij} \otimes \mathbb{I})U^{\dagger} \in \mathcal{A}_L$. In order for $\mathcal{L}$ and $\mathcal{A}_L$ to be quasi-orthogonal, the trace needs to factorise in such that:

$$\frac{1}{d^2}\mathrm{tr}(p_{\mathcal{A}}p_{\mathcal{L}}) = \frac{1}{d^4}\mathrm{tr}(p_{\mathcal{L}})\mathrm{tr}(p_{\mathcal{A}})$$

The left hand side is equal to:

$$\frac{1}{d^2}\mathrm{tr}(p_{\mathcal{A}}p_{\mathcal{L}}) = \frac{1}{d}\sum_{i,j,k,l=0}^{d} \mathrm{tr}(U(e_{kl} \otimes \mathbb{I})U^{\dagger}(e_{ij} \otimes \mathbb{I})) \tag{A.1}$$

This trace has already been computed in the proof of Theorem 3.0.1. Using this one arrives at:

$$\frac{1}{d}\mathrm{tr}(p_{\mathcal{L}}p_{\mathcal{A}}) = \frac{1}{d}\sum_{i,j,k,l=1}^{d} U^R(U^R)^{\dagger})_{kj}^{li}. \tag{A.2}$$

The right hand side will be computed in the following:

$$
\begin{aligned}
\frac{1}{d^4}\mathrm{tr}(p_{\mathcal{L}})\mathrm{tr}(p_{\mathcal{A}}) &= \frac{1}{d^3}\sum_{i,j=0}^{d}\mathrm{tr}((e_{ij}\otimes \mathbb{I}))\sum_{k,l=0}^{d}\mathrm{tr}(U(e_{kl}\otimes \mathbb{I})U^{\dagger}) \\
&= \frac{1}{d^2}\sum_{i,j=0}^{d}\mathrm{tr}(|i\rangle\langle j|)\sum_{k,l=0}^{d}\mathrm{tr}(U(|k\rangle\langle l|\otimes\sum_{r=0}^{d}|r\rangle\langle r|)U^{\dagger}) \\
&= \frac{1}{d}\sum_{k,l,r=0}^{d}\mathrm{tr}(U|kr\rangle\langle lr|U^{\dagger}) \\
&= \frac{1}{d}\sum_{k,l,r=0}^{d}\sum_{m,t=0}^{d}\langle mt|U|kr\rangle\langle lr|U^{\dagger}|mt\rangle \\
&= \frac{1}{d}\sum_{k,l,r=0}^{d}\sum_{m,t=0}^{d}U^{mt}_{kr}(U^{\dagger})^{lr}_{mt} \\
&= \frac{1}{d}\sum_{k,l,r=0}^{d}(UU^{\dagger})^{lr}_{kr}
\end{aligned}
$$

But since U is a d^2-dimensional unitary this equals to:

$$\sum_{k,l,r=0}^{d}(UU^{\dagger})^{lr}_{kr} = d^2. \tag{A.3}$$

One thus finds that the following has to hold:

$$\sum_{i,j,k,l=1}^{d}(U^{R}(U^{R})^{\dagger})^{li}_{kj} = d^2. \tag{A.4}$$

On the other hand one has:

$$\sum_{i,j,k,l=1}^{d}|U^{R}(U^{R})^{\dagger})^{li}_{kj}|^2 = d^2. \tag{A.5}$$

Therefore, if $\mathcal{L}$ and $\mathcal{A}$ are quasi-orthogonal, the following equation has to be satisfied:

$$\sum_{i,j,k,l=1}^{d}(U^{R}(U^{R})^{\dagger})^{li}_{kj} = \sum_{i,j,k,l=1}^{d}|U^{R}(U^{R})^{\dagger})^{li}_{kj}|^2 = d^2. \tag{A.6}$$

But this is only possible, if $(U^R(U^R)^\dagger)^{li}_{kj}$ equals to either 0 or 1 for all i, j, k, l. Since the sum equals to d^2 there have to be d^2 1's and because the Schatten norm is invariant under unitary transformations, one can conclude that $U^R(U^R)^\dagger$ has to be the identity matrix in dimension d^2 and thus U^R is unitary.

A.2 Additional Calculations to Theorem 3.0.3

I. Trace condition for $\mathcal{A}_R$ and $\mathcal{R}$

Let

$$P_{\mathcal{R}} = d \sum_{i,j=1}^{d} |\mathbb{I}_{d^2} \otimes E_{ij}\rangle \langle \mathbb{I}_{d^2} \otimes E_{ij}|$$

the projection onto the right subalgebra and

$$P_{U\mathcal{R}U^\dagger} = d \sum_{i,j=1}^{d} |U(\mathbb{I}_{d^2} \otimes E_{ij})U^\dagger\rangle \langle U(\mathbb{I}_{d^2} \otimes E_{ij})U^\dagger|$$

be the projection onto $\mathcal{A}_R$. Compute:

$$\begin{aligned}
\mathrm{Tr}(P_{U\mathcal{R}U^\dagger} P_{\mathcal{R}}^\dagger) &= d^2 \sum_{i,j,k,l=1}^{d} |\langle (U\mathbb{I}_{d^2} \otimes E_{ij}U^\dagger)|\mathbb{I}_{d^2} \otimes E_{kl}\rangle|^2 \\
&= d^2 \sum_{i,j,k,l=1}^{d} |\tau\big((U\mathbb{I}_{d^2} \otimes E_{ij}U^\dagger)(\mathbb{I}_{d^2} \otimes E_{kl})\big)|^2 \\
&= d^2 \sum_{i,j,k,l=1}^{d} |\frac{1}{d^3}\mathrm{tr}\big((U\mathbb{I}_{d^2} \otimes E_{ij}U^\dagger)(\mathbb{I}_{d^2} \otimes E_{kl})\big)|^2 \\
&= \frac{1}{d^4} \sum_{i,j,k,l=1}^{d} |\mathrm{tr}\big((U\mathbb{I}_{d^2} \otimes E_{ij}U^\dagger)(\mathbb{I}_{d^2} \otimes E_{kl})\big)|^2.
\end{aligned}$$

Further compute:

$$\begin{aligned}
\operatorname{tr}\Big((U\mathbb{I}_{d^2}\otimes E_{ij}U^\dagger)(\mathbb{I}_{d^2}\otimes E_{kl})\Big) &= \operatorname{tr}\Big(\sum_{r,s,t,u=1}^{d}(UE_{tt}\otimes E_{rr}\otimes E_{ij}U^\dagger)(E_{uu}\otimes E_{ss}\otimes E_{kl})\Big)\\
&= \operatorname{tr}\Big(\sum_{r,s,t,u=1}^{d} U\,|tri\rangle\,\langle trj|\,U^\dagger\,|usk\rangle\,\langle usl|\Big)\\
&= \sum_{r,s,t,u=1}^{d}\langle usl|\,U\,|tri\rangle\,\langle trj|\,U^\dagger\,|usk\rangle\\
&= \sum_{r,s,t,u=1}^{d} U^{usl}_{tri}(U^\dagger)^{trj}_{usk}\\
&= \sum_{r,s,t,u=1}^{d} U^{usl}_{tri}(U^*)^{usk}_{trj}. \qquad \text{(A.7)}
\end{aligned}$$

Line (A.7) can be transformed in various ways:

$$\begin{aligned}
(A.7) &= \sum_{r,s,t,u=1}^{d}(U^{R_{1,6}})^{isl}_{tru}(U^{R_{1,6}*})^{jsk}_{tru}\\
&= \sum_{r,s,t,u=1}^{d}(U^{R_{1,6}})^{isl}_{tru}((U^{R_{1,6}})^\dagger)^{tru}_{jsk}\\
&= \sum_{s=1}^{d}(U^{R_{1,6}}(U^{R_{1,6}})^\dagger)^{isl}_{jsk},
\end{aligned}$$

or, analogously,

$$\begin{aligned}
(A.7) &= \sum_{r=1}^{d}(U^{R_{3,4}}(U^{R_{3,4}})^\dagger)^{krj}_{lri},\\
(A.7) &= \sum_{t=1}^{d}(U^{R_{3,5}}(U^{R_{3,5}})^\dagger)^{tkj}_{tli},\\
(A.7) &= \sum_{u=1}^{d}(U^{R_{2,6}}(U^{R_{2,6}})^\dagger)^{uil}_{ujk}.
\end{aligned}$$

With that one gets:

$$\mathrm{Tr}(P_{U\mathcal{L}U^\dagger}P_{\mathcal{L}}^\dagger) = \frac{1}{d^4}\sum_{i,j,k,l=1}^{d}\left\{\begin{array}{l} |\sum_{s=1}^{d}(U^{R_{1,6}}(U^{R_{1,6}})^\dagger)_{jsk}^{isl}|^2 \\ |\sum_{r=1}^{d}(U^{R_{3,4}}(U^{R_{3,4}})^\dagger)_{lri}^{krj}|^2 \\ |\sum_{t=1}^{d}(U^{R_{3,5}}(U^{R_{3,5}})^\dagger)_{tli}^{tkj}|^2 \\ |\sum_{u=1}^{d}(U^{R_{2,6}}(U^{R_{2,6}})^\dagger)_{ujk}^{uil}|^2 \end{array}\right.$$

$$= \frac{1}{d^4}\sum_{i,j,k,l=1}^{d}\left\{\begin{array}{l} \left|\left(\mathrm{tr}_2\left(U^{R_{1,6}}(U^{R_{1,6}})^\dagger\right)\right)_{jk}^{il}\right|^2 \\ \left|\left(\mathrm{tr}_2\left(U^{R_{3,4}}(U^{R_{3,4}})^\dagger\right)\right)_{kj}^{li}\right|^2 \\ \left|\left(\mathrm{tr}_1\left(U^{R_{3,5}}(U^{R_{3,5}})^\dagger\right)\right)_{kj}^{li}\right|^2 \\ \left|\left(\mathrm{tr}_1\left(U^{R_{2,6}}(U^{R_{2,6}})^\dagger\right)\right)_{jk}^{il}\right|^2 \end{array}\right.$$

$$= \frac{1}{d^2}\left\{\begin{array}{l} \left\|\mathrm{tr}_2\left(U^{R_{1,6}}(U^{R_{1,6}})^\dagger\right)\right\|_2^2 \\ \left\|\mathrm{tr}_2\left(U^{R_{3,4}}(U^{R_{3,4}})^\dagger\right)\right\|_2^2 \\ \left\|\mathrm{tr}_1\left(U^{R_{3,5}}(U^{R_{3,5}})^\dagger\right)\right\|_2^2 \\ \left\|\mathrm{tr}_1\left(U^{R_{2,6}}(U^{R_{2,6}})^\dagger\right)\right\|_2^2 \end{array}\right.$$

II. Trace condition for $\mathcal{A}_R$ and $\mathcal{M}$

Next, the aim is to compute $\mathrm{Tr}(P_{U\mathcal{R}U^\dagger}P_{\mathcal{M}}^\dagger)$. The calculation proceeds as in the beginning of this proof. Compared to Eq. (A.7), the indices l and k are in the third position, instead of in the first position. One finds:

$$\begin{aligned}
\mathrm{Tr}(P_{U\mathcal{R}U^\dagger}P^\dagger_{\mathcal{M}}) &= \frac{1}{d^4}\sum_{i,j,k,l=1}^{d} |\mathbf{tr}\big((U\mathbb{I}_{d^2}\otimes E_{ij}U^\dagger)(\mathbb{I}_d\otimes E_{kl}\otimes \mathbb{I}_d)\big)|^2 \\
&= \frac{1}{d^4}\sum_{i,j,k,l=1}^{d} |\mathbf{tr}\big(\sum_{r,s,u,t=1}^{d}(UE_{rr}\otimes E_{tt}\otimes E_{ij}U^\dagger)(E_{ss}\otimes E_{kl}\otimes E_{uu})\big)|^2 \\
&= \frac{1}{d^4}\sum_{i,j,k,l=1}^{d} |\mathbf{tr}\big(\sum_{r,s,u,t=1}^{d} U\left|rti\right\rangle\left\langle rtj\right| U^\dagger \left|sku\right\rangle\left\langle slu\right|\big)|^2 \\
&= \frac{1}{d^4}\sum_{i,j,k,l=1}^{d} |\sum_{r,s,t,u=1}^{d} U^{slu}_{rti}(U^*)^{sku}_{rtj}|^2 \qquad \text{(A.8)}
\end{aligned}$$

This expression can be transformed in multiple ways:

$$(A.12) = \frac{1}{d^4}\sum_{i,j,k,l=1}^{d} |\sum_{t=1}^{d}(U^{R_{2,4}}(U^{R_{2,4}})^\dagger)^{ktj}_{lti}|^2,$$

$$(A.12) = \frac{1}{d^4}\sum_{i,j,k,l=1}^{d} |\sum_{u=1}^{d}(U^{R_{1,6}}(U^{R_{1,6}})^\dagger)^{ilu}_{jku}|^2,$$

$$(A.12) = \frac{1}{d^4}\sum_{i,j,k,l=1}^{d} |\sum_{r=1}^{d}(U^{\Gamma_{2,5}}(U^{\Gamma_{2,5}})^\dagger)^{rkj}_{rli}|^2,$$

and

$$(A.12) = \frac{1}{d^4}\sum_{i,j,k,l=1}^{d} |\sum_{s=1}^{d}(U^{\Gamma_{3,6}}(U^{\Gamma_{3,6}})^\dagger)^{sli}_{skj}|^2.$$

This gives us:

$$\mathrm{Tr}(P_{U\mathcal{R}U^\dagger}P^\dagger_{\mathcal{M}}) = \frac{1}{d^2}\begin{cases} ||\mathbf{tr}_1(U^{\Gamma_{3,6}}(U^{\Gamma_{3,6}})^\dagger)||_2^2 \\ ||\mathbf{tr}_1(U^{\Gamma_{2,5}}(U^{\Gamma_{2,5}})^\dagger)||^2 \\ ||\mathbf{tr}_3(U^{R_{1,6}}(U^{R_{1,6}})^\dagger)||_2^2 \\ ||\mathbf{tr}_2(U^{R_{2,4}}(U^{R_{2,4}})^\dagger)||_2^2 \end{cases}.$$

III. Trace condition for $\mathcal{A}_M$ and $\mathcal{M}$

Finally, one has:

$$\begin{aligned}
\mathrm{Tr}(P_{U\mathcal{M}U^\dagger}P_{\mathcal{M}}^\dagger) &= \frac{1}{d^4}\sum_{i,j,k,l=1}^{d} |\mathrm{tr}\big((U\mathbb{I}_d\otimes E_{ij}\otimes \mathbb{I}_d U^\dagger)(\mathbb{I}_d\otimes E_{kl}\otimes \mathbb{I}_d)\big)|^2 \\
&= \frac{1}{d^4}\sum_{i,j,k,l=1}^{d} |\mathrm{tr}\big(\sum_{r,s,u,t=1}^{d}(UE_{rr}\otimes E_{ij}\otimes E_{tt}U^\dagger)(E_{ss}\otimes E_{kl}\otimes E_{uu})\big)|^2 \\
&= \frac{1}{d^4}\sum_{i,j,k,l=1}^{d} |\mathrm{tr}\big(\sum_{r,s,u,t=1}^{d} U\,|rit\rangle\,\langle rjt|\,U^\dagger\,|sku\rangle\,\langle slu|\big)|^2 \\
&= \frac{1}{d^4}\sum_{i,j,k,l=1}^{d} |\sum_{r,s,u,t=1}^{d} U_{rit}^{slu}(U^*)_{rjt}^{sku}|^2 \qquad \text{(A.9)}
\end{aligned}$$

This expression can again be transformed in multiple ways:

$$(A.9) = \frac{1}{d^4}\sum_{i,j,k,l=1}^{d} |\sum_{r=1}^{d}(U^{R_{2,6}}(U^{R_{2,6}})^\dagger)_{ril}^{rjk}|^2,$$

$$(A.9) = \frac{1}{d^4}\sum_{i,j,k,l=1}^{d} |\sum_{t=1}^{d}(U^{R_{2,4}}(U^{R_{2,4}})^\dagger)_{lit}^{kjt}|^2,$$

$$(A.9) = \frac{1}{d^4}\sum_{i,j,k,l=1}^{d} |\sum_{u=1}^{d}(U^{R_{1,5}}(U^{R_{1,5}})^\dagger)_{jku}^{ilu}|^2,$$

and

$$(A.9) = \frac{1}{d^4}\sum_{i,j,k,l=1}^{d} |\sum_{s=1}^{d}(U^{R_{3,5}}(U^{R_{3,5}})^\dagger)_{skj}^{sli}|^2.$$

Hence one is left with:

$$\mathrm{Tr}(P_{U\mathcal{M}U^\dagger}P_{\mathcal{M}}^\dagger) = \frac{1}{d^2}\begin{cases} ||\mathrm{tr}_1(U^{R_{3,5}}(U^{R_{3,5}})^\dagger)||_2^2 \\ ||\mathrm{tr}_3(U^{R_{1,5}}(U^{R_{1,5}})^\dagger)||_2^2 \\ ||\mathrm{tr}_3(U^{R_{2,4}}(U^{R_{2,4}})^\dagger)||_2^2 \\ ||\mathrm{tr}_1(U^{R_{2,6}}(U^{R_{2,6}})^\dagger)||_2^2 \end{cases}.$$

IV. Trace condition for $\mathcal{A}_M$ and $\mathcal{R}$

Next, the aim is to compute $\text{Tr}(P_{U\mathcal{M}U^\dagger}P_{\mathcal{R}}^\dagger)$. The calculation proceeds as in the beginning of this proof. Compared to Eq. (A.7), the indices l and k are in the third position, instead of in the first position. One finds:

$$\begin{aligned}
\text{Tr}(P_{U\mathcal{M}U^\dagger}P_{\mathcal{R}}^\dagger) &= \frac{1}{d^4}\sum_{i,j,k,l=1}^{d} |\text{tr}\big((U\mathbb{I}_d \otimes E_{kl} \otimes \mathbb{I}_d U^\dagger)(\mathbb{I}_{d^2} \otimes E_{ij})\big)|^2 \\
&= \frac{1}{d^4}\sum_{i,j,k,l=1}^{d} |\text{tr}\big(\sum_{r,s,u,t=1}^{d} (UE_{rr} \otimes E_{kl} \otimes E_{tt}U^\dagger)(E_{ss} \otimes E_{uu} \otimes E_{ij})\big)|^2 \\
&= \frac{1}{d^4}\sum_{i,j,k,l=1}^{d} |\text{tr}\big(\sum_{r,s,u,t=1}^{d} U\,|rkt\rangle\,\langle rlt|\,U^\dagger\,|sui\rangle\,\langle suj|\big)|^2 \\
&= \frac{1}{d^4}\sum_{i,j,k,l=1}^{d} |\sum_{r,s,t,u=1}^{d} U_{rkt}^{suj}(U^*)_{rlt}^{sui}|^2 \qquad \text{(A.10)}
\end{aligned}$$

This expression can be transformed in multiple ways:

$$(A.12) = \frac{1}{d^4}\sum_{i,j,k,l=1}^{d} |\sum_{t=1}^{d}(U^{R_{3,4}}(U^{R_{3,4}})^\dagger)_{jkt}^{ilt}|^2,$$

$$(A.12) = \frac{1}{d^4}\sum_{i,j,k,l=1}^{d} |\sum_{u=1}^{d}(U^{R_{1,5}}(U^{R_{1,5}})^\dagger)_{lui}^{kuj}|^2,$$

$$(A.12) = \frac{1}{d^4}\sum_{i,j,k,l=1}^{d} |\sum_{r=1}^{d}(U^{\Gamma_{3,5}}(U^{\Gamma_{3,5}})^\dagger)_{rkj}^{rli}|^2,$$

and

$$(A.12) = \frac{1}{d^4}\sum_{i,j,k,l=1}^{d} |\sum_{s=1}^{d}(U^{\Gamma_{2,5}}(U^{\Gamma_{2,5}})^\dagger)_{sli}^{skj}|^2.$$

This gives us:

$$\text{Tr}(P_{U\mathcal{M}U^\dagger}P_{\mathcal{R}}^\dagger) = \frac{1}{d^2}\begin{cases} ||\text{tr}_3(U^{\Gamma_{3,4}}(U^{\Gamma_{3,4}})^\dagger)||_2^2 \\ ||\text{tr}_1(U^{\Gamma_{2,5}}(U^{\Gamma_{2,5}})^\dagger)||^2 \\ ||\text{tr}_2(U^{R_{1,5}}(U^{R_{1,5}})^\dagger)||_2^2 \\ ||\text{tr}_1(U^{R_{3,5}}(U^{R_{3,5}})^\dagger)||_2^2 \end{cases}.$$

V. Trace condition for $\mathcal{A}_R$ and $\mathcal{L}$

Next, the aim is to compute $\mathrm{Tr}(P_{U\mathcal{R}U^\dagger}P_{\mathcal{L}}^\dagger)$. The calculation proceeds as in the beginning of this proof. Compared to Eq. (A.7), the indices l and k are in the third position, instead of in the first position. One finds:

$$\begin{aligned}
\mathrm{Tr}(P_{U\mathcal{R}U^\dagger}P_{\mathcal{L}}^\dagger) &= \frac{1}{d^4}\sum_{i,j,k,l=1}^{d} |\mathrm{tr}\big((U\mathbb{I}_{d^2}\otimes E_{ij}U^\dagger)(E_{kl}\otimes\mathbb{I}_{d^2})\big)|^2 \\
&= \frac{1}{d^4}\sum_{i,j,k,l=1}^{d} |\mathrm{tr}\big(\sum_{r,s,u,t=1}^{d}(UE_{rr}\otimes E_{tt}\otimes E_{ij}U^\dagger)(E_{kl}\otimes E_{ss}\otimes E_{uu})\big)|^2 \\
&= \frac{1}{d^4}\sum_{i,j,k,l=1}^{d} |\mathrm{tr}\big(\sum_{r,s,u,t=1}^{d} U\,|rti\rangle\,\langle rtj|\,U^\dagger\,|ksu\rangle\,\langle lsu|\big)|^2 \\
&= \frac{1}{d^4}\sum_{i,j,k,l=1}^{d} |\sum_{r,s,t,u=1}^{d} U_{rti}^{lsu}(U^*)_{rtj}^{ksu}|^2 \qquad \text{(A.11)}
\end{aligned}$$

This expression can be transformed in multiple ways:

$$(A.12) = \frac{1}{d^4}\sum_{i,j,k,l=1}^{d} |\sum_{u=1}^{d}(U^{R_{2,6}}(U^{R_{2,6}})^\dagger)_{kju}^{liu}|^2,$$

$$(A.12) = \frac{1}{d^4}\sum_{i,j,k,l=1}^{d} |\sum_{r=1}^{d}(U^{R_{1,5}}(U^{R_{1,5}})^\dagger)_{rli}^{rkj}|^2,$$

$$(A.12) = \frac{1}{d^4}\sum_{i,j,k,l=1}^{d} |\sum_{t=1}^{d}(U^{\Gamma_{1,4}}(U^{\Gamma_{1,4}})^\dagger)_{lti}^{ktj}|^2,$$

and

$$(A.12) = \frac{1}{d^4}\sum_{i,j,k,l=1}^{d} |\sum_{s=1}^{d}(U^{\Gamma_{3,6}}(U^{\Gamma_{3,6}})^\dagger)_{ksj}^{lsi}|^2.$$

This gives us:

$$\mathrm{Tr}(P_{U\mathcal{R}U^\dagger}P_{\mathcal{M}}^\dagger) = \frac{1}{d^2}\begin{cases} ||\mathrm{tr}_2(U^{\Gamma_{3,6}}(U^{\Gamma_{3,6}})^\dagger)||_2^2 \\ ||\mathrm{tr}_2(U^{\Gamma_{1,4}}(U^{\Gamma_{1,4}})^\dagger)||^2 \\ ||\mathrm{tr}_1(U^{R_{1,5}}(U^{R_{1,5}})^\dagger)||_2^2 \\ ||\mathrm{tr}_3(U^{R_{2,6}}(U^{R_{2,6}})^\dagger)||_2^2 \end{cases}.$$

VI. Trace condition for $\mathcal{A}_M$ and $\mathcal{L}$

Next, the aim is to compute $\mathrm{Tr}(P_{U\mathcal{M}U^\dagger}P_{\mathcal{L}}^\dagger)$. The calculation proceeds as in the beginning of this proof. Compared to Eq. (A.7), the indices l and k are in the third position, instead of in the first position. One finds:

$$\begin{aligned}
\mathrm{Tr}(P_{U\mathcal{M}U^\dagger}P_{\mathcal{L}}^\dagger) &= \frac{1}{d^4}\sum_{i,j,k,l=1}^{d} |\mathrm{tr}\big((U\mathbb{I}_d \otimes E_{kl} \otimes \mathbb{I}_d U^\dagger)(E_{ij}\otimes \mathbb{I}_{d^2})\big)|^2 \\
&= \frac{1}{d^4}\sum_{i,j,k,l=1}^{d} |\mathrm{tr}\big(\sum_{r,s,u,t=1}^{d} (UE_{rr} \otimes E_{kl} \otimes E_{tt} U^\dagger)(E_{ij}\otimes E_{uu} \otimes E_{ss})\big)|^2 \\
&= \frac{1}{d^4}\sum_{i,j,k,l=1}^{d} |\mathrm{tr}\big(\sum_{r,s,u,t=1}^{d} U\,|rkt\rangle\,\langle rlt|\,U^\dagger\,|ius\rangle\,\langle jus|\big)|^2 \\
&= \frac{1}{d^4}\sum_{i,j,k,l=1}^{d} |\sum_{r,s,t,u=1}^{d} U_{rkt}^{jus}(U^*)_{rlt}^{ius}|^2 \qquad \text{(A.12)}
\end{aligned}$$

This expression can be transformed in multiple ways:

$$(A.12) = \frac{1}{d^4}\sum_{i,j,k,l=1}^{d} |\sum_{u=1}^{d}(U^{R_{3,5}}(U^{R_{3,5}})^\dagger)_{iul}^{juk}|^2,$$

$$(A.12) = \frac{1}{d^4}\sum_{i,j,k,l=1}^{d} |\sum_{r=1}^{d}(U^{R_{1,6}}(U^{R_{1,6}})^\dagger)_{rkj}^{rli}|^2,$$

$$(A.12) = \frac{1}{d^4}\sum_{i,j,k,l=1}^{d} |\sum_{t=1}^{d}(U^{\Gamma_{1,4}}(U^{\Gamma_{1,4}})^\dagger)_{jkt}^{ilt}|^2,$$

and

$$(A.12) = \frac{1}{d^4}\sum_{i,j,k,l=1}^{d} |\sum_{s=1}^{d}(U^{\Gamma_{2,5}}(U^{\Gamma_{2,5}})^\dagger)_{ils}^{jks}|^2.$$

This gives us:

$$\mathrm{Tr}(P_{U\mathcal{M}U^\dagger}P_{\mathcal{L}}^\dagger) = \frac{1}{d^2}\left\{\begin{array}{l} ||\mathrm{tr}_3(U^{\Gamma_{1,4}}(U^{\Gamma_{1,4}})^\dagger)||_2^2 \\ ||\mathrm{tr}_3(U^{\Gamma_{2,5}}(U^{\Gamma_{2,5}})^\dagger)||^2 \\ ||\mathrm{tr}_3(U^{R_{1,4}}(U^{R_{1,4}})^\dagger)||_2^2 \\ ||\mathrm{tr}_2(U^{R_{3,5}}(U^{R_{3,5}})^\dagger)||_2^2 \end{array}\right. .$$

A.3 Multiunitaries and Delocalised Subalgebras in Dimension 16

Proposition A.0.1. *Consider the matrix algebra* $\mathcal{M}_{d^4}(\mathbb{C}) \cong \mathcal{M}_d(\mathbb{C}) \otimes \mathcal{M}_d(\mathbb{C}) \otimes \mathcal{M}_d(\mathbb{C}) \otimes \mathcal{M}_d(\mathbb{C})$ *and let* $\mathcal{L} = \mathcal{M}_d(\mathbb{C}) \otimes \mathbb{I}_{d^3}$ *be the left subalgebra,* $\mathcal{R} = \mathbb{I}_{d^3} \otimes \mathcal{M}_d(\mathbb{C})$ *be the right subalgebra and* $\mathcal{M}_1 = \mathbb{I}_d \otimes \mathcal{M}_d(\mathbb{C}) \otimes \mathbb{I}_{d^2}$ *and* $\mathcal{M}_2 = \mathbb{I}_{d^2} \otimes \mathcal{M}_d(\mathbb{C}) \otimes \mathbb{I}_d$ *be the "middle subalgbras". Now consider* $U \in U(n^4)$ *and set* $\mathcal{A}_L := U\mathcal{L}U^\dagger$*,* $\mathcal{A}_R := U\mathcal{R}U^\dagger$*,* $\mathcal{A}_{M_1} := U\mathcal{M}_1U^\dagger$ *and* $\mathcal{A}_{M_2} := U\mathcal{M}_2U^\dagger$*.*

If U *is multiunitary in the sense that there are 16 rearrangements of* U *that are unitary, then* $\mathcal{A}_L$*,* $\mathcal{A}_R$*,* $\mathcal{A}_{M_1}$ *and* $\mathcal{A}_{M_2}$ *are delocalised.*

Proof. Let $\sqrt{d}e_{ij} = \sqrt{d}\,|i\rangle\langle j|$ be an ONB in $\mathcal{M}_d(\mathbb{C})$ and $\mathbb{I}_{d^3}$ be the identity operator of $\mathcal{L}(H_{M_1}) \otimes \mathcal{L}(H_{M_2}) \otimes \mathcal{L}(H_R) \cong \mathcal{M}_{d^3}(\mathbb{C})$. Then

$$P_{\mathcal{L}} = d \sum_{i,j=1}^{d} |e_{ij} \otimes \mathbb{I}_{d^3}\rangle \langle e_{ij} \otimes \mathbb{I}_{d^3}|$$

is the projection onto the left subalgebra. Similarly, one has

$$P_{U\mathcal{L}U^\dagger} = d \sum_{i,j=1}^{d} |U(e_{ij} \otimes \mathbb{I}_{d^3})U^\dagger\rangle \langle U(e_{ij} \otimes \mathbb{I}_{d^3})U^\dagger|$$

as projection onto $\mathcal{A}$. Following the proof of Prop. 3.0.1, one then computes:

$$\begin{aligned}
\mathrm{Tr}(P_{U\mathcal{L}U^\dagger} P_{\mathcal{L}}^\dagger) &= d^2 \sum_{i,j,k,l=1}^{d} |\langle (Ue_{ij} \otimes \mathbb{I}_{d^3} U^\dagger) | e_{kl} \otimes \mathbb{I}_{d^3}\rangle|^2 \\
&= d^2 \sum_{i,j,k,l=1}^{d} |\tau\big((Ue_{ij} \otimes \mathbb{I}_{d^3} U^\dagger)(e_{kl} \otimes \mathbb{I}_{d^3})\big)|^2 \\
&= d^2 \sum_{i,j,k,l=1}^{d} |\frac{1}{d^4}\mathrm{tr}\big((Ue_{ij} \otimes \mathbb{I}_{d^3} U^\dagger)(e_{kl} \otimes \mathbb{I}_{d^3})\big)|^2 \\
&= \frac{d^2}{d^8} \sum_{i,j,k,l=1}^{d} |\mathrm{tr}\big((Ue_{ij} \otimes \mathbb{I}_{d^3} U^\dagger)(e_{kl} \otimes \mathbb{I}_{d^3})\big)|^2 \\
&= \frac{1}{d^6} \sum_{i,j,k,l=1}^{d} |\mathrm{tr}\big((Ue_{ij} \otimes \mathbb{I}_{d^3} U^\dagger)(e_{kl} \otimes \mathbb{I}_{d^3})\big)|^2.
\end{aligned}$$

Further compute:

$$\mathrm{tr}\Big((Ue_{ij}\otimes \mathbb{I}_{d^3}U^{\dagger})(e_{kl}\otimes \mathbb{I}_{d^3})\Big) = \mathrm{tr}\Big(\sum_{\substack{r_1,r_2,\\ s_1,s_2,\\ t,u=1}}^{d}(Ue_{ij}\otimes e_{r_1r_1}\otimes e_{r_2r_2}\otimes e_{tt}U^{\dagger})$$

$$\times(e_{kl}\otimes e_{s_1s_1}\otimes e_{s_2s_2}\otimes e_{uu})\Big).$$

This can be transformed into:

$$\mathrm{tr}\Big(\sum_{\substack{r_1,r_2,\\ s_1,,s_2,\\ t,u=1}}^{d} U\,|ir_1r_2t\rangle\,\langle jr_1r_2t|\,U^{\dagger}\,|ks_1s_2u\rangle\,\langle ls_1s_2u|\Big) = \sum_{r_1,r_2,s_1,s_2,t,u=1}^{d}\langle ls_1s_2u|\,U\,|ir_1r_2t\rangle\,\langle jr_1r_2t|$$

$$= \sum_{r_1,r_2,s_1,s_2,t,u=1}^{d} U_{ir_1r_2t}^{ls_1s_2u}(U^{\dagger})_{ksu}^{jr_1r_2t}$$

$$= \sum_{r_1,r_2,s_1,s_2,t,u=1}^{d} U_{ir_1r_2t}^{ls_1s_2u}(U^{*})_{jr_1r_2t}^{ks_1s_2u}.$$

Hence one gets:

$$\mathrm{Tr}(P_{U\mathcal{L}U^{\dagger}}P_{\mathcal{L}}^{\dagger}) = \frac{1}{d^6}\sum_{i,j,k,l=1}^{d}\Big|\sum_{r_1,r_2,s_1,s_2,t,u=1}^{d} U_{ir_1r_2t}^{ls_1s_2u}(U^{*})_{jr_1r_2t}^{ks_1s_2u}\Big|^2.$$

This expression can be transformed in various ways. Labeling the upper indices with $1,2,3,4$ and the lower indices with $5,6,7,8$, one can perform the following index swaps in order to simplify the expression:

$1 \leftrightarrow 6$

$1 \leftrightarrow 7$

$1 \leftrightarrow 8$

$5 \leftrightarrow 2$

$5 \leftrightarrow 3$

$5 \leftrightarrow 4$

Similarly, one gets

$$\mathrm{Tr}(P_{U\mathcal{L}U^\dagger}P_{\mathcal{R}}^\dagger) = \frac{1}{d^6}\sum_{i,j,k,l=1}^{d} \Big| \sum_{r_1,r_2,s_1,s_2,t,u=1}^{d} U_{ir_1r_2t}^{s_1s_2ul}(U^*)_{jr_1r_2t}^{s_1s_2uk}\Big|^2.$$

with possible index shifts:

$4 \leftrightarrow 6$

$4 \leftrightarrow 7$

$4 \leftrightarrow 8$

$5 \leftrightarrow 1$

$(5 \leftrightarrow 2)$

$(5 \leftrightarrow 3)$

Moreover, one finds:

$$\mathrm{Tr}(P_{U\mathcal{L}U^\dagger}P_{\mathcal{M}_1}^\dagger) = \frac{1}{d^6}\sum_{i,j,k,l=1}^{d} \Big| \sum_{r_1,r_2,s_1,s_2,t,u=1}^{d} U_{ir_1r_2t}^{s_1ls_2u}(U^*)_{jr_1r_2t}^{s_1ks_2u}\Big|^2.$$

with possible index shifts:

$2 \leftrightarrow 6$

$2 \leftrightarrow 7$

$2 \leftrightarrow 8$

$(5 \leftrightarrow 1)$

$(5 \leftrightarrow 3)$

$(5 \leftrightarrow 4)$

Lastly, one has:

$$\mathrm{Tr}(P_{U\mathcal{L}U^\dagger}P_{\mathcal{M}_2}^\dagger) = \frac{1}{d^6}\sum_{i,j,k,l=1}^{d} \Big| \sum_{r_1,r_2,s_1,s_2,t,u=1}^{d} U_{ir_1r_2t}^{s_1s_2lu}(U^*)_{jr_1r_2t}^{s_1s_2ku}\Big|^2.$$

with possible index shifts:

$3 \leftrightarrow 6$

$3 \leftrightarrow 7$

$3 \leftrightarrow 8$

$(5 \leftrightarrow 1)$

$(5 \leftrightarrow 2)$

$(5 \leftrightarrow 4)$

These index shifts correspond to 16 rearrangements of the matrix $U \in U(d^4)$. Analogous calculations hold for the trace conditions of $\mathcal{A}_R$, $\mathcal{A}_{M_1}$ and $\mathcal{A}_{M_2}$.

From here, proceed like in the proof for $k = 3$ with the prefactor d^6 instead of d^4. In the following the proof that $\mathcal{A}_L$ is quasi-orthogonal to $\mathcal{L}$ if $U^{R^{1,6}}$ is unitary will be sketched as an example.

One can rewrite the trace condition as follows:

$$\operatorname{Tr}\left(P_{U\mathcal{L}U^\dagger} P_{\mathcal{L}}^\dagger\right) = \frac{1}{d^6} \sum_{i,j,k,l=1}^{d} \left| \sum_{r_1,s_1 s_1,s_1=1}^{d} U_{ir_1r_1t}^{ls_1s_2u} \left(U^*\right)_{js_1r_2t}^{ks_1s_2u} \right|^2$$

$$= \frac{1}{d^6} \sum_{i,j,k,l=1}^{d} | \left(\sum_{r_1,t=1}^{d} U^{R_{1,6}} \left(U^{R_{1,6}}\right)^\dagger \right))_{ilr_2t}^{jkr_2t} |^2$$

$$= \frac{1}{d^6} \sum_{i,j,k,l=1}^{d} \left| \operatorname{tr}_{CD} \left(U^{R_{1,6}} \left(U^{R_{1,6}}\right)^\dagger \right)_{il}^{jk} \right|^2$$

Now assuming that $U^{R_{1,6}}$ is unitary, one finds:

$$\begin{aligned} \operatorname{Tr}\left(P_{U\mathcal{L}U^\dagger} P_{\mathcal{L}}^\dagger\right) &= \frac{1}{d^6} \sum_{i,j,k,l=1}^{d} \left| \operatorname{tr}_{CD} \left(\mathbb{I}_{d^4}\right)_{il}^{jk} \right|^2 \\ &= \frac{1}{d^6} d^4 \sum_{i,i,k,l=1}^{d} \left| \left(\mathbb{I}_{d^2}\right)_{il}^{jk} \right|^2 \\ &= 1 \end{aligned}$$

Hence $\mathcal{A}_L$ is quasi-orthogonal to $\mathcal{L}$. □

A.4 Additional calculations for Theorem 3.0.4

Similarly, to the calculations in the proof of Theorem 3.0.4, once can derive the following trace conditions for the subalgebra $\mathcal{A}_R$:

$$\mathrm{Tr}(P_{\mathcal{A}_R} P^\dagger_{\mathcal{L}}) = \frac{1}{d^{2(k-1)}} \sum_{i,j,m,l=1}^{d} | \sum_{\substack{r_1,..,r_{k-1},\\ s_1,..,s_{k-1}=1}}^{d} U^{ls_1\ldots s_{k-1}}_{r_1\ldots r_{k-1}i} (U^*)^{ms_1\ldots s_{k-1}}_{r_1\ldots r_{k-1}j} |^2, \tag{A.13}$$

$$\mathrm{Tr}(P_{\mathcal{A}_R} P^\dagger_{\mathcal{R}}) = \frac{1}{d^{2(k-1)}} \sum_{i,j,m,l=1}^{d} | \sum_{\substack{r_1,..,r_{k-1},\\ s_1,..,s_{k-1}=1}}^{d} U^{s_1\ldots s_{k-1}l}_{r_1\ldots r_{k-1}i} (U^*)^{s_1\ldots s_{k-1}m}_{r_1\ldots r_{k-1}j} |^2, \tag{A.14}$$

$$\mathrm{Tr}(P_{\mathcal{A}_R} P^\dagger_{\mathcal{M}_\dashv}) = \frac{1}{d^{2(k-1)}} \sum_{i,j,m,l=1}^{d} | \sum_{\substack{r_1,..,r_{k-1},\\ s_1,..,s_{k-1}=1}}^{d} U^{s_1..s_{a-1}ls_a..s_{k-1}}_{r_1\ldots r_{k-1}i} (U^*)^{s_1..s_{a-1}ms_a..s_{k-1}}_{r_1\ldots r_{k-1}j} |^2. \tag{A.15}$$

The trace conditions for the subalgebras $\mathcal{A}_{M_a}$ for $a \in [k-2]$ are given by:

$$\mathrm{Tr}(P_{\mathcal{A}_{M_a}} P^\dagger_{\mathcal{L}}) = \frac{1}{d^{2(k-1)}} \sum_{i,j,m,l=1}^{d} | \sum_{\substack{r_1,..,r_{k-1},\\ s_1,..,s_{k-1}=1}}^{d} U^{ls_1\ldots s_{k-1}}_{r_1..r_a i r_{a-1}..r_{k-1}} (U^*)^{ms_1\ldots s_{k-1}}_{r_1..r_a j r_{a-1}..r_{k-1}} |^2, \tag{A.16}$$

$$\mathrm{Tr}(P_{\mathcal{A}_{M_a}} P^\dagger_{\mathcal{R}}) = \frac{1}{d^{2(k-1)}} \sum_{i,j,m,l=1}^{d} | \sum_{\substack{r_1,..,r_{k-1},\\ s_1,..,s_{k-1}=1}}^{d} U^{s_1\ldots s_{k-1}l}_{r_1..r_a i r_{a-1}..r_{k-1}} (U^*)^{s_1\ldots s_{k-1}m}_{r_1..r_a j r_{a-1}..r_{k-1}} |^2, \tag{A.17}$$

$$\mathrm{Tr}(P_{\mathcal{A}_{M_a}} P^\dagger_{\mathcal{M}_\lfloor}) = \frac{1}{d^{2(k-1)}} \sum_{i,j,m,l=1}^{d} | \sum_{\substack{r_1,..,r_{k-1},\\ s_1,..,s_{k-1}=1}}^{d} U^{s_1..s_{b-1}ls_b..s_{k-1}}_{r_1..r_a i r_{a-1}..r_{k-1}} (U^*)^{s_1..s_{b-1}ms_a..s_{b-1}}_{r_1..r_a j r_{a-1}..r_{k-1}} |^2. \tag{A.18}$$

B Additional Material for Section 3.3, Chapter 3

B.1 SageMath Notebooks

In the following, some SageMath notebooks containing some calculations and implementation of algorithms supplementary to Section 3.3 will be displayed:

I. Self Complementary Orthonormal Bases in $\mathbb{F}_{2^m}/\mathbb{F}_2$.

II. 2-Unitaries From Doubly Perfect Sequences for All Dimension (except $d^2 = 36$).

III. Doubly Perfect Sequences of length 36 - a sparse and a symmetric solution.

These notebooks can also be found on the present author's GitHub repository [35].

I) Self Complementary Orthonormal Bases in $\mathbb{F}_{2^m}/\mathbb{F}_2$

[256]:
```
import numpy as np
```

Fix dimension (m has to be an odd integer):

[257]:
```
m= 3
```

Define base fields and matrix spaces over these fields:

[258]:
```
F2m = GF(2^m)
F22 = GF(2^2)
F22m = GF(2^(2*m))
F2 = GF(2)
M = MatrixSpace(F2, m,m)
Mm = MatrixSpace(F2m, m,m)
```

Define normal basis α and its generator α_0 using GAP:

[259]:
```
# normal basis

alpha = [F2m(element) for element in list(gap(F2m).NormalBase())]

alpha
```

[259]:
```
[z3 + 1, z3^2 + 1, z3^2 + z3 + 1]
```

[260]:
```
# generator

alpha_0 = alpha[0]

alpha_0
```

[260]:
```
z3 + 1
```

The following function takes as input an element $\mathbb{F}_{2^m}$ and and integer m and outputs the trace of the field extension $\mathbb{F}_{2^m}/\mathbb{F}_2$:

[261]:
```
def trace(element, dim):
    return sum([element**(2**i) for i in range(0,dim)])
```

Define permutation matrix S:

[262]:
```
def S(dim):
    l = []
    for i in range(0,dim):
        for j in range(0,dim):
            if i == mod(j-1,dim):
                l.append(1)
            else:
```

```
                l.append(0)
    return(M(np.array(l).reshape((dim,dim))))

# test

S(m)
```

[262]:
```
[0 1 0]
[0 0 1]
[1 0 0]
```

Define matrix $A = \mathrm{tr}(\alpha\alpha')$:

[263]:
```
def A(dim,Basis):
    a_prime = list(vector(Basis)*S(dim))
    return Matrix([[trace(element1*element2,dim) for element1 in Basis]for␣
↪element2 in a_prime])

A = A(m, alpha)
```

[264]:
```
A
```

[264]:
```
[0 0 1]
[1 0 0]
[0 1 0]
```

Compute inverse A^{-1}:

[265]:
```
A_inv = A.inverse()
A_inv
```

[265]:
```
[0 1 0]
[0 0 1]
[1 0 0]
```

Define matrix $D = \sum_{i=0}^{n-1} \alpha_0^{2^i} S^i$:

[266]:
```
def D(element, perm, dim):
    return Matrix(sum([ (element**(2**j))*(perm**j) for j in range(0,dim) ]))

D(alpha_0, S(m), m)
```

[266]:
```
[       z3 + 1       z3^2 + 1 z3^2 + z3 + 1]
[z3^2 + z3 + 1         z3 + 1      z3^2 + 1]
[     z3^2 + 1 z3^2 + z3 + 1         z3 + 1]
```

Define $\omega = (D^2)_{0,0}$:

[267]:
```
w = (D(alpha_0, S(m), m)**2)[0,0]

w
```

[267]:
```
z3^2 + 1
```

Define vector $\omega = ((D^2)_{0,i})_{i\in[n]}$:

[268]:
```
omega = [(D(alpha_0, S(m), m)**2)[0,i] for i in range(0,m) ]

omega
```

[268]:
```
[z3^2 + 1, z3 + 1, z3^2 + z3 + 1]
```

Now a self-complementary normal basis can be computed via: $\Gamma = \omega \cdot A^{-1}$.

[269]:
```
SCN = list(vector(omega)*A_inv)

SCN
```

[269]:
```
[z3^2 + z3 + 1, z3^2 + 1, z3 + 1]
```

Verify that basis is equal to dual basis, i. e. self-complementary:

[270]:
```
F2m.dual_basis(SCN) == SCN
```

[270]:
```
True
```

Extend the basis to the field $\mathbb{F}_{2^{2m}}$. For this take a random element $a \in \mathbb{F}_{2^2}$ and compute its square:

[271]:
```
extension = []
for element in F22:
    if F22(trace(element,2))==1:
        extension.append(element)
        extension.append(element**2)
        break

extension
```

[271]:
```
[z2, z2 + 1]
```

Extend SCN basis by multiplying $\{a, a^2\}$ and α:

[272]:
```
SCN_even = flatten([[ F22m(element1*element2) for element1 in extension ]for␣
↪element2 in SCN])
```

[273]:
```
SCN_even
```

[273]:
```
[z6^3,
 z6^5 + z6^3 + z6 + 1,
```

```
 z6^5 + z6^3 + 1,
 z6^5 + z6^4 + z6^3 + z6^2 + z6 + 1,
 z6^5 + z6^3 + z6^2 + z6 + 1,
 z6^4 + z6^3 + z6 + 1]
```

Check if it is self-complementary:

[274]:
```
SCN_even == F22m.dual_basis(SCN_even)
```

[274]:
```
True
```

Now construct matrix with non-zero determinant. For this choose arbitrary element $\beta \in \mathbb{F}_{2^m}$ such that $\beta \neq 1, 0$:

[275]:
```
for element in F2m:
    if (element != 0 and element != 1):
        beta = element
        break


beta
```

[275]:
```
z3
```

Define matrix $G = \mathrm{tr}(\alpha_i \beta \alpha_j)$, where α is a SCN basis:

[276]:
```
def G(Basis, Beta, dim):
    return matrix([[trace(element1*Beta*element2,dim) for element1 in Basis] for␣
 ↪element2 in Basis])
```

Construct $m \times m$ - matrix using the SCN basis of $\mathbb{F}_{2^m}/\mathbb{F}_2$:

[277]:
```
G_odd = G(SCN, beta, m)
```

Construct $2m \times 2m$ - matrix using the SCN basis of $\mathbb{F}_{2^{2m}}/\mathbb{F}_2$:

[278]:
```
G_even = G(SCN_even, beta, 2*m)

G_even
```

[278]:
```
[0 0 1 0 0 0]
[0 0 0 1 0 0]
[1 0 1 0 1 0]
[0 1 0 1 0 1]
[0 0 1 0 1 0]
[0 0 0 1 0 1]
```

Define matrices

$$N = \begin{pmatrix} G & \mathbb{I}_n \\ \mathbb{I}_n & G \end{pmatrix} \quad \text{and} \quad N + J = \begin{pmatrix} G & 0 \\ 0 & G \end{pmatrix}. \tag{1}$$

[279]:
```
def N(dim, matr):
    return matrix(np.vstack((np.hstack((identity_matrix(dim), np.array(matr))),␣
↪np.hstack(( np.array(matr), identity_matrix(dim) )))))
```

Define the $2m \times 2m$-matrix N (odd case):

[280]:
```
N(m, G_odd)
```

[280]:
```
[1 0 0 0 1 0]
[0 1 0 1 1 1]
[0 0 1 0 1 1]
[0 1 0 1 0 0]
[1 1 1 0 1 0]
[0 1 1 0 0 1]
```

Check determinant:

[281]:
```
N(m, G_odd).determinant()
```

[281]:
```
1
```

Define the $4m \times 4m$-matrix N' (even case):

[282]:
```
N(2*m, G_even)
```

[282]:
```
[1 0 0 0 0 0 0 0 1 0 0 0]
[0 1 0 0 0 0 0 0 0 1 0 0]
[0 0 1 0 0 0 1 0 1 0 1 0]
[0 0 0 1 0 0 0 1 0 1 0 1]
[0 0 0 0 1 0 0 0 1 0 1 0]
[0 0 0 0 0 1 0 0 0 1 0 1]
[0 0 1 0 0 0 1 0 0 0 0 0]
[0 0 0 1 0 0 0 1 0 0 0 0]
[1 0 1 0 1 0 0 0 1 0 0 0]
[0 1 0 1 0 1 0 0 0 1 0 0]
[0 0 1 0 1 0 0 0 0 0 1 0]
[0 0 0 1 0 1 0 0 0 0 0 1]
```

Check determinant:

[283]:
```
N(2*m, G_even).determinant()
```

[283]:
```
1
```

Define matrix J:

[284]:
```
def J(dim):
    return Matrix(F2, np.hstack((np.vstack((np.zeros((dim, dim)),␣
↪-identity_matrix(dim))), np.vstack((identity_matrix(dim), np.zeros((dim,␣
↪dim))))))
```

Compute the $2m \times 2m$-matrix $N + J$ (odd case):

[285]:
```
N(m, G_odd)+ J(m)
```

[285]:
```
[1 0 0 1 1 0]
[0 1 0 1 0 1]
[0 0 1 0 1 0]
[1 1 0 1 0 0]
[1 0 1 0 1 0]
[0 1 0 0 0 1]
```

Check determinant:

[286]:
```
(N(m, G_odd)+ J(m)).determinant()
```

[286]:
```
1
```

Compute the $4m \times 4m$-matrix $N + J$ (even case):

[287]:
```
N(2*m, G_even)+ J(2*m)
```

[287]:
```
[1 0 0 0 0 0 1 0 1 0 0 0]
[0 1 0 0 0 0 0 1 0 1 0 0]
[0 0 1 0 0 0 1 0 0 0 1 0]
[0 0 0 1 0 0 0 1 0 0 0 1]
[0 0 0 0 1 0 0 0 1 0 0 0]
[0 0 0 0 0 1 0 0 0 1 0 0]
[1 0 1 0 0 0 1 0 0 0 0 0]
[0 1 0 1 0 0 0 1 0 0 0 0]
[1 0 0 0 1 0 0 0 1 0 0 0]
[0 1 0 0 0 1 0 0 0 1 0 0]
[0 0 1 0 0 0 0 0 0 0 1 0]
[0 0 0 1 0 0 0 0 0 0 0 1]
```

Check determinant:

[288]:
```
(N(2*m, G_even)+ J(2*m)).determinant()
```

[288]:
```
1
```

II. 2-Unitaries From Doubly Perfect Sequences for All Dimension (except $d^2 = 36$)

[17]:
```
import numpy as np
import itertools
```

I. Definition of basic functions

Fix dimensions in the following.

(For $d = 2$ and suitable matrices N, we get solutions for even dimensions.)

[18]:
```
d = 3 # change dimension here

m = 1 # change m value here
```

Example $2m \times 2m$ matrices N can be defined below:

[19]:
```
N = identity_matrix(2*m) # change matrix here
```

Define symbolic variables of length $2m$ with symbolic entries in $\mathbb{F}_d$

[20]:
```
a = var('a', n= 2*m, latex_name='a')
b = var('b', n= 2*m, latex_name='b')
```

The following function is used to define a list of all possible combinations of choices for a tuple a consisting of 2m elements with entries from a number field of dimension d.

[21]:
```
def iteration_list(m,d):
    return list(itertools.product([j for j in range(0,d)], repeat=2*m))
```

The following function defines a matrix that generates symplectic product taking as input two tuples consisting of symbolic variables and the parameters d and m. The function outputs the symplectic product of these tuples interpreted as vectors.

[22]:
```
def symplectic_product(vec_a,vec_b, m, d):
    F.<w> = CyclotomicField(d)
# for d = 2, omega becomes the imaginary unit
    if d==2:
        w = I
    J = Matrix(ZZ, np.hstack((np.vstack((np.zeros((m, m)),␣
↪-identity_matrix(m))), np.vstack((identity_matrix(m), np.zeros((m, m)))))))
    return w**(vec_a*J*vec_b)

# test

symplectic_product(vector(a),vector(b),m, d)
```

[22]:
```
(1/2*I*sqrt(3) - 1/2)^(-a1*b0 + a0*b1)
```

The next function defines a sequence taking as input a tuple of symbolic variables and a matrix N. The function outputs the values of the sequence for each choice of numbers.

[23]:
```
def sequence(vec,N,d):
    F.<w> = CyclotomicField(d)
# for d = 2, omega becomes the imaginary unit
    if d==2:
        w = I
    return w**(vec*N*vec)
```

The following function output all values of the sequence as a list by taking as input the function that generates the sequence values and the parameters m and d.

[24]:
```
def sequence_list(seq,N, m,d):
    return [seq(vector(values),N, d) for values in iteration_list(m,d)]


# test

print(sequence_list(sequence,N,m,d))
```

```
[1, w, w, w, -w - 1, -w - 1, w, -w - 1, -w - 1]
```

The next function defines the absolute value of the sequence by taking as input a tuple of symbolic variables, the parameters d and m and a matrix N and outputting the absolute value of the sequence for each choice of numbers for the tuple a as a list.

[25]:
```
def sequence_absolute_value(N, seq, m, d):
    return [seq(vector(values), N, d)*conjugate(seq(vector(values),N, d)) for␣
 ↪values in iteration_list(m,d)]


# test

print(sequence_absolute_value(N, sequence, m, d))
```

```
[1, 1, 1, 1, 1, 1, 1, 1, 1]
```

The next function defines the cross correlation of the sequence by taking as input two tuples of symbolic variables, the parameters d and m and a matrix N and outputting the cross correlation of the sequence for each choice of numbers for the tuple a as a list.

[26]:
```
def cross_correlation(N, seq, m, d):
    output_list = []
    for values_b in iteration_list(m,d):
        sum_counter = 0
        for values_a in iteration_list(m,d):
            sum_counter +=␣
 ↪seq(vector(values_a)+vector(values_b),N,d)*conjugate(seq(vector(values_a),N,d))
        output_list.append(sum_counter)
    return output_list
```

[27]:
```
# test

print(cross_correlation(N, sequence, m , d))
```

```
[9, 0, 0, 0, 0, 0, 0, 0, 0]
```

The next function defines the twisted cross correlation of the sequence by taking as input two tuples of symbolic variables, the parameters d and m and a matrix N and outputting the twisted cross correlation of the sequence for each choice of numbers for the tuple a as a list.

[28]:
```
def twisted_cross_correlation(N, seq, m , d):
    output_list = []
    for values_b in iteration_list(m,d):
        sum_counter = 0
        for values_a in iteration_list(m,d):
            sum_counter += seq(vector(values_a)+vector(values_b),N,␣
↪d)*conjugate(seq(vector(values_a),N,␣
↪d))*symplectic_product(2*vector(values_a),vector(values_b),m, d)

        output_list.append(sum_counter)
    return output_list

# test

print(twisted_cross_correlation(N, sequence, m ,d))
```

```
[9, 0, 0, 0, 0, 0, 0, 0, 0]
```

Define a function that takes as input two tuples of symbolic variables, the parameters d adn m and a matrix N, computes the absolute value, the cross correlation and the twisted cross correlation of the corresponding sequence and outputs true if the sequence is perfect and false otherwise.

[29]:
```
def is_perfect_sequence(N, seq, m, d):
    CC = cross_correlation(N, seq, m, d)
    TWCC = twisted_cross_correlation(N,seq, m ,d)
    Abs = sequence_absolute_value(N, seq, m, d)
    if (TWCC[0] != d**(2*m) or CC[0] != d**(2*m) or Abs[0] != 1):
        return false
    for k in range(1,len(CC)):
            if (Abs[k] != 1 or TWCC[k] != 0 or CC[k] != 0):
                return false
    return true
```

[30]:
```
# test

is_perfect_sequence(N, sequence, m , d)
```

[30]: True

The following function constructs a unitary out of the perfect sequence, taking as input the sequence, the matrix N and the parameters d and m and outputting a d^{2m}-dimensional matrix.

[31]:
```
def matrix_generator(N,d,m, seq):
    return Matrix(np.
↪array(flatten([[seq(vector(values_a)-vector(values_b),N,d)*symplectic_product(2*vector(values
↪d)for values_a in iteration_list(m,d)]for values_b in iteration_list(m,d)])).
↪reshape((d**(2*m), d**(2*m))))
```

[33]:
```
# test

H = (1/(d**m))*matrix_generator(N,d,m,sequence)
```

Define a function that computes the reshuffle of a matrix:

[34]:
```
def matrix_reshuffle(M,d,m):
    dim = d**m
    matrix_reshaped = np.array(M).reshape((dim, dim, dim, dim))
    return Matrix(np.array([[[[matrix_reshaped[l,j,k,i] for i in range(0,dim)]␣
↪for j in range(0,dim)] for k in range(0,dim)] for l in range(0,dim)]).
↪reshape((dim**2,dim**2)))
```

Define a function that checks if a matrix is dual unitary:

[35]:
```
def is_dual_unitary(M,d,m):
    return matrix_reshuffle(M,d,m).is_unitary()

# test


is_dual_unitary(H,d,m)
```

[35]:
```
True
```

Define a function that computes the partial transpose of a matrix:

[36]:
```
def matrix_partial_transpose(M,d,m):
    dim = d**m
    matrix_reshaped = np.array(M).reshape((dim, dim, dim, dim))
    return Matrix(np.array([[[[matrix_reshaped[k,j,i,l] for i in range(0,dim)]␣
↪for j in range(0,dim)] for k in range(0,dim)] for l in range(0,dim)]).
↪reshape((dim**2,dim**2)))
```

Define a function that checks if a matrix is Γ-dual unitary:

[37]:
```
def is_gamma_dual_unitary(M,d,m):
    return matrix_partial_transpose(M,d,m).is_unitary()

# test
```

```
is_gamma_dual_unitary(H,d,m)
```

[37]: True

Define function thats checks 2-unitarity by checking if matrix itself, dual and gamma dual matrices are unitary:

[38]:
```
def is_2unitary(M,d,m):
    return (M.is_unitary() and is_dual_unitary(M,d,m) and␣
 ↪is_gamma_dual_unitary(M,d,m))
```

[39]:
```
# test is_2unitary

is_2unitary(H,d,m)
```

[39]: True

II.

In the following it will be demonstrated for low dimensions that the identity matrix generates a perfect sequence for odd dimensions.

[40]:
```
for dim in range(1,10,2):
    N = identity_matrix(2*m)
    print("d = ", dim, " Perfect sequence: ", is_perfect_sequence(N, sequence,␣
 ↪m, dim))
```

```
d =  1  Perfect sequence:  True
d =  3  Perfect sequence:  True
d =  5  Perfect sequence:  True
d =  7  Perfect sequence:  True
d =  9  Perfect sequence:  True
```

III.

In the following it will be demonstrated that the kite-matrix generates doubly perfect sequences for even dimensions up to $d^m = 2^{500}$:

[43]:
```
for m in range(2,500):
    M2 = MatrixSpace(GF(2), 2*m, 2*m)
    list = []
    for i in range(0,2*m):
        for j in range(0,2*m):
            if (i+j <= 2*m-1):
                list.append(1)
            else:
                list.append(0)

    N = M2(np.array(list).reshape((2*m,2*m)))
```

```
    J =  Matrix(ZZ, np.hstack((np.vstack((np.zeros((m, m)),␣
↪identity_matrix(m))), np.vstack((identity_matrix(m), np.zeros((m, m)))))))
    M = M2(N+J)
    if (N.determinant()==0 or M.determinant() == 0):
        if(mod(m-1,3) == 0):
            print(m, 'true', '\n')
```

```
4 true

7 true
```

III. Doubly Perfect Sequences of length 36 - a sparse and a symmetric solution

[20]:
```
import numpy as np
import itertools

K.<w> = CyclotomicField(3)
F.<f> = CyclotomicField(6)
```

In the following both the Chinese remainder isomorphism chinese_rem(a), that takes as input an element $a \in \mathbb{Z}_6$ and outputs a tuple $(k, x) \in \mathbb{Z}_3 \times \mathbb{Z}_2$, and its inverse inv_chinese_rem(k,x), that takes as input two numbers $k \in \mathbb{Z}_3$ and $x \in \mathbb{Z}_2$ and outputs a number $a \in \mathbb{Z}_6$, are defined:

[2]:
```
def chinese_rem(a):
    return [mod(a,3), mod(a,2)]

# test

chinese_rem(2)
```

[2]: [2, 0]

[3]:
```
def inv_chinese_rem(k,x):
    return mod(4*k + 3*x,6)

# test

inv_chinese_rem(2,0)
```

[3]: 2

Next define the list of all possible combiantions of two elements $a_1, a_2 \in \mathbb{Z}_6$ when factorised by the Chinese remainder isomorphism into two tuples (k, x), $(l, y) \in \mathbb{Z}_3 \times \mathbb{Z}_2$:

[4]:
```
iteration_list = []
for a1 in range(0,6):
    for a2 in range(0,6):
        k = chinese_rem(a1)[0]
        l = chinese_rem(a2)[0]
        x = chinese_rem(a1)[1]
        y = chinese_rem(a2)[1]
        iteration_list.append([k,l,x,y])

# length check

len(iteration_list)
```

[4]: 36

Define the sequence values for the symmetric and the sparse solution as functions that take as input four numbers k, l, x, y, where $k, l \in \mathbb{Z}_3$ and $x, y \in \mathbb{Z}_2$ and ouput the sequence value for these numbers.

[5]:
```
def sequence_sym(k,l,x,y):
    if (mod(x,2) == 1 and mod(y,2) ==1):
        return K(w**mod(2*(k**2 + l**2),3))
    else:
        return K(w**mod(2*(k**2 + l**2 - (k+l+ mod(x,3)-mod(y,3))**2),3))
```

[6]:
```
def sequence_sparse(k,l,x,y):
    if (mod(x,2) == 1 and mod(y,2) ==1):
        return K(w**(2*(k**2 + l**2)))
    else:
        return K(w**(2*(k**2 + l**2 + (l + mod(x,3)-mod(y,3))**2)))
```

The function sequence_list(seq) takes as input a function that generates a sequence value and outputs the whole sequence as a list:

[7]:
```
def sequence_list(seq):
    list_out = []
    for values in iteration_list:
            list_out.append(seq(values[0], values[1], values[2], values[3]))
    return list_out
```

[21]:
```
# test symmetric

print(sequence_list(sequence_sym))
```

```
[1, -w - 1, 1, w, 1, 1, 1, w, -w - 1, -w - 1, w, w, 1, -w - 1, -w - 1, 1, w, w,
w, -w - 1, -w - 1, 1, 1, -w - 1, 1, -w - 1, w, -w - 1, -w - 1, -w - 1, -w - 1,
w, -w - 1, -w - 1, -w - 1, w]
```

[22]:
```
# test sparse

print(sequence_list(sequence_sparse))
```

```
[1, -w - 1, w, -w - 1, w, w, w, w, w, -w - 1, 1, w, -w - 1, w, 1, w, 1, 1, -w -
1, -w - 1, -w - 1, 1, w, -w - 1, -w - 1, w, 1, w, 1, 1, w, w, w, -w - 1, 1, w]
```

The function sequence_abs(seq) takes as input a function that generates sequence values and outputs the absolute value of each sequence value as a list:

[10]:
```
def sequence_abs(seq):
    list_out = []
    for values in iteration_list:
        list_out.append(seq(values[0], values[1], values[2],␣
 ↪values[3])*conjugate(seq(values[0], values[1], values[2], values[3])))
    return list_out
```

[23]:
```
# test symmetric

print(sequence_abs(sequence_sym))
```

```
[1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1,
1, 1, 1, 1, 1, 1, 1, 1, 1, 1]
```

[24]:
```
# test sparse

print(sequence_abs(sequence_sparse))
```

```
[1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1,
1, 1, 1, 1, 1, 1, 1, 1, 1, 1]
```

The function cross_correlation(seq) takes as input a function that generates sequence values and outputs the cross correlation of the sequence as a list:

[13]:
```
def cross_correlation(seq):
    list_out =[]
    for values_b in iteration_list:
        t=0
        for values_a in iteration_list:
            t += conjugate(seq(values_a[0]+values_b[0], values_a[1]+values_b[1],␣
 ↪values_a[2]+values_b[2], values_a[3]+ values_b[3]))*seq(values_a[0],␣
 ↪values_a[1], values_a[2], values_a[3])
        list_out.append(K(t))
    return list_out
```

[25]:
```
# test symmetric

print(cross_correlation(sequence_sym))
```

```
[36, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
0, 0, 0, 0, 0, 0, 0, 0, 0, 0]
```

[26]:
```
# test sparse

print(cross_correlation(sequence_sparse))
```

```
[36, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
0, 0, 0, 0, 0, 0, 0, 0, 0, 0]
```

The function twisted_cross_correlation(seq) takes as input a function that generates sequence values and outputs the twisted cross correlation of the sequence as a list:

[16]:
```
def twisted_cross_correlation(seq):
    list_out =[]
    for values_b in iteration_list:
        t = 0
        for values_a in iteration_list:
```

```
            t += K(seq(values_a[0]+values_b[0], values_a[1]+values_b[1],␣
↪values_a[2]+values_b[2], values_a[3]+ values_b[3])*conjugate(seq(values_a[0],␣
↪values_a[1], values_a[2],␣
↪values_a[3]))*w**(inv_chinese_rem(values_b[1]*values_a[0]-values_b[0]*values_a[1],mod(values_
        list_out.append(K(t))
    return list_out
```

[27]:

```
# test symmetric

print(twisted_cross_correlation(sequence_sym))
```

```
[36, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
0, 0, 0, 0, 0, 0, 0, 0, 0, 0]
```

[28]:

```
#test sparse

print(twisted_cross_correlation(sequence_sparse))
```

```
[36, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
0, 0, 0, 0, 0, 0, 0, 0, 0, 0]
```

As one can see, the sequences defined through the functions sequence_sym(k,l,x,y)} and sequence_sparse(k,l,x,y) are unimodular and doubly perfect.

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