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Mutually Unbiased Bases in Composite Dimensions – A Review

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Maximal sets of mutually unbiased bases are useful throughout quantum physics, both in a foundational context and for applications. To date, it remains unknown if complete sets of mutually unbiased bases exist in Hilbert spaces of dimensions different from a prime power, i.e. in composite dimensions such as six or ten. Fourteen mathematically equivalent formulations of the existence problem are presented. We comprehensively summarise analytic, computer-aided and numerical results relevant to the case of composite dimensions. Known modifications of the existence problem are reviewed and potential solution strategies are outlined.

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Given a value of q ,
all possible values of p are *equally likely*.¹
Pascual Jordan – 1927

1 Introduction

1.1 Motivation

Given a particle with momentum p moving along a straight line, what can we say about its position? If we are dealing with a *classical* point particle, we know that it will occupy a precise location which a measurement would reveal with certainty. In contrast, the position q of a *quantum* particle with momentum p cannot be predicted with certainty. The particle will be found with *equal* probability

$$\text{prob}(q, dq) = |\langle p|q \rangle|^2 dq = \frac{1}{2\pi} dq, \quad (1.1)$$

irrespective of the chosen interval of length dq about the value q . An analogous statement holds upon exchanging the roles of position and momentum, with $\text{prob}(p, dp) = |\langle q|p \rangle|^2 dp$.

For a free particle on the line, the basis formed by the momentum eigenstates $|p\rangle, p \in \mathbb{R}$, is called *unbiased* with respect to the basis of the position eigenstates $|q\rangle, q \in \mathbb{R}$, since the transition probabilities from each state $|q\rangle$ into any state $|p\rangle$ do not depend on the value of q . Due to their symmetry, the bases are, in fact, *mutually unbiased* (MU) since an equivalent statement applies to the situation in which the roles of position and momentum are swapped. Any pair of orthonormal bases with this property—certainty about the value of one observable implies complete uncertainty about the value of the other observable, and *vice versa*—is called MU.

Mutual unbiasedness captures an important aspect of Bohr’s concept of complementarity [66]. It provides a precise mathematical formulation of what it means for observables such as position $\hat{q}$ and momentum $\hat{p}$ to be a *complementary* pair. Importantly, it carries over naturally to bases of *finite-dimensional* Hilbert spaces $\mathcal{H} \simeq \mathbb{C}^d$ which are used to describe quantum systems with d orthogonal states. Let us now define the notion central to this review.

¹Originally in German: “Bei einem gegebenen Wert von q sind alle möglichen Werte von p *gleich wahrscheinlich*.” [208, p. 814].

Definition 1.1 (Pairs of MU bases). Two orthonormal bases $\mathcal{B}$ and $\mathcal{B}'$ of the d -dimensional Hilbert space $\mathcal{H} \simeq \mathbb{C}^d$ are *mutually unbiased* if the transition probabilities between any two states $|v\rangle \in \mathcal{B}$ and $|v'\rangle \in \mathcal{B}'$ are equal,

$$|\langle v|v'\rangle|^2 = \frac{1}{d}, \quad v, v' = 0, 1, \dots, d-1. \quad (1.2)$$

The constant value cannot be chosen arbitrarily: completeness of the basis $\mathcal{B}$ implies that the sum of the values $|\langle v|v'\rangle|^2$ over v equals one, forcing the right-hand-side of Eq. (1.2) to take the value $1/d$. The eigenstates of any two Cartesian components of the spin operator of a spin $1/2$ provide the simplest example of a pair of mutually unbiased bases: they form a pair of orthonormal bases such that the squared modulus of the overlap of any two vectors taken from different bases equals $1/2$. As a relation between states and bases, mutual unbiasedness is *symmetric* but neither reflexive nor transitive, hence not an equivalence relation.

It is natural to associate *complex Hadamard matrices* (see Sec. 5.2 for details) with mutually unbiased bases. To see why, consider the d orthonormal basis vectors of the bases $\mathcal{B}$ and $\mathcal{B}'$ as columns of two unitary matrices V and V' , respectively, each of size d . A suitable unitary transformation maps this pair to the pair $\{\mathbb{I}, H\}$, where $\mathbb{I}$ is the identity matrix corresponding to the standard basis in $\mathbb{C}^d$, and H is a unitary matrix the entries of which have modulus $1/\sqrt{d}$, expressing the fact that its column vectors are mutually unbiased to the column vectors of the identity matrix.

Definition 1.2 (Complex Hadamard matrix). A *complex Hadamard matrix* of order d is a $d \times d$ unitary matrix H whose entries satisfy $|H_{jk}| = 1/\sqrt{d}$ for all $j, k = 1 \dots d$.

Returning to the case of a spin $1/2$, the eigenstates of all three Cartesian spin components actually provide an example of *three* pairwise mutually unbiased bases. This observation immediately raises the question of whether there is a limit on the number of pairwise MU bases in the Hilbert space $\mathbb{C}^d$. The answer is known: a d -dimensional complex Hilbert space supports at most $(d+1)$ pairwise mutually unbiased bases, forming what is known as a complete or maximal set.

Definition 1.3 (Complete sets of MU bases). A *complete* (or *maximal*) *set of mutually unbiased bases* in the Hilbert space $\mathbb{C}^d$ consists of $(d+1)$ orthonormal bases $\mathcal{B}_b$, $b = 0, 1, 2, \dots, d$, which are pairwise mutually unbiased.

More explicitly, a complete set of MU bases requires the scalar products between all its pairs of states to take the values

$$|\langle v_b|v'_{b'}\rangle|^2 = \begin{cases} \frac{1}{d} & b \neq b' \\ \delta_{vv'} & b = b' \end{cases}, \quad v, v' = 0 \dots d-1. \quad (1.3)$$

If the dimension d of the underlying Hilbert space is given by a power of a prime number,

$$d = p^k, \quad p \in \mathbb{P}, \quad k \in \mathbb{N}, \quad (1.4)$$

then explicit constructions of maximal sets are known, some of which are summarised in Appendix A, both as a backdrop and for easy reference. It will be useful to denote the set of prime powers by $\mathbb{PP}$ —read: prime power—so that Eq. (1.4) would abbreviate to $d \in \mathbb{PP}$. We will call integer numbers d *composite* if they are *not equal to the power of a prime*, i.e. $d \notin \mathbb{PP}$. Thus, our usage of the term differs from the convention in number theory where all numbers except primes are considered to be composite.

With pairs of mutually unbiased bases capturing the idea of complementarity, larger sets can be thought of as realising *multiple complementarity*. Complete sets of mutually unbiased bases, made from states satisfying the conditions of (1.3), are then required to achieve “maximal complementarity” in a d -dimensional state space. In this way, the traditional concept of complementarity, which was limited to *pairs* of non-commuting observables such as position and momentum, opens up in an unexpected direction.

Somewhat surprisingly, it is not known whether a complete set of mutually unbiased bases exists in state spaces of *composite* dimension, $d \notin \mathbb{PP}$, i.e. whenever the number d is *not* equal to a power of a prime or explicitly,

$$d = \prod_{j=1}^r p_j^{n_j}, \quad p_j \in \mathbb{P}, \quad n_j \in \mathbb{N}, \quad r \geq 2, \quad (1.5)$$

involving at least *two* different prime numbers, $p_1 \neq p_2$. A list of small integers seems to suggest that composite numbers are rare: up to $d = 11$, for example, we encounter only two, $d = 6$ and

$d = 10$. However, the opposite is true: composite dimensions abound since the proportion of prime numbers—and hence prime-powers—among all integers below a given number $N \in \mathbb{N}$ decreases with N (see Sec. 2.3).

The upper bound allows for up to seven and eleven MU bases in the spaces $\mathbb{C}^6$ and $\mathbb{C}^{10}$, respectively, but in both cases, no more than *three* mutually unbiased bases have been found so far. The construction of these *triples* of mutually unbiased bases hinges on the lowest factor $p_1 = 2$ in the prime decomposition (1.5) of six and ten, as will be explained in more detail later (cf. in Sec. 6.2). More generally, the number of MU bases we are able to construct in a space of dimension d depends on its prime decomposition and is significantly smaller than the maximum of $(d + 1)$ bases. Thus, we are led to the main question which has been driving the research reviewed here.

Problem 1.1 (*Existence problem in composite dimensions*). Do complete sets of mutually unbiased bases exist in *composite* dimensions $d \notin \mathbb{PP}$, i.e. whenever $d \neq p^k$, $p \in \mathbb{P}$, $k \in \mathbb{N}$?

For composite dimensions $d \notin \mathbb{PP}$, all known results—be they in closed form, computer-algebraic or numerical—point to the *non-existence* of $(d + 1)$ MU bases. More specifically, for dimension six, all findings are compatible with *Zauner’s conjecture* (cf. Sec. 2.3) that only three of the seven potential MU bases exist. Lifting the conjecture from $d = 6$ to arbitrary composite dimensions in a sweeping speculative move, the existence of complete sets in arbitrary composite dimensions is called into question.

Conjecture 1.1 (*Non-existence*). *Complete sets of mutually unbiased bases do not exist in composite dimensions $d \notin \mathbb{PP}$, i.e. whenever $d \neq p^k$, $p \in \mathbb{P}$, $k \in \mathbb{N}$.*

A natural attempt to upper-bound the number of MU bases, related to the prime decomposition of $d \notin \mathbb{PP}$, turns out to be *false*.

Claim (False upper bound). No more than $(p_1^{n_1} + 1)$ mutually unbiased bases exist in the *composite* dimension $d = p_1^{n_1} p_2^{n_2} \dots$, where $p_j \in \mathbb{P}$, $n_j \in \mathbb{N}$, and $p_1^{n_1}$ is the smallest prime-power present in the decomposition of d .

Thm. 6.11 of Sec. 6.9 provides counterexamples to this claim in specific dimensions such as $d = 2^2$.

13^2 : a construction using Latin squares leads to $(p_1^{n_1} + 2)$ MU bases. A universal *lower* bound on the number of MU bases in composite dimension is stated in Thm. 6.1 of Sec. 6.2.

The existence problem of complete sets of MU bases has made it into the list of the “ten most annoying questions in quantum computing” [1]. It also figures on another long-standing list of open problems in quantum information [240], and a solution wins you a prize [193].

1.2 Goals, scope and outline

The *goal* of this review is to collect what is known about mutually unbiased bases in composite dimensions $d \notin \mathbb{PP}$, complementing earlier surveys [133, 225] which were focused on prime-power dimensions, $d \in \mathbb{PP}$. Accordingly, we can afford to be brief on topics such as the construction of complete sets (see Appendix A).

This review will feel much less conclusive than the substantial monograph by Durt *et al.* [133], simply because mutually unbiased bases in composite dimensions have not yet revealed their secret. With a steady number of papers directly addressing MU bases, and an increasing interest in using MU bases (see Fig. 1.1), it seems desirable to describe the state of play, in spite—or because—of the limited progress concerning the existence problem. We wish to provide a reliable snapshot of the current state of the art (summer 2024), as well as an easy-to-navigate resource for future work.

There is much more to say about mutually unbiased bases in composite dimensions than just stating our inability to construct complete sets. We will show that considerable ingenuity has led to many results which, for example, restrict the possible form of a complete set (see the summary in Sec. 10.1), although they do not settle the central existence question. In the absence of an over-arching theory, we can still point to quite a few relevant—if seemingly disconnected—observations, and to a surprising wealth of mathematical concepts. They have been published in journals specialising in pure mathematics, combinatorics, computer science or physics, mostly quantum information and, hence, are not always easy to track down. We hope that this review allows researchers wishing to think about MU bases in composite dimensions to easily access what is known.

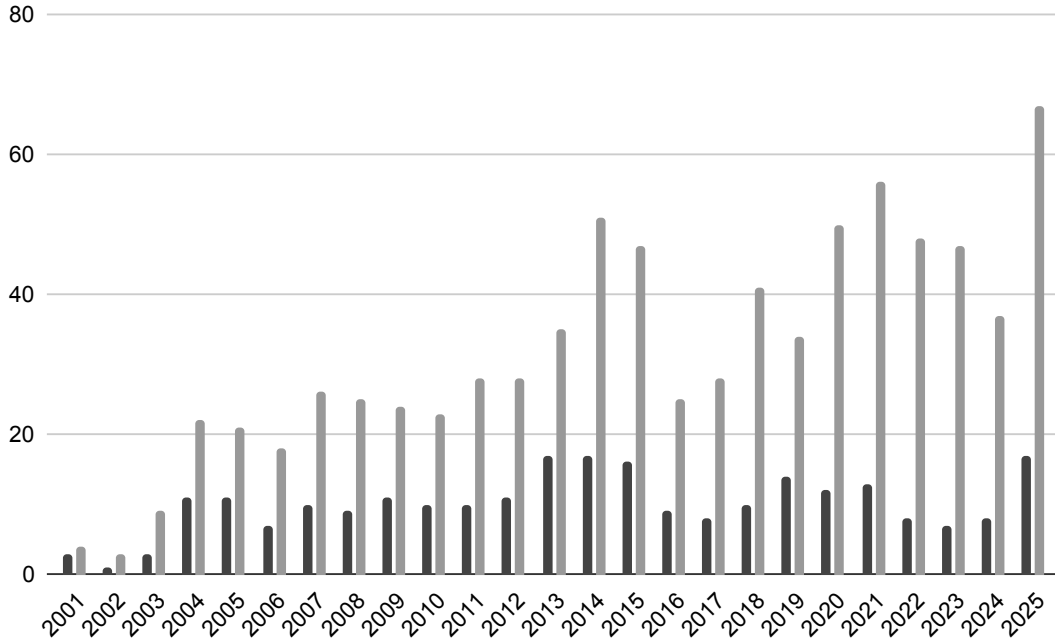


Figure 1.1: Number of preprints uploaded annually to arXiv.org in the sections computer sciences, mathematics and physics containing the expression ‘mutually unbiased’ in the *title* (dark) and in the *abstract* (light), respectively.

The impatient reader may wish to jump to Secs. 6 and 7, which constitute the core of the survey containing rigorous results in general composite dimensions and dimension six, respectively. Sec. 8 summarises results based on numerical work. MU bases for continuous variable systems require infinite-dimensional Hilbert spaces and will be discussed in Sec. 9, along with other modifications of the original existence problem.

Readers with more time on their hands may wish to explore other parts of the survey. Let us briefly *outline* its overall structure. Sec. 2 summarises the history of mutually unbiased bases in a non-technical way, which we hope newcomers to the field will find useful. Divided into three parts, it tracks down instances of mutual unbiasedness before the name was coined (Sec. 2.1), then describes the emergence of results for the case of prime-power dimensions (Sec. 2.2) and for composite dimensions (Sec. 2.3). Next, in Sec. 3 we explain why physicists are interested in mutually unbiased bases, especially within quantum theory. We cover a broad range of topics including quantum state spaces, Kochen-Specker type arguments, inequalities saturated by complete sets of MU bases, and we report experiments in which the states forming MU bases have been created successfully. Applications of (complete sets of)

MU bases can be found in Sec. 4, containing both traditional and more recent achievements.

Over time, a variety of alternative characterisations of mutually unbiased bases have been discovered. They range from specific sets of coupled polynomial equations and Hadamard matrices to Lie algebras with specific properties and so-called quantum designs. Fourteen *Equivalences*, which rigorously express complete sets of MU bases in a different mathematical setting, are described in Sec. 5. Each equivalence gives rise to a separate conjecture which captures the existence problem of MU bases in terms of a related mathematical structure. Proving or disproving any of these conjectures is tantamount to solving the original problem.

The next two sections bring together rigorous results obtained for mutually unbiased bases in composite dimensions, obtained either by analytic or computer-algebraic methods for general composite dimensions (Sec. 6), or specifically dimension six (Sec. 7). It is shown, for example, that certain types of mutually unbiased bases do not extend to complete sets. Numerical results are presented in Sec. 8. While they provide no proof of the non-existence of maximal sets, they strongly suggest their absence in the dimensions studied. We pull together evidence which has

been accumulated mainly for the case $d = 6$ but also for some other small composite dimensions.

Since the existence problem has, so far, defied all attempts to be solved in its current form, we will, in Sec. 9, draw attention to various ways in which it has been modified. The common underlying strategy is to test how robust the problem is under a partial change in the relations defining it, and ideally to gain insights which also apply to the original problem. For example, one can set the problem in a real instead of a complex Hilbert space, use a p -adic number field, change the constraints on the overlaps between states, or set the problem in a Hilbert space of countably infinite dimension.

Readers wishing to actively investigate the open existence problem might find some inspiration in Sec. 10 where, in order to be as explicit as possible, we first summarise the properties a complete set of seven MU bases in $\mathbb{C}^6$ must have. Then, we list promising strategies to solve the existence problem which have not yet been fully explored, some of which could be improved simply by using more powerful computational resources. Next, the section lists “stepping stones”, i.e. less general problems that may be helpful on the way towards a solution of the existence problem, as well as other open questions related to MU bases. Finally, we will speculate about future directions of the field.

Appendix A summarises existing constructions of complete sets of mutually unbiased bases and discusses the fact that maximal sets are not always unique. Properties of complex Hadamard matrices are collected in Appendix B, while Appendix C describes how MU bases relate to both SIC-POVMs (see Sec. 3.9) and affine planes.

2 Conceptual history of MU bases

2.1 MU bases *avant la lettre*

In 1822, Fourier [149, p. 525] described a new method to represent a function $f(x)$ depending on the variable $x \in \mathbb{R}$, by expressing it as a linear combination of continuously many wave trains with real coefficients $f(\alpha)$,

$$f(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\alpha f(\alpha) \int_{-\infty}^{\infty} dp \cos(px - p\alpha). \quad (2.1)$$

This mathematical relation, which we now interpret as a definition of Dirac’s delta distribution,

$$\delta(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dp e^{ipx}, \quad (2.2)$$

illustrates the concept of complementarity of two conjugate variables, called x and p here, albeit in a non-quantum setting. In order to localise a function about a point in x -space, we must superpose infinitely many components in Fourier- or p -space, with all coefficients having *equal* moduli. Since there is no conceptual difference between the original and the Fourier space, this argument also applies after swapping the variables. Thus, mutual unbiasedness represents a mathematical relation, independent of quantum theory. This observation suggests casting our net wide in Sec. 5 where we will gather alternative formulations of mutual unbiasedness.

Another early appearance of MU bases dates back to an 1844 paper by Hesse [184] who discusses the geometric properties of a configuration of nine points and twelve lines in a projective plane. This geometric structure showcases an intimate connection between a collection of nine equiangular vectors—known today as the *Hesse SIC* discussed in Sec. 3.9—and a related set of twelve vectors which partition into four orthogonal bases of $\mathbb{C}^3$ [55]. The overlaps between the vectors of these four bases satisfy Eqs. (1.3), resulting in (perhaps) the first instance of a complete set of MU bases.

Sylvester describes pairs of MU bases in arbitrary finite dimensions d in a paper² published in 1867 [354]: His “inverse orthogonal matrices” effectively satisfy the same conditions as complex Hadamard matrices. Sylvester conjectures (erroneously) that the construction provided exhausts all matrices of the desired form. The approach leads to matrices of order d with the first row and column being real, i.e. they are given in “dephased” form (cf. Appendix B).

In prime dimensions, $d \in \mathbb{P}$, Sylvester obtains the *Fourier matrices* F_d with entries $F_{d,jk} = \omega^{jk}/\sqrt{d}$ in row j and column k , where $j, k = 0 \dots d-1$, and ω is a d -th root of unity (see

²The introduction of the paper ends by specifying the wide-ranging audience which Sylvester has in mind: he states that his results would be “furnishing interesting food for thought, or substitute for the want of it, alike to the analyst at his desk and the fine lady in her boudoir” ([354], p. 461).

Sec. 6.1). The Fourier matrices F_3 and F_5 are displayed explicitly. Furthermore, for any decomposition of the number $d = d_1 d_2 \dots$, the construction of inverse orthogonal matrices results in direct products $F_{d_1} \otimes F_{d_2} \otimes \dots$ of Fourier matrices, some of which are now known to be equivalent to each other. Sylvester pays particular attention to dimensions which are powers of two, with explicit expressions given for $d = 2, 4, 8$. In the case of $d = 4$, both F_4 and $F_2 \otimes F_2$ are displayed. The Fourier matrices will play an important role throughout the discussion of mutually unbiased bases (e.g. see Sec. 7.3).

Nearly thirty years later, Hadamard searches for the maximal value of matrix determinants given that the moduli of their entries do not exceed a given value [176]. Choosing the bound to be 1, he shows that Sylvester’s “inverse orthogonal matrices” produce the desired maximum, describing them as Vandermonde determinants formed by the roots of unity. Hadamard points out that these are not the only solutions: In dimension four he adds a collection of matrices depending on one continuous parameter, known today as the Fourier family (see Sec. 6.1 for details). This set contains the special cases already considered by Sylvester, and it provides—in modern parlance—the first examples of complex Hadamard matrices with entries other than roots of unity. The paper concludes with the question “for which values of n there exist maximal determinants with real elements” ([176, p. 246]) which—under the heading of the *Hadamard conjecture*—has fascinated mathematicians ever since [182]. Sets of real Hadamard matrices with all elements ± 1 define mutually unbiased bases consisting of real vectors only; they have been studied in their own right (see Sec. 9.1) without shedding much light on the existence problem in complex spaces.

One main driving force behind further studies of mutually unbiased bases has been quantum theory (see Sec. 3). The motto of this review stems from Jordan’s fundamental paper [208] in 1927, where he rolls the four variants of quantum theory existing at the time into a single one; his remark may be one of the first explicit descriptions of unbiasedness. We are not aware of other authors stating mutual unbiasedness before 1927.

The interplay between position and momentum measurements also appears in von Neumann’s classic book, published originally in 1932:

If q has a very small dispersion in an ensemble, then the p measurement with the accuracy (i.e., dispersion) ε sets up a q dispersion of at least $h/4\pi\varepsilon$ [...], i.e., everything is ruined [428, pp. 305-6 (footnote 162)].

Note the negative connotation of the word “ruin” (‘verderben’ in the German version³) used to describe the effect of measuring the observable complementary to position.

In their well-known paper from 1935, Einstein, Podolski and Rosen [134] use an entangled state of two particles to argue that quantum theory is incomplete. Their reasoning starts by describing the impossibility to attribute a definite value of position to a single quantum particle which resides in a momentum eigenstate, and it invokes Born’s probability interpretation of the squared overlaps of states [69]. Their discussion closely follows Weyl’s 1928 book on group theory and quantum mechanics [394, 395] in which he points out that the x -component of the momentum of a particle “*cannot assume a definite value with certainty when x [the x -component of its position] does, and conversely*” (p. 55; original emphasis). This statement also captures mutual unbiasedness but not as precisely as Jordan’s wording.

An important step in the history of mutually unbiased bases is due to Schwinger in 1960, building on Weyl’s work. The influential study of unitary operator bases [331] opens up three new vistas: (i) MU bases are defined and subsequently constructed in a finite-dimensional space; (ii) the generators of a pair of MU bases in a finite-dimensional Hilbert space $\mathcal{H}$ can be used to construct a basis of the unitary operators acting on $\mathcal{H}$; (iii) mutual unbiasedness is linked to the finite-dimensional Heisenberg-Weyl group on the space $\mathbb{C}^d$.

Introducing a pair of unitary operators U and V by the requirement that they cyclically permute their respective eigenstates, Schwinger de-

³“Wenn q in einer Gesamtheit kaum streut, so wird die p -Messung mit der Genauigkeit (d. h. Streuung) ε die q -Streuung auf mindestens $h/4\pi\varepsilon$ heraufsetzen [...]-d. h. alles verderben.” [427, p. 256 (footnote 162)]

rives the commutation relation

$$VU = e^{\frac{2\pi i}{d}} UV, \quad (2.3)$$

which implies that the operators U and V are maximally incompatible, i.e., their eigenstates form orthonormal bases and come with pairwise constant overlaps, Eq. (1.3). When d is a prime number, suitable products of U and V form a basis of the bounded operators $\mathcal{B}(\mathbb{C}^d)$ acting on the space $\mathbb{C}^d$, and their eigenstates define a set of $(d+1)$ MU bases (see Sec. 5.4). A finite-dimensional equivalent of the relation Eq. (2.2) exists for the eigenstates of U and V , which goes hand in hand with interpreting them as d eigenstates of finite displacements and of momentum boosts, respectively. It becomes plain to see that the Fourier transformation underpins the concept of mutual unbiasedness in both finite- and infinite-dimensional spaces.

Also in 1962, Schlögl [329] points out that the eigenstates of the Pauli matrices in $\mathbb{C}^2$ form a triple of MU bases. In a finite-dimensional setting, he searches for non-commuting observables which are pairwise “informations-fremd” (“information-agnostic”), a concept which captures the idea of mutual unbiasedness while avoiding confusion with the notion of “complementary” observables. It is shown that no more than two observables with this property can exist in dimensions $d > 2$ —by allowing *Hermitian* operators only, he misses the fact that the eigenbases of *unitary* operators may also form sets of states which are “informations-fremd”. In dimension $d = 2$, however, he identifies the triple of MU bases associated with the three observables corresponding to orthogonal spin components which are, of course, both Hermitian and unitary.

Hadamard’s influential paper generated a large body of research limited to matrices with real elements only, although Sylvester’s earlier work allowed for complex matrix elements of modulus one. Historically speaking, a more accurate naming convention would be to call “complex Hadamard matrices” *Sylvester matrices*, and to reserve the label *Hadamard matrices* to those with real entries only. In 1962, Butson [90] brought Sylvester’s *complex* Hadamard matrices back to the fold, by initiating the study of complex-valued Hadamard matrices with entries given by finite roots of unity (cf. Sec. 9.2).

It took another 20 years for further contributions relevant for MU bases to emerge. Then,

however, within about two years, we witness progress in several unrelated fields: *signal processing*, *Lie* or, more generally, *matrix algebras*, and *maximal Abelian subalgebras*. These developments all revolve around the mathematical structure which underpins mutual unbiasedness. MU bases also resurface in quantum theory, in the context of *quantum state determination* (see Sec. 2.2 for this topic).

Correlations of complex signals—Periodic sequences of complex numbers and their correlations were studied in great detail in the 1970’s, to set up efficient communication protocols with radar signals. Given sets of sequences of d complex numbers, it is important to control both the overlap between a sequence and its (shifted) complex conjugate and between two different sequences within one set. These quantities are known as *auto-* and *cross-correlations*, respectively. In 1979, Sarwate [327] shows that a trade-off relation between good auto-correlations and good cross-correlations exists. Since “good” in this context means “small”, the two types of correlations should be minimised simultaneously. This requirement gives rise to an additive type of uncertainty relation, structurally similar to the one which applies to the position and momentum variables of a quantum particle, for example.

For odd prime values of d , Sarwate identifies $(d-1)$ equimodular sequences which minimise the trade-off relation. He points out that, by adding the standard basis of the space $\mathbb{C}^d$, there are d sets of sequences in total which saturate the trade-off relation. The conditions satisfied by these sequences are equivalent to those satisfied by d MU bases in the space $\mathbb{C}^d$. Since d MU bases uniquely determine an additional basis MU to the given ones (see Sec. 6.3), Sarwate had, in fact, implicitly constructed a complete set of MU bases.

The existence of sequences with desirable *auto-correlations* in terms of complex exponentials depending on quadratic polynomials had already been noticed by Chu in 1972 [118]. Sarwate’s contribution consists of adding a condition on the *cross-correlations* between different sequences, ensuring the mutual unbiasedness of different bases.

Alltop [9] constructs $(d+1)$ periodic sequences in $\mathbb{C}^d$ for prime numbers d greater than three (cf. Appendix A.3). His result is based on the prop-

erties of complex third-order polynomials as arguments of exponential functions. In addition to these *cubic* phase sequences, he also constructs *quadratic* phase sequences, pointing out that they essentially reproduce Sarwate's result of d sequences.

Orthogonal decompositions of Lie algebras—Still in 1972, Kostrikin *et al.* [237] initiated a search for orthogonal decompositions of the Lie groups of type A_d , having Lie algebras sl_{d+1} . Observations made for values of $d \leq 8$ resulted in the *Winnie-the-Pooh problem* (5.1) and the conjecture that decompositions would only exist for prime-powers, i.e. when $d + 1 = p^n$, for any $p \in \mathbb{P}$, $n \in \mathbb{N}$. In Sec. 5.5 we describe the problem in detail and explain how it achieved its name. A direct link between orthogonal decompositions of certain Lie algebras and complete sets of MU bases was established only in 2005 [73].

Maximal Abelian subalgebras (MASAs)—In 1983, Popa [312] investigates mutually orthogonal and maximal Abelian $*$ -subalgebras (MASAs) of von Neumann algebras. The results pertaining to finite-dimensional matrix algebras are, with hindsight, statements about the existence of MU bases (cf. Sec. 5.6). Effectively, Popa constructs $(p+1)$ MASAs for complex matrices of order $p \times p$, i.e. in dimensions $d = p$. When the dimension d is not a prime, at least $(p_1 + 1)$ MASAs are constructed, with p_1 being the smallest prime divisor of d . It is stated clearly that there are at least three MASAs in *all* dimensions greater than two, $d \geq 2$, and that there cannot be more than $(d + 1)$ MASAs for dimension d . In today's quantum parlance, Popa's arguments are based on the Heisenberg-Weyl algebra, using “clock-and-shift” operators.

Popa conjectures that in prime dimensions all pairs of MASAs are equivalent to the standard Fourier pair. This claim was disproved first by de la Harpe and Jones [423] who show that for dimensions $p \geq 13$ and $p \equiv 1 \pmod{4}$, other pairs exist. Munemasa and Watatani [290] extend this result to primes p equal to or larger than seven if they are of the form $p \equiv 3 \pmod{4}$. Thus, pairs of MU bases inequivalent to the standard Heisenberg-Weyl pair exist in *all* odd prime dimensions $d \geq 7$. Interestingly, these constructions make use of graph theory—Payley graphs in particular—a topic which has figured in the context of MU bases only rarely.

A decade later, Haagerup [174] showed in a *tour de force* that in dimension $d = 5$, all pairs of MU bases are unitarily equivalent to the standard Fourier pair. This had been the only open case left after the work in the sequel of Popa's conjecture. Just as with Sylvester and Kraus [239] (cf. below), Haagerup “dephases” Hadamard matrices in order to remove trivial equivalences. As an aside, he also introduced a necessary criterion for the equivalence of Hadamard matrices of the same order. Given an $n \times n$ Hadamard matrix H , construct its *Haagerup set* $\Lambda(H)$ defined in Eq. (B.1), which contains the products of four matrix elements H_{jk} , $j, k = 1, \dots, n$. By construction, this set of products is invariant under dephasing transformations so that two Hadamard matrices with different Haagerup sets cannot be equivalent; there exist, however, inequivalent Hadamard matrices with identical Haagerup sets (see Appendix B).

Haagerup also establishes a close connection between MU bases and the problem of *cyclic n -roots*, i.e., the solutions of a highly symmetrical set of n equations (see Sec. 6.4) introduced by Björck [62] in 1985. The equations arise when searching for all ‘*bi-equimodular*’ vectors $x \in \mathbb{C}^n$, i.e. *all x with coordinates of constant absolute value such that the Fourier transform of x is a vector with coordinates of constant absolute value* [60, p. 331], and it was solved for small values of n using computer-algebraic methods. When $n = 5$, for example, only “classical” roots (i.e. of Fourier-type) exist. In contrast, among the 156 cyclic 6-roots given by Björck and Fröberg [60], Haagerup identifies 48 which are of modulus one, and thus are relevant in the context of MASAs or, equivalently, MU bases. Twelve of these roots are the expected “classical” ones and the remaining 36 (which Haagerup spells out explicitly) are of a different type (see Sec. 7.3 for further analysis).

Kraus, in 1987, considered quantum systems with finite-dimensional state spaces and, referring back to Schwinger [331], used mutual unbiasedness to define pairs of *complementary* observables: *exact knowledge of the measured value of one observable implies maximal uncertainty of the measured value of the other* [239, p. 3070]. He shows that all pairs for $d = 2$ and $d = 3$, respectively, are equivalent and explains how to construct complementary pairs of bases in systems of product dimensions $d = p_1 p_2$, namely by

tensoring MU bases of the factors $\mathbb{C}^{p_j}$, $j = 1, 2$, of the space $\mathbb{C}^{p_1 p_2}$. However, this construction does not necessarily exhaust all MU pairs, as he shows for the case $p_1 = p_2 = 2$. The set of all inequivalent pairs of MU bases in dimension $d = 4$ is presented in the form of a dephased complex Hadamard matrix (see Sec. 5.2) which depends on *one* free real parameter. Kraus states that a similar construction for $d = 8$ leads to a family of MU pairs depending on *five* real parameters, while declaring the general classification to be an (allegedly complicated) open problem. Thus, Kraus provides early examples both of non-unique complementary *pairs* in product dimensions and of the existence of continuous families of such pairs (cf. Sec. 3.3 for his contribution in the context of complementarity and Sec. 3.13 for the general definition of equivalence classes of sets of MU bases).

2.2 Prime-power dimensions

Nearly 30 years after Weyl's and Schwinger's work, the concept underlying MU bases re-emerged in the 1980's in contributions addressing a fundamental problem of quantum theory: *quantum state reconstruction*, which asks for a unique characterisation of arbitrary mixed quantum states in terms of expectation values.

In 1981, Ivanović exploited the properties of Gauss sums to construct states which form $(p+1)$ MU bases in spaces with prime dimensions $p \in \mathbb{P}$ [203]. More specifically, he decomposed the space of unitary operators into orthogonal hyperplanes which are associated with sets of commuting operators suitable for quantum state determination. Ivanović appears to be the first to show that no more than $(p+1)$ MU bases can exist in the space $\mathbb{C}^p$. This result goes beyond Schwinger who also constructed $(p+1)$ MU bases but did not show this to be maximal.

A few years later, Wootters and Fields extended Ivanović's contribution from Hilbert spaces with prime dimension to spaces of prime-power dimension $d \in \mathbb{PP}$, both even and odd [401]. The authors introduce the notion of *mutual unbiasedness* both for sets of states forming orthonormal bases and for the associated measurements, i.e. sets of commuting projections onto one-dimensional orthogonal subspaces of a Hilbert space $\mathbb{C}^d$. The construction rests on properties of *Galois* (or *finite*) *fields* with d elements,

which exist as long as the dimension of the space is a power of a prime number. It is also shown that the outlined method of state reconstruction is *optimal* in the sense that the required measurements come with the smallest possible statistical errors. Furthermore, the upper limit of $(d+1)$ MU bases in the space $\mathbb{C}^d$ is derived.

Today, many other ways to construct complete sets of MU bases in prime-power dimensions are known, some of which we present in Appendix A (see also the review [133]). According to Godsil and Roy [157], nearly all complete sets of MU bases known (in 2009) could, effectively, be obtained from one single construction presented by Calderbank *et al.* [92] in their study of *symplectic spreads* and $\mathbb{Z}_4$ -Kerdock codes used for error correction. Abdukhalikov [3] introduced an independent construction of complete sets of MU bases and classified the existing methods.

Are complete sets of MU bases unique for a given prime-power dimension? Two sets of MU bases are said to be *equivalent* under unitary transformations if there is a single unitary which maps one set to the other. For example, all complete sets of MU bases in $\mathbb{C}^d$, with $2 \leq d \leq 5$, are equivalent [77, 174]; in other words, there exists only a single set of $(d+1)$ MU bases in each of these dimensions (apart from trivial dephased versions).

The smallest dimension in which *inequivalent* complete sets of MU bases are known to occur is $d = 27$, as pointed out by Kantor in 2012 [212]. To reach this conclusion, Kantor first showed that a symplectic spread determines a complete set of MU bases and, secondly, uses the fact that two spreads are equivalent to each other if and only if these spreads can be mapped to each other by a symplectic transformation (cf. [92]). Inequivalent symplectic spreads were identified already in 1983, for example, if $d = 2^n$ with an odd number $n > 3$, in the context of coding theory [217]. Explicit examples of inequivalent maximal sets of MU bases have been given in [152], for $d = p^n \in \mathbb{PP}$, with an odd prime p . Some erroneous examples are presented in [335].

The focus of our review is the notable *lack* of MU bases in *composite* dimensions rather than the structure of MU bases in prime-power dimensions. Initially barely worth mentioning, the curious non-existence of complete sets in those dimensions has evolved into a formidable and long-

standing open problem. In the following section we retrace the steps which led researchers to become aware of this problem.

2.3 Composite dimensions $d \notin \mathbb{PP}$

Many early papers on MU bases were focused on the explicit construction of complete sets in prime and prime-power dimensions, $d \in \mathbb{PP}$. Checking the first few integers for the relative frequencies of prime and composite numbers suggests that composite dimensions ($d \notin \mathbb{PP}$) are rare: up to $d = 27$, say, five out of six number are primes or prime-powers. However, this observation is deceptive: fewer than 0.1% of the numbers below 10^{1000} are primes or prime-powers. In fact, the probability for a randomly sampled positive integer less than N to be composite approaches the value one for $N \rightarrow \infty$,

$$\text{prob}(\text{composite } d < N) \simeq 1 - \frac{1}{\log N}. \quad (2.4)$$

This relation follows from Hadamard’s and de la Vallée Poussin’s *prime-number theorem* upon ignoring the minute contribution of the prime-powers. The punchline is that for most quantum system with a large, randomly chosen dimension d we currently are *not* in a position to construct a complete set of MU bases. Let us review how the important insight into this shortcoming emerged and describe some of the attempts to clarify the unexpected situation.

In the early 1960’s, both Schwinger’s construction of unitary operator bases [331] and Butson’s construction of complex Hadamard matrices [90] were set in spaces of arbitrary integer dimensions d . However, it did not occur to them to look for a possible difference between spaces of prime-power and composite dimensions; effectively, they were interested in problems which translate into a search for *pairs* of MU bases known to exist in *all* dimensions $d \in \mathbb{N}$.

Nearly two decades later and only *en passant*, Sarwate [327] and Alltop [9] mention the case of complex sequences with periods given by *composite* numbers, $d \notin \mathbb{PP}$. They point out that their techniques can still be used to construct some sequences with the desired properties but only a small number, limited by the lowest prime factor p_1 of d if the dimension is given by $d = p_1 p_2 \dots p_r$, with $p_1 < p_2 < \dots < p_r$.

Soon after, Kostrikin *et al.* [237] envisage—apparently for the first time—that complex Hilbert spaces of composite and prime-power dimensions, respectively, might differ fundamentally when constructing specific mathematical objects. If there is no solution to Winnie-the-Pooh’s problem (cf. Sec. 5.5), i.e. the desired orthogonal decomposition of the relevant Lie algebra does not always exist, then the number of MU bases in a Hilbert space of composite dimension must drop *below* $(d + 1)$, the strict upper bound on their number in any dimension.

In the context of MASAs (cf. Sec. 2.1), Popa [312] obtained a similar result about MU bases in spaces of composite dimension d : he showed how to construct at least $(p_1 + 1)$ MASAs where p_1 is the smallest prime divisor of d . In addition, he clearly states in his paper from 1983—possibly for the first time—that there are at least three MASAs, and hence MU bases, in *all* dimensions $d \geq 2$.

Independently of Sarwate and Alltop, Kraus [239] spells out in 1987 the tensor-product construction of pairs of complementary observables for bipartite finite quantum systems of dimension $d = p_1 p_2$. As already mentioned, he was aware of the fact that pairs of MU bases in $\mathbb{C}^{p_1 p_2 \dots}$ can be found from tensoring MU bases, but he does not launch a systematic investigation into the construction of larger sets in composite dimensions.

While Wootters and Fields successfully construct complete sets of MU bases in all prime-power dimensions [401], they also point out in their 1989 paper that the method will *not* work in composite dimensions $d \notin \mathbb{PP}$. Since “there is no finite field whose number of elements is not a power of a prime”, any method producing a complete set of MU bases in other dimensions “must be very different from the procedures used here” [401, p. 376]. Lacking such a complete set would rule out, for example, the optimal state reconstruction method presented in their paper.

In an unpublished diploma thesis completed in 1991, Zauner proposes a “Vermutung”—i.e. an educated guess—which states that “there are no four non-commuting 6×6 matrices, each having six different eigenvalues, which are independent with respect to $\mathbb{I}/6$ ” [411, p. 75]. His notion of independence is an alternative way to demand that the matrices represent MU bases, with their column vectors possessing the correct overlaps.

The main thrust of Zauner’s study had been to develop the concept of independent observables in quantum theory in close analogy to the concept of independent observables in classical probability theory.

Retrospectively—as pointed out by Klappe-necker and Rötteler [229] in 2004—the main novelty in Zauner’s work is the explicit conjecture that in the Hilbert space of composite dimension $d = 6$, the number of MU bases is limited to *three* (and not *seven*, which the prime-power case would suggest). In his thesis from 1999, the author surmises that such a limitation exists, using the language of quantum designs [412] (see [413] for an English translation). Here we reproduce the original statement corresponding to the non-existence conjecture presented in Sec. 1.1.

Conjecture 2.1 (Zauner 1999). *Presumably a complex, affine quantum design with $b = g = 6$, $r = 1$, $\lambda = 1/6$, and $k = 4$ does not exist either. [413, p. 494]*

A *quantum design* (see Sec. 5.8) consists of k sets of g orthogonal projection matrices in a b -dimensional complex Hilbert space. The rank of each projector is r , and the scalar product of two projectors belonging to different sets is given by λ . The case of rank-one projectors, $r = 1$, corresponds to the case of MU bases if $\lambda = 1/d$, and the design is *affine* (or of degree 2) if the scalar products between any two projectors are equal to either zero or λ .

Zauner’s construction of three MU bases in the space $\mathbb{C}^6$ is based on the triple existing in dimension two, i.e. the smallest factor of six. More generally, this method leads to $(p_1^{n_1} + 1)$ MU bases where $p_1^{n_1}$ is the smallest prime-power factor in the decomposition of the dimension $d = p_1^{n_1} p_2^{n_2} \dots p_r^{n_r}$ [229]. This suggests the (false) *Claim* in Sec. 1.1 that the upper-bound on the number of MU bases in a composite dimension is $(p_1^{n_1} + 1)$.

In a long and influential paper published in 1997, Haagerup [174] explores the existence of Hadamard matrices—and thus MU bases—in composite dimensions. He shows that for dimensions $d = pq$ it is possible to construct families of Hadamard matrices depending on $(p - 1)(q - 1)$ parameters; the implied two-parameter set for $d = 6$ is given explicitly. Two further Hadamard matrices are constructed which are inequivalent

to the 6×6 Fourier matrix. These results are important, of course, because each known complex Hadamard matrix may represent a basis in a larger set of MU bases. From 2004, onwards, new 6×6 Hadamard matrices have appeared sporadically, including Diță’s one-parameter family [130], a three-parameter family by Karlsson that encompasses all earlier non-isolated examples [220], and a non-constructive proof by Bondal and Zhdanovskiy that a four-parameter family exists [67].

In 2005, Archer [20] attempted to systematically transfer known constructions of complete sets of MU bases in prime-power dimensions to composite dimensions, without success. This negative outcome explains the growing interest in alternative ways to search for larger sets of MU bases, championed mainly by researchers with a background in quantum theory.

Around the same time, Grassl used *computer-algebraic methods* (Sec. 7.3) to prove that no pair of Heisenberg-Weyl-type MU bases can be extended to more than three bases in $d = 6$ [166]. This important result, confirming the findings obtained for cyclic n -roots (see Sec. 6.4), paved the way for further computer-assisted studies carried out in the quantum community. In 2007, Bengtsson *et al.* [49] searched *numerically* for Butson-type Hadamard matrices of order six by restricting the elements to d -th or $(2d)$ -th roots of unity, based on the observation that all known complete sets of MU bases were of this particular form. This paper also introduced a *distance* between bases in a Hilbert space, allowing one to frame the search for MU bases in terms of a global minimum of a scalar function (Sec. 8.2). Butterly and Hall took up the idea in an attempt to identify *four* MU bases in dimension six [91] but failed to find such a set. A measure of unbiasedness related to the average success probability of quantum random access codes was shown by Aguilar *et al.* [7] to be useful for the same purpose.

The numerical approach was refined soon after by introducing the concept of *MU constellations* [78], defined as sets of vectors which are either MU or orthogonal, but not necessarily forming entire orthonormal bases. The increased flexibility leads to considerable computational simplifications. In dimension six, for example, it is much less onerous to numerically search for a single state that is mutually unbiased to three

MU bases than to deal with a set of four MU bases. The results are among the most extensive numerical data, strongly supporting the non-existence of constellations containing more than three MU bases (cf. Sec. 8.3).

Some success—in the form of analytic results—has been achieved by strategies that impose additional constraints on sets of MU bases. For example, we now have analytic proofs that no more than three *nice* [21], *monomial* [73], or *product* [285] MU bases exist in a Hilbert space of dimension six (cf. Secs. 6.5–6.7). Bases are “nice” or “monomial” if the unitary operator basis from which they are constructed is a nice error basis or a monomial basis, respectively. Both of these properties are shared by all known complete sets of MU bases in prime-power dimensions.

It is also possible to express the existence problem as a *semi-definite program* [80] (cf. Sec. 10.2). But again, no results have been obtained which go beyond a proof of principle, i.e. the reproduction of known results in low dimensions.

It is instructive to compare the number of *free parameters* in $(d+1)$ arbitrary bases of the space $\mathbb{C}^d$ with the number of constraints which these $d(d+1)$ states must satisfy to represent a complete set of MU bases [78]. In dimension seven, for example, 56 pure states—which depend on 288 independent parameters—have to satisfy 1176 constraints. This example shows that the surprising feature of MU bases is, actually, not the *absence* of complete sets in composite dimensions but their *existence* in prime-power dimension, for any $d > 2$. The constraints must align with some fundamental structure prevailing in the space $\mathbb{C}^7$ and degenerate in some way, which then allows for the existence of a complete set. It is likely that the number-theoretic consequences of d being prime—such as the existence of a suitable Galois field—play a central role. This perspective explains, in some sense, why it will be hard to prove Zauner’s conjecture: spaces of composite dimensions do not support structures which, in the case of prime-power dimensions, allow for the existence of complete sets.

Could it be that the existence of maximal sets of MU bases is an *undecidable* question? The answer is no: by coarse-graining the parameter space, Jaming *et al.* [205, 206] showed that the existence problem can be expressed in terms of a set of rigorous inequalities which, in principle,

can be checked numerically to hold (or not) in any composite dimension (cf. the discussion of Thm. 7.7). However, the resources required to implement this *algorithm* are formidable, even for $d = 6$. As a proof of principle, a restricted case—rather than the general existence problem in dimension six—has been studied successfully: it is impossible to extend pairs consisting of the identity and any member of the Fourier family to a quadruple of MU bases. Other algorithmic approaches to the existence problem exist which do not rely on numerical approximations but remain unfeasible from a practical point of view [119].

In view of the overall difficulty to resolve the existence problem, various authors have introduced *variations* of the original problem which will be reviewed in Sec. 9. The modifications either relax the original constraints or impose additional ones to define new but structurally similar existence problems. For example, the problem may be set in a real, quaternionic, p -adic or infinite-dimensional Hilbert space, instead of the standard *complex* Hilbert space. Alternatively, one can search for measurements which satisfy an approximate condition of unbiasedness, or non-projective measurements which satisfy another form of complementarity.

3 MU bases in quantum theory

This section will illustrate the role played by mutually unbiased bases in quantum physics. We describe their relation to other important concepts, ranging from foundational aspects such as Kochen-Specker’s theorem to experimental realisations of MU bases. Applications of MU bases, i.e. scenarios in which they are crucial to achieve specific tasks such as quantum cryptography or quantum state reconstruction, will be considered separately, in Sec. 4. Nevertheless, both sections aim at answering the question raised in 2005 [53]: “Given a complete set of MU bases, what can we do with them?”—and thereby motivating the search for complete sets in composite dimensions.

3.1 Quantum degrees of freedom

In his paper on the representations of the Heisenberg-Weyl group, Schwinger [331] considered Hilbert spaces of finite dimension d , with prime decomposition $d = p_1 p_2 \dots p_k$. He pro-

posed to associate one degree of freedom to each of the factors. This suggestion is motivated by the idea that a quantum degree of freedom should be associated with an irreducible representation of operators satisfying the canonical commutation relations, as the position and momentum of a quantum particle do. However, in a finite-dimensional Hilbert space only “integrated” versions of these commutation relations exist, satisfied by operators forming the Heisenberg-Weyl algebra. Hence, a quantum system with a six-dimensional state space $\mathbb{C}^6$ would have two degrees of freedom.⁴

While natural, the conceptual advantage of defining degrees of freedom in this way remains unclear, and it is not obvious whether observable consequences follow. Some quantum systems may have six orthogonal levels because they are indeed composed of two distinct physical systems with two and three orthogonal states, respectively; hence, two degrees of freedom may be introduced naturally as they are associated with the subsystems. However, the decomposition into distinct parts may not be of interest [158] or, in the case of a—yet to be discovered—elementary particle with spin $s = 5/2$, no physical constituents may exist.

It is an intriguing idea to associate degrees of freedom to irreducible representations. However, combined with a hypothetical lack of complete sets of MU bases in composite dimensions, an awkward *structural* discrepancy would emerge [78], raising physicists’ eyebrows. Consider systems with four and six levels, for example, both of which would be endowed with two degrees of freedom. Nevertheless, the collections of observables in these systems possess fundamentally distinct properties if a complete set of MU bases exists only for one of them. Such a difference seems acceptable only when the number of degrees of freedom differs, e.g. when comparing systems of dimensions five and six.

⁴Connes is reported to have expressed this idea in the context of quantum field theory when stating that he “was immediately led to the idea that somehow passing from the integers to the primes is very similar to passing from quantum field theory, as we observe it, to the elementary particles, whatever they are” [324, p. 204].

3.2 Quantum state-space geometry

In 1981, Ivanović sets up a procedure to determine unknown quantum states (cf. Sec. 4.1) for systems with Hilbert space $\mathbb{C}^d$ [203]. He points out that a complete set of $(d + 1)$ MU bases (if it exists) induces a highly symmetric, orthogonal decomposition of the quantum state space, i.e. the density operators of the system.

To derive this decomposition, the set of $d \times d$ Hermitian matrices is considered as a real Euclidean space with dimension d^2 , the scalar product of two Hermitian matrices being defined by the trace of their product. Non-negative density matrices ρ of a d -level system are a subset of that space satisfying the normalisation condition $\text{Tr}(\rho \mathbb{I}/d) = 1/d$; hence, they live in a $(d^2 - 1)$ -dimensional hyperplane of the space. The projectors $P_b(v) = |v_b\rangle\langle v_b|$ and $P_{b'}(v') = |v'_{b'}\rangle\langle v'_{b'}|$ on states contained in different MU bases, i.e. for $b \neq b'$, are *not* orthogonal to each other according to Eq. (1.3), since

$$\text{Tr}(P_b(v) P_{b'}(v')) = \frac{1}{d}. \quad (3.1)$$

However, the scalar products between their “shifted” versions $\bar{P}_b(v) = |v_b\rangle\langle v_b| - \mathbb{I}/d$, etc. do vanish, which means each MU basis is confined to a plane orthogonal to the plane associated with any other MU basis. Taken together, the $(d + 1)$ planes provide—upon adding in the identity $\mathbb{I}$ —an orthogonal decomposition of the state space, explaining the usefulness of MU bases for quantum state reconstruction.

This geometric picture has been developed further by Bengtsson and Ericsson [50, 53]. By defining the so-called *complementarity polytope*, the existence problem of MU bases can be expressed in an entirely geometric setting. A complete set of MU bases gives rise to this convex polytope in the space of Hermitian matrices in the following way: construct $(d + 1)$ regular simplices by associating d equidistant vertices to the projectors of each MU basis and form the convex hull of the $(d^2 + d)$ vertices characterising the non-overlapping simplices.

As a geometric object, the *complementarity polytope* may be rotated in the Euclidean space of Hermitian matrices. In general, its vertices will move in such a way that they are no longer associated with rank-one projection operators but other non-positive Hermitian matrices, except

when $d = 2$. In other words, the rotated complementarity polytope will not necessarily sit inside the body of density matrices. However, every construction of a complete set of MU bases successfully embeds the complementarity polytope in the set of density matrices, associating projection operators with its vertices.

Turning this observation around, the existence problem of complete sets of MU bases can be expressed in the following form: given a complementarity polytope in the d^2 -dimensional Euclidean space, is it possible to rotate it in such a way that it will fit inside the body of density matrices? This geometric picture links the existence problem with another problem known to be difficult, namely to efficiently characterise the structure of the convex body of density matrices of quantum systems. Already for a qutrit, the eight-dimensional analog of the Bloch ball turns out to be an intricate geometrical object (see e.g. [136]).

3.3 Complementarity

Early insights into the properties of pairs of quantum mechanical observables which give rise to MU bases were mentioned in Sec. 2.1. However, the buzzword of the times was *complementarity*, proposed by Bohr in 1927 as a fundamental property of quantum systems, albeit expressed in a rather non-technical fashion (see the write-up of his Como lecture [66], for example). Complementarity is at the heart of uncertainty relations: if one measures one observable of a complementary pair—the position of a quantum particle, say—then the outcomes of a subsequent measurement of the other observable—momentum—are maximally uncertain. In Bohr’s words:

The momentum of a particle, on the other hand, can be determined with any desired degree of accuracy [...], but then the determination of the space coordinates of the particle becomes correspondingly less accurate. [66, p. 582]

One way to give meaning to the statement that two observables are complementary is to say that their eigenstates form a *pair of mutually unbiased bases* satisfying Eq. (1.2) of Definition 1.1. This is a neat and satisfactory approach to complementarity which, however, has not yet made its

way into the average textbook. Many of the traditional ways to think about complementary observables have been reviewed in [87].

Weyl and Jordan made early *qualitative* statements about the complementary observables of a quantum particle (cf. Sec. 2.1). In 1960, Schwinger provided a *quantitative* analysis of this concept by setting it in a state space of finite dimension d . He considers a pair of “properties U and V ” described by unitary operators satisfying the relation (2.3), and shows that the transition probabilities between their eigenstates are constant,

$$p(u', v'') = |\langle u' | v'' \rangle|^2 = \frac{1}{d}, \quad (3.2)$$

where u' and v'' label the eigenvalues of the unitaries U and V , respectively. Next, Schwinger considers the expression

$$p(u', v, u'') = \sum_{v'} p(u', v') p(v', u'') = \frac{1}{d}, \quad (3.3)$$

i.e. the probability to find a specific value of u' given that the system starts out in another eigenstate of U with label u'' , say, and assuming an intermediate measurement in the V basis. The independence of the probability $p(u', v, u'')$ of all its arguments expresses the fact that the intermediate measurement of V completely erases any information about the initial state. In Schwinger’s own words, Eq. (3.3) shows that “the properties U and V exhibit the maximum degree of incompatibility” [331, p. 575]. Finally, he remarks that this property is tantamount to “the attribute of complementarity” (p. 579, footnote 3).

Observables which either satisfy the canonical commutation relations or their integrated version (2.3) are necessarily complementary in the sense that their eigenbases are mutually unbiased, i.e. the squared moduli of their overlaps are state independent, as in Eq. (3.2). Accardi observed in 1984 that the converse statement is not necessarily true: constant transition probabilities between all states of two bases can also arise from operators which do not satisfy the canonical commutation relations [4]. Accordingly, he suggests classifying all pairs of observables with this property, in both finite- and infinite-dimensional Hilbert spaces. This problem is still open since, in the finite-dimensional case, it means listing all complex Hadamard matrices of order d , a task not yet realised even for dimension six (see *Problem 10.4*

in Sec. 10.2). In 2002, Cassinelli and Varadarajan [100] answered another question raised by Accardi’s question, regarding the uniqueness of complementary projection-valued measures, both in the finite- and the infinite-dimensional setting.

Schwinger’s paper apparently prompted Kraus to systematically classify pairs of complementary observables in low dimensions [239], without mentioning Accardi. As described at the end of Sec. 2.1, Kraus established the existence of parameter-dependent, *unitarily inequivalent* families of MU bases for $d = 4$ and $d = 8$, while he found pairs of complementary observables to be unique in dimensions two and three, up to unitary equivalences.

In a paper written on the occasion of Carl Friedrich von Weizsäcker’s 90th birthday, Brukner and Zeilinger revisit his idea of the “ur” as an elementary carrier of information, endowed with a two-dimensional (complex) Hilbert space. They consider “mutually complementary measurements” which are associated with the orthogonal components of a quantum spin, thereby using the triple of MU bases for a spin- $\frac{1}{2}$ [83]. Their argument aligns with Weizsäcker’s tenet that a fundamental link might exist between (i) us necessarily performing experiments in *three-dimensional* Euclidean space and (ii) a corresponding number of complementary measurements.

In a study of amplitude and phase operators, Klimov *et al.* (2005) introduce the notion of “mutually complementary observables” to denote sets of operators with MU eigenbases [231]. Therefore, a Hilbert space of dimension d can support up to $(d + 1)$ pairwise complementary observables. *Mutatis mutandis*, this terminology also applies to a *triple* of pairwise canonically conjugate observables [390] used to construct three MU bases for a quantum particle described by a pair of canonically conjugate observables (cf. Sec. 9.13 for details on MU bases for continuous variables).

To quantify complementarity, the authors of Ref. [32] introduce a measure of the non-commutativity of sharp observables based on an operational approach, in a setting typical for quantum key distribution. Their measure $Q(O)$ attains its maximum if the observables in a set $O = \{O_1, \dots, O_\mu\}$, $\mu \leq d + 1$, are pairwise mutually unbiased, i.e. when they have mutually unbiased eigenbases. This result could be used to

prove non-existence of sets of MU bases in composite dimensions $d \notin \mathbb{PP}$ by showing that the bound cannot be saturated. In dimension $d = 6$, for example, it would be sufficient to show that no four observables $O_1, \dots, O_4$, exist which achieve this maximum value.

On a conceptual point, the close link between MU bases and complementarity raises the question of the extent to which these concepts are genuinely quantum mechanical. As a mathematical property, unbiasedness arises in non-quantum settings as well, via Fourier transforms and Sarwate’s trade-off relations between auto- and cross-correlations, for example. These observations notwithstanding, complementarity has not played an important role in the description of classical systems.

Within quantum theory, *incompatibility* and *entropic uncertainty relations* have, over time, supplanted the notion of complementarity as they are more flexible and easier to handle, especially for systems with finite-dimensional Hilbert spaces. The next two sections explain how MU bases relate to these concepts.

3.4 Incompatibility

In quantum theory, certain sets of measurements exhibit incompatibility, meaning that they cannot be measured jointly on a single device [183]. In particular, incompatible measurements cannot be obtained from the marginals of a single (parent) positive operator-valued measure (POVM). For projective measurements this property is equivalent to non-commutativity but for general measurements, described by POVMs, joint measurability does not imply commutativity. Interestingly, incompatibility shares a one-to-one correspondence with Einstein-Podolsky-Rosen (EPR) steering (cf. Sec. 3.12)—a type of uni-directional correlation between a quantum state split between two parties [398]—and has close connections to non-locality, state discrimination and quantum coherence.

One can quantify the incompatibility of a set of observables in terms of its *noise robustness*, defined as the minimum amount of uniform noise needed to ensure the set is jointly measurable. For a pair of observables P and Q , the robustness

is given by

$$I(P, Q) = \inf\{\lambda > 0 \mid (P_\lambda, Q_\lambda) \text{ are compatible}\}, \quad (3.4)$$

where *noisy* versions of the original observables are defined as

$$P_\lambda = (1 - \lambda)P + \lambda \mathbb{I}/d, \quad (3.5)$$

and Q_λ , analogously. In general, it is difficult to evaluate $I(P, Q)$ analytically unless the observables exhibit a high degree of symmetry, like mutually unbiased bases. Usually, semidefinite programming techniques are required, but even this is limited to relatively small dimensions.

The incompatibility robustness of qubit measurements has been treated exhaustively by Busch in 1986 [88]; a few decades later the special case of MU bases connected by a Fourier transformation (in arbitrary dimensions) was considered [98], followed by a solution for any pair of MU bases as well as complete sets [128]. Finally, the region of joint measurability for a pair of MU bases with *different* noise parameters, i.e. P_λ and Q_ν , was determined using state discrimination methods and an incompatibility witness [99]. The same noise bounds can be derived by a relation between incompatibility and quantum coherence (cf. Sec. 3.6). The joint measurement at this noise boundary can be implemented sequentially by quantum instruments [227].

Complete sets of $(d + 1)$ MU bases seem to be among the most incompatible observables with respect to the robustness measure of Eq. (3.4). When considering fewer measurements, POVMs have been found which exhibit a stronger degree of incompatibility than MU bases [41]. However, other quantifiers of incompatibility have been introduced for which pairs of MU bases are found to be maximally incompatible [127, 289, 370].

Incompatibility robustness can also be used to prove the existence of operationally inequivalent sets of MU bases since the degree of incompatibility depends on the particular choice of MU bases (for sets with cardinality greater than two) [128]. A further distinction between equivalence classes of MU bases arises from the construction of extremal sets of compatible observables, as not all MU bases lead to such sets [97].

3.5 Entropic uncertainty relations

Over time, the traditional variance-based approach to uncertainty relations has been com-

plemented by the introduction of entropic uncertainty relations. This development is partly driven by the focus on finite-dimensional quantum systems where no two Hermitian operators exist which satisfy the equivalent of the relation $i[\hat{p}, \hat{q}] = \hbar$, the canonical commutation relations for particle position and momentum observables. Nevertheless, systems consisting of quantum particles and qudits, respectively, are conceptually similar since mutual unbiasedness of orthonormal bases does not rely on the existence of suitable Hermitian operators. The unifying feature is the constant (i.e. basis-independent) overlap between states taken from different orthonormal bases.

To establish an uncertainty relation in a Hilbert space of dimension d , Kraus [239] uses the *information-theoretic* or *Shannon entropy* of an observable P ,

$$S_\rho(P) = - \sum_{j=1}^d p_j \ln p_j, \quad p_j = \text{Tr}[P(j)\rho], \quad (3.6)$$

where $P(j)$ denotes the projection operator onto the j -th eigenstate of P . The entropy $S_\rho(P)$ depends solely on the probabilities p_j , $j = 1 \dots d$, to obtain the j -th eigenvalue of the observable P when measuring it in a system prepared in state ρ . Improving earlier results [129, 305], Kraus conjectures that given any two observables P and Q in the space $\mathbb{C}^d$, their entropies must satisfy the inequality

$$S_\rho(P) + S_\rho(Q) \geq \ln d. \quad (3.7)$$

For $d \leq 4$, he found this *entropic uncertainty relation* to be saturated if the observables P and Q form a complementary pair (cf. Sec. 3.3), i.e. if all outcomes upon measuring the observable Q are equally likely given that a system resides in an eigenstate of P , and *vice versa*. In other words, the eigenstates of the operators P and Q are necessarily MU. For arbitrary dimensions d , the relation (3.7) was proved by Maassen and Uffink [266] in 1988 as a special case of more general inequalities satisfied by probability distributions with finitely many outcomes.

Ivanović raised the question of whether the entropic uncertainty inequality (3.7) generalises to more than two MU bases [204]. A complete set of MU bases corresponding to the observables

$P_1, P_2, \dots, P_{d+1}$, is shown to obey the inequality

$$\sum_{n=1}^{d+1} S_\rho(P_n) \geq (d+1) \ln \left(\frac{d+1}{2} \right), \quad (3.8)$$

which, for $d \geq 4$, strengthens an immediate bound obtained from Eq. (3.7) by suitably grouping the terms in the sum. This result means that the multi-complementarity uncertainty cannot be reduced to the uncertainty resulting from pairs of MU bases, an observation which is also valid in the case of a triple of pairwise complementary observables (see Sec. 9.13) for a quantum particle [221]. Somewhat unexpectedly, the bound (3.8) distinguishes between even and odd dimensions since there are no states which attain it for even dimensions [359].

Entropic uncertainty relations for both complete and smaller sets of MU bases [23, 405], as well as others valid in specific dimensions, have been surveyed in Ref. [29]. A host of additional state-dependent and state-independent uncertainty relations were derived for MU bases using the Rényi and Tsallis entropies [316].

It is important to identify those states that minimise a given uncertainty relation. For the Rényi entropy (of order 2), the minimal uncertainty states for a complete set of MU bases include all fiducial vectors of a Heisenberg-Weyl SIC-POVM (see Sec. 3.9) in prime dimensions [15] and the MUB-balanced states [12, 14, 402]. A MUB-balanced state is a pure state which has the same outcome probability distribution regardless of which MU basis from the complete set is measured.

Upper bounds on entropic sums, known as *certainty* relations, have been derived for arbitrarily many observables and any pure state. Clearly, a state maximises a certainty relation if it is unbiased to all measurement bases, therefore certainty relations for extendible sets of MU bases yield only trivial upper bounds. This result is also true for an arbitrary *pair* of orthonormal bases due to the existence of at least one vector mutually unbiased to both bases (see Sec. 6.2). Examples of non-trivial certainty relations have been obtained both for complete sets of MU bases [359] and for sets of orthonormal bases with cardinality greater than two [94, 313]. It has been conjectured that complete sets of MU bases (if they exist) achieve the smallest difference between upper and lower bounds for the av-

erage entropy among all sets of $(d+1)$ measurements with d outcomes.

3.6 Coherence in measurements

Coherence, typically considered a resource of quantum states [40, 350] (see Sec. 3.7), can be treated as a measurement resource, where the free resources are incoherent measurements (diagonal in the incoherent basis) [27, 227, 302]. Measurements which are *maximally coherent*, i.e. the “most valuable” from a resource perspective, are those which are mutually unbiased to the incoherent basis.

To see this, consider a general measurement described by a POVM (positive operator-valued measure) $M = \{M(i)\}_{i \in \Omega}$, i.e. a collection of positive semidefinite operators indexed by the outcome set Ω such that $\sum_{i \in \Omega} M(i) = \mathbb{I}$. A measure of coherence known as the *entry-wise coherence* of a measurement is defined as

$$\text{coh}_{nm}(M) = \sum_{i \in \Omega} |\langle n | M(i) | m \rangle|, \quad (3.9)$$

for each $n, m \in \{1, \dots, d\}$, where $\{|n\rangle\}$ is the incoherent basis. This quantity, which cannot increase with free operations, and satisfies $0 \leq \text{coh}_{nm}(M) \leq 1$, implies that a measurement is *maximally coherent* if the upper bound is saturated for all m, n .

It was shown in [227] that a POVM M with d outcomes is maximally coherent if and only if M is mutually unbiased to the incoherent basis. For example, the measurement $M(\pm) = \frac{1}{2}(\mathbb{I} \pm \sigma_x)$ is maximally coherent with respect to the eigenbasis of σ_z , since $\text{coh}_{nm}(M) = 1$ for all $n, m \in \{1, 2\}$. In light of this correspondence, one can reformulate the problem of finding pairs of MU bases as the problem of finding maximally coherent observables.

Measurement coherence turns out to be intimately connected to incompatibility (Sec. 3.4). In particular, necessary and sufficient conditions can be derived—with the aid of MU bases—that determine the amount of coherence needed for pairs of observables to be incompatible [227]. To understand the fundamental role of MU bases in this connection, consider a pair of observables P and Q that are mutually unbiased (and therefore incompatible in the sense of Sec. 3.4), with P the observable whose eigenstates define the incoherent basis. The pair can be modified by adding

noise in the form of pure decoherence (which is more general than the convex mixing approach described in Eq. (3.5)), such that P remains incoherent, and the coherence of Q is reduced. The interesting point is that if the noisy observables are jointly measurable (i.e. the noise has destroyed the incompatibility of the initial pair), then incompatibility is also lost if we start with *any* observable in place of the complementary observable Q . Hence, MU bases are both maximally coherent and maximally incompatible in this setting. Consequently, they provide a means to verify joint measurability for more general observables.

3.7 Coherence in states

MU bases also play a role in the resource theory of coherence in states, where the free resources are states diagonal in the incoherent basis. Many different resource theories of coherence have been introduced in the literature, mainly due to the freedom to choose between distinct classes of free operations which map the set of incoherent states to itself [40, 350]. Examples of these operations include *maximally incoherent operations* (MIO), which cannot create coherence, and a proper subset thereof: the *incoherent operations* (IO) which admit a Kraus decomposition so that each Kraus operator K_i cannot create coherence from the incoherent basis, i.e. $K_i|m\rangle \sim |n\rangle$.

Quantifiers of state coherence were first introduced to require monotonicity under IO, and included the relative entropy of coherence, the l_1 norm of coherence and the trace norm of coherence. Since coherence is a basis-dependent quantity, to determine the maximum value of the coherence attributed to a state requires an optimisation over all bases. This is equivalent to optimising the coherence $C(\rho)$ over all unitary transformations of a given quantum state ρ , i.e.

$$C_{\max}(\rho) = \sup_U C(U\rho U^\dagger), \quad (3.10)$$

defining the maximally coherent state(s) $\rho_{\max} = V\rho V^\dagger$, where V is the unitary maximising Eq. (3.10).

The relative entropy of coherence, which is also an MIO monotone, is given by

$$C_R(\rho) = S(\rho_I) - S(\rho) \leq \log d - S(\rho), \quad (3.11)$$

where S is the von Neumann entropy and ρ_I is the diagonal part of ρ . The upper bound is saturated for bases which are mutually unbiased to the eigenvectors of ρ [408]. This is also true for other coherence measures, including the robustness of coherence, the coherence weight and the modified Wigner-Yanase skew information measure [196]. On the other hand, the l_1 -norm of coherence,

$$C_{l_1}(\rho) = \sum_{i \neq j} |\rho_{ij}|, \quad (3.12)$$

is an IO monotone that violates MIO monotonicity, and is not maximised by MU bases [408].

More generally, for *any* MIO monotone, bases mutually unbiased to the eigenstates of ρ are always optimal. In particular, among all states with a fixed spectrum $\{\lambda_i\}$, the maximally coherent state (with respect to any MIO monotone C) is given by $\rho_{\max} = \sum_i \lambda_i |\phi_i\rangle\langle\phi_i|$, where $\{|\phi_i\rangle\}$ is MU to the incoherent basis [351]. The unitary which achieves the maximum is given by $V = \sum_i |\phi_i\rangle\langle\psi_i|$, with $|\psi_i\rangle$ the eigenstates of ρ . It follows that $\rho_{\max}$ is a resource state among all states with the same spectrum. Somewhat surprisingly, maximally coherent states link the resource theories of coherence and purity. In particular, for any MIO monotone, the corresponding purity of a quantum state ρ is the maximal coherence $C_{\max}(\rho)$ [351].

3.8 Quantum channels

Any orthonormal basis $\{|v\rangle, v = 0 \dots d-1\}$ of the space $\mathbb{C}^d$ defines a *quantum channel* which acts by projecting a density matrix ρ onto the associated diagonal matrix,

$$\Psi(\rho) = \sum_{v=0}^{d-1} \langle v|\rho|v\rangle |v\rangle\langle v|. \quad (3.13)$$

Given more than one orthonormal basis of $\mathbb{C}^d$, convex mixtures of the identity map $\mathbb{I}$ and the channels $\Psi_b(\rho)$, $b = 1, 2, \dots$, of type (3.13) are also channels,

$$\Phi = s\mathbb{I} + \sum_b t_b \Psi_b. \quad (3.14)$$

Using MU bases in this construction, the channel Φ can be shown to be *completely positive* and *trace preserving* for suitable choices of the parameters s and t [295]. The resulting *Pauli diagonal channels constant on axes* leave the completely

mixed state invariant, thus generalising *unital* qubit channels to higher-dimensional spaces.

Whenever complete sets of MU bases exist, i.e. for channels acting on states living in a Hilbert space of dimension $d \in \mathbb{PP}$, a link between quantum channels and orthogonal unitary operator bases (see Sec. 5.4) emerges, entailing a generalised Bloch sphere representation of qudits in the space $\mathbb{C}^d$. Further properties and applications of Pauli channels have been studied in [344], and in the references provided there.

3.9 SIC-POVMs, MU bases and frames

Symmetric informationally-complete POVMs (or SICs, for short) are defined by prescribing the moduli of the transition amplitudes between the pure states forming them, just as for sets of MU bases. However, the condition that the states $\{\phi_1, \phi_2, \dots, \phi_{d^2}\}$ give rise to a SIC, i.e.,

$$|\langle \phi_k | \phi_{k'} \rangle|^2 = \frac{1}{d+1}, \quad (3.15)$$

$k, k' = 1 \dots d^2$, $k \neq k'$, exhibits a greater degree of symmetry than Eqs. (1.3), since *all* pairs of states are treated in the same way; there is no subdivision of the states into orthonormal bases of $\mathbb{C}^d$.

SICs are currently thought to exist in Hilbert spaces of arbitrary dimension d as they have been found when $d \leq 193$ partly by hand and partly by computer-algebraic methods [150, 164, 334], and for some specific dimensions such as $d = n^2 + 3 \in \mathbb{P}$ [17] or $d = 4p = n^2 + 3$, $p \in \mathbb{P}$ [51]. Both MU bases and SICs form complex projective 2-designs (see Sec. 5.11) containing $d(d+1)$ and d^2 elements, respectively. In spite of some surprising connections, the existence problems for these structures do not seem to illuminate each.

For example, Wootters [403] points out that the geometric connection between an affine plane and a complete set of MU bases (cf. Appendix C) is mirrored by a SIC when the roles of the d^2 points and $d(d+1)$ lines are swapped. Beneduci *et al.* [47] shed further light on this connection, providing an operational link between SICs and MU bases for prime-power dimensions. In particular, by introducing the notion of *mutually unbiased POVMs* (cf. Sec. 9.10), they show that a complete set of MU bases arises when a set of commutative MU-POVMs is obtained from the marginals of a SIC.

Other connections between these superficially similar sets of states can be made, unrelated to the existence question. For example, Heisenberg-Weyl covariant SICs can be created once a so-called *fiducial* vector has been found, simply by applying d^2 phase-space displacement operators. Dang, Appleby and Fuchs [15] show that, in prime dimensions d , the probabilities that characterise a fiducial vector with respect to measurements in a complete set of MU bases satisfy a simple condition within each basis: a fiducial vector must be a minimum uncertainty state measured in terms of the quadratic Renyi entropy. However, the argument holds only in one direction: not every state with minimal uncertainty will be a fiducial vector of a SIC. If it did, the result could be used to construct SICs in all prime dimensions. Another surprising connection has been identified in the space $\mathbb{C}^4$ [365], while in $\mathbb{C}^3$, a state-independent Kochen-Specker inequality exists which elegantly combines the elements of a complete set of four MU bases and the nine states of a SIC (cf. Sec. 3.10).

Finite tight frames—a generalisation of orthonormal bases—provide a framework to study collections of vectors on finite dimensional Hilbert spaces, often with a high degree of symmetry [380]. A *finite frame* is a collection of vectors which span the Hilbert space, extending the notion of a basis to overcomplete spanning sets of vectors. A frame is *tight* if the projections onto the frame elements sum to a multiple of the identity. Orthogonal bases as well as collections of MU bases are examples of tight frames. A SIC is a special type of frame known as an *equiangular* tight frame, and contains the maximal number of vectors defining equiangular lines in the underlying space. MU bases and SICs often appear as illustrative examples of tight frames, e.g. [113, 380, 381]. The notion of unbiasedness has been extended to equiangular tight frames [145], and generalised further to *MU frames* [314], as described in Sec. 9.11.

3.10 Contextuality

A state-independent Kochen-Specker (KS) inequality has been constructed by combining the twelve states of a complete set of MU bases in the Hilbert space $\mathbb{C}^3$ with the nine states of a SIC-POVM [48]. By dropping the rules characteristic for value assignments in the KS set-

ting, one can also obtain a state-independent *non-contextual* inequality, using the same SIC-POVM and four MU bases. Since these constructions have no obvious generalisations to higher dimensions, it remains open whether the interplay between MU bases and SICs is a dimensional coincidence only. Related higher-dimensional constructions that build on MU bases—including systematic KS sets and explicit examples in $d = 4, 5$ —can be found in [296].

Another proof that quantum systems with dimension $d \geq 4$ violate non-contextuality has been formulated in [250], using complete sets of MU bases. If these sets also existed in composite dimensions $d \notin \mathbb{PP}$, the underlying inequality assuming non-contextual value assignments could be violated in *all* dimensions, not just those with d being a prime-power.

3.11 Quantum correlations

Entanglement in quantum systems can be characterised in a variety of ways, leading to a complex hierarchy of quantum correlations. Some entangled states, for example, admit a local hidden-state model and are therefore unsteerable (cf. Sec. 3.12) while others violate Bell inequalities (Bell non-locality) and are highly entangled. Methods that detect entangled states (including bound entanglement) via MU bases are discussed in Sec. 4.2.

For any dimension $d \geq 2$, there are tailor-made Bell inequalities which are maximally violated by d -element MU bases [366]. This property can be used to set up a weak form of device-independent self-testing for pairs of MU bases as well as a means to certify the presence of a maximally entangled state. These specific Bell inequalities also allow for the distribution of a key at an optimal rate, in a device-independent way, using measurements with d outcomes (see Sec. 4.3 for other approaches to quantum cryptography based on MU bases). Self-testing via Bell inequalities is also possible for three and four MU bases in two-qutrit systems [68, 211]. Performing random MU bases in low dimensions has been shown to provide a high probability of achieving Bell violations [360].

The existence of quantum correlations in arbitrary bipartite non-product states can be confirmed using a measure based on MU bases which exploits their complementarity [173]. In another approach, MU product bases (cf. Sec. 7.4) for

bipartite systems have been used to quantify quantum correlations and entanglement [267] (see also Sec. 4.2). The measures used were the mutual information, the Pearson coefficient and the sum of conditional probabilities between the complementary bases. For two-qutrit systems, an experiment based on four MU bases has simultaneously certified entanglement, non-locality and steering [197].

3.12 Steering

Schrödinger first realised that composite quantum systems can exhibit surprising non-classical behaviour. The phenomenon of “steering” is closely related to entanglement but conceptually distinct from quantum correlations. In a two-qubit setting, say, the set of steerable states is found to be smaller than the set of entangled states but larger than the set of states violating Bell’s inequality.

In the steering scenario, a bipartite state ρ_{AB} is shared between Alice and Bob who then measure observables on each of their respective subsystems. After a measurement (POVM) by Alice, taken from the set $\{M_b(v)\}$, where v labels the possible outcomes and b the available measurements, Bob’s state is given by $\sigma_{v|b} = \text{Tr}_A[M_b(v) \otimes \mathbb{I} \rho_{AB}]$. The assemblage $\{\sigma_{v|b}\}$ of all possible states at Bob’s end (and hence the state ρ_{AB}) is said to be *steerable* by Alice’s measurements if $\{\sigma_{v|b}\}$ does not admit a *local hidden-state model*. An assemblage has a local hidden-state model capable of simulating the statistics of the quantum states if there exists a set of positive operators $\{\sigma_\lambda\}$ with $\sum_\lambda \sigma_\lambda = \mathbb{I}$, such that $\sigma_{v|b} = \sum_\lambda D(v|b, \lambda) \sigma_\lambda$, for all v and b , where $D(v|b, \lambda) \geq 0$ and $\sum_v D(v|b, \lambda) = 1$ describes a stochastic transformation.

A pure state with full Schmidt rank is steerable if and only if Alice’s measurements are incompatible [315, 376]. This suggests that MU bases, which are highly incompatible (see Sec. 3.4), play a significant role in demonstrating steerability. Indeed, many of the approaches to steering rely on MU bases, as summarised in the review article by Cavalcanti and Skrzypczyk [101].

One way to convince Bob that a state is steerable is to construct inequalities which hold if a local hidden-state model exists. For example, a recent inequality [418] detects if an assemblage of *any* size is steerable—as well as quantifying the

steering robustness (and hence the incompatibility robustness)—while it exhibits *maximal* violations only if Alice uses MU bases (under the restriction of projective measurements). In this scenario, the absence of complete sets of MU bases in composite dimensions $d \notin \mathbb{P}$ poses an intriguing open problem: how many bases are needed to construct a maximally incompatible (steerable) assemblage in composite dimensions?

Other steerability criteria have been obtained for bipartite qubit-qudit systems based on *mutually unbiased measurements* [210], i.e. collections of *non-projective* POVMs that satisfy a modified form of the overlap conditions for MU bases (cf. Sec. 9.9). Experimental demonstrations of steering using MU bases include loop-hole free steering [399] and higher dimensional steering [415].

3.13 Equivalence classes

Two sets of μ MU bases in $\mathbb{C}^d$ are *equivalent*,

$$\{\mathcal{B}_0, \dots, \mathcal{B}_{\mu-1}\} \sim \{\mathcal{B}'_0, \dots, \mathcal{B}'_{\mu-1}\}, \quad (3.16)$$

if any combination of the following operations transform one set to the other: (i) a fixed unitary (or anti-unitary) applied to all states; (ii) permuting the states within a basis; (iii) multiplying each state with an individual phase factor; (iv) swapping any two bases within the set. As a consequence, and without loss of generality, it is standard practice to assume that the first basis $\mathcal{B}_0$ is the canonical basis so that the remaining bases can be represented as complex Hadamard matrices (see Secs. 1.1 and 5.2). The equivalence relations imply that the second basis $\mathcal{B}_1$ can be written as a *dephased* Hadamard matrix H with its first column and row given by $H_{i1} = H_{1i} = 1/\sqrt{d}$ for $i = 1 \dots d$. A detailed discussion on the constructions of different equivalence classes is given in Sec. 6.1.

In the results described so far, unbiasedness of a set of bases—independent of the choice of equivalence class—is the essential property behind their practical utility. However, in some cases, the choice of equivalence class can lead to different outcomes. One discrepancy between inequivalent sets is their incompatibility content. As already noted in Sec. 3.4, inequivalent sets of MU bases can exhibit different degrees of incompatibility [128]. A further discrepancy arises from quantifying the information extraction capabilities of sets of measurements [421]. In particular,

the estimation fidelity can distinguish inequivalent MU bases in $d = 4$, as has been demonstrated experimentally [407]. Entropies of inequivalent sets of MU bases also do not have to coincide [336].

Tangible differences in the outcomes of practical tasks can also be seen in the QRAC protocol (described in Sec. 5.9): using inequivalent classes yield different average success probabilities, although it is conjectured there exists a set of MU bases that always optimises the average success probability. Similarly, entanglement witnesses constructed from MU bases (Sec. 4.2) can depend on the chosen equivalence class [186]. In some instances, unextendible MU bases (Sec. 6.10) detect entanglement more efficiently than extendible ones.

What is more, there are situations in which it is not necessary to alter the equivalence class to observe different outcomes. When using MU bases to detect entanglement, permutations of the basis elements significantly modify the entanglement witness and its ability to detect bound entangled states [25] (see Sec. 4.2). A similar phenomenon has been observed for a guessing game described in [131].

For a discussion on inequivalent complete sets of MU bases, see Appendix A.8.

3.14 Mathematical topics

MU bases have found their way into a number of mathematical topics with no immediate physical motivation. Some of the relations mentioned in Sec. 5 such as Lie theory and projective 2-designs are fitting examples. Furthermore, large collections of MU bases prove useful for probability theory in the context of random matrices [103], as well as to estimate the value of the trace of a matrix [148]. They have also inspired the construction of new arithmetic functions which are multiplicative, i.e. $f(mn) = f(m)f(n)$ holds whenever the greatest common divisor of the integers m and n is equal to one [104], and of maximal orthoplectic fusion frames [65]. A notion of MU bases was formulated in the category of sets and relations (**Rel**), and a classification was provided via connections to mutually orthogonal Latin squares [138].

3.15 Experiments with MU bases

Quantum states forming MU bases have been created in a number of dimensions using various physical systems. For $d = 2$, pairs and triples of MU bases were obtained in a quantum optical setting, exploiting the fact that wave plates cause suitable phase shifts [194]. D'Ambrosio *et al.* [123] embedded a photonic quantum system of dimension $d = 6$ in a Hilbert space associated with photon polarisation coupled to some orbital angular momentum. The 18 product states which form three MU bases were prepared and certified. Another quantum optical approach to create and manipulate complete sets of $(d + 1)$ MU bases for dimensions $d < 5$ has been implemented by Lukens *et al.* [262].

Various tasks at the core of quantum information have been carried out successfully using MU bases. Two protocols for *quantum key distribution* (cf. Sec. 4.3) with photons based on MU bases were realised experimentally [39]; the security of the protocols is linked to quantum cloning and a temporal variant of steering. Generating photons with suitable orbital angular momentum has been verified as a feasible approach, making it possible to implement higher-dimensional quantum key distribution protocols [71, 269, 288]. A high dimensional implementation of MU bases ($d > 9$) using traverse modes of spatial light has been applied to verify that ignorance about a certain aspect of the whole system does not imply ignorance of its parts [222]. Self-testing of two four-dimensional MU measurements has been demonstrated [139]. A scalable implementation of MU bases is proposed in [200], where the number of interferometers scales logarithmically with d . This scheme is relevant to quantum key distribution when $d = 4$.

The theoretically appealing idea that MU bases are highly suitable for *quantum tomography* (cf. Sec. 4.1) has been demonstrated experimentally for two-qubit polarisation states [5], with increased fidelity of the reconstructed states when compared to standard techniques, and for higher-dimensional photonic qudits [258]. Local tomography based on MU bases for the individual parts of a composite quantum system has led to the successful reconstruction of the states of bipartite entangled systems [155], again using the orbital angular momentum of photons. In a similar spirit, *quantum process tomography* is feasible,

either with complete sets of MU bases for prime dimensions d or using MU bases obtained from tensoring in the composite dimension $d = 6$ [349] (cf. Sec. 4.1).

MU bases have been used to confirm the first reported quantum *teleportation* of a qutrit state [264] as well as both loop-hole free *steering* [399] and higher dimensional steering [415] (see Sec. 3.12). They have also been instrumental to experimentally verify bipartite bound entanglement in two-photon qutrits [185]. A link between pairs of MU bases for discrete and continuous variables (cf. Sec. 9.13) was established in [364], along with a quantum optical implementation of the resulting coarse-grained observables. The findings have been extended both theoretically and experimentally from two to three measurements [308].

There is a natural link between MU bases and a discretised model of plane paraxial geometric optics which may be implemented experimentally. Hadamard matrices arise as representations of *discrete linear canonical transforms* that describe the action of an optical system on d -component signals [181].

4 Applications of complete sets

We will now summarise applications of complete sets of MU bases in the field of quantum information: quantum state tomography, quantum key distribution, secret sharing, the Mean-King problem, entanglement detection, and quantum random access codes. They provide strong motivation to search for complete sets in composite dimensions $d \notin \mathbb{PP}$. In the absence of complete sets, one needs to turn to workarounds, some of which are discussed when available.

4.1 Quantum state reconstruction

A widely known and important application of MU bases is the solution it provides to the problem of *quantum state determination / reconstruction*, or *quantum tomography*. The idea of complete sets of MU bases for prime and prime-power dimensions was, in fact, rediscovered when addressing the problem of optimal quantum state reconstruction. MU bases play a key role when estimating a given quantum state since they minimise the statistical error [203, 401].

The reconstruction of a quantum state typically starts by assuming that there is a large but finite ensemble of identically prepared systems with d levels. The state of the system is described by a density matrix $\rho \in \mathcal{S}(\mathcal{H})$, a positive trace class operator with trace one. To determine the state ρ , the ensemble is divided into $(d+1)$ sub-ensembles of equal sizes. On each sub-ensemble we repeatedly perform measurements of a different observable with d outcomes. In the limit of an infinitely large ensemble, the resulting $(d-1)(d+1)$ independent outcome probabilities characterise the unknown pre-measurement state ρ unambiguously. This result conforms with Schrödinger’s conception of the wave function as a “catalogue of expectations”⁵

Any informationally complete set of observables [89] will be sufficient to determine the state ρ . However, given a *finite* ensemble, statistical errors are unavoidable but are minimised by choosing $(d+1)$ *pair-wise complementary* measurements [401]. In this case, measuring the b -th observable projects the initial state onto the elements of an orthonormal basis (associated with d orthogonal projection operators $\{P_b(v)\}_{v=0}^{d-1}$) which is mutually unbiased to the those of the other d measurements.

In the simplest case of a two-dimensional Hilbert space, one wishes to reconstruct a density matrix $\rho = (\mathbb{I} + \vec{r} \cdot \vec{\sigma})/2$, with $\mathbb{I}$ being the 2×2 identity matrix, while $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)^T$ is the operator-valued spin vector constructed from the Pauli matrices, and the vector $\vec{r}$ runs through all points of the unit ball in $\mathbb{R}^3$. Measuring the complementary spin observables σ_x , σ_y and σ_z separately on three sub-ensembles, one obtains the components of the vector $\vec{r}$ which determines the unknown state ρ unambiguously. However, since every measurement comes with some degree of statistical inaccuracy, the reconstructed value of each component $r_j, j = x, y, z$, is confined to a “fuzzy” estimate of the exact plane only. The intersection of all three ‘slabs’ determines the region of the unit ball which is compatible with the (inaccurate) measurements. As one expects intuitively, the overall statistical error is minimised if the planes are pair-wise perpendicular, corresponding to a measurement defined by *mutually unbiased* bases. The argument carries through

for dimensions larger than $d = 2$, underlining the specific role played by MU bases for quantum state tomography.

In a bipartite setting, methods of quantum state *verification*—rather than reconstruction—are more efficient than traditional tomographic approaches, especially when using complete sets of MU bases. Efficient protocols for both pure [253] and maximally entangled states have been developed [419].

For quantum process tomography, in which a *quantum channel* is reconstructed, a large number of parameters must be determined through measurements. Complete sets of MU bases have been used in different ways to achieve this goal. One may adapt quantum tomographic methods in prime-power dimensional Hilbert spaces to determine the parameters characterising the channel in hand [144]. Alternatively, one can exploit the fact that they form a 2-design (cf. Sec. 5.11) [46]. This generalises to non-prime-power dimensions [349] if one tensors complete sets of MU bases. A quantum optical experiment for quantum process tomography in this scenario has been proposed, with the quantum state of a d -level system encoded as the position of photons in the transversal direction, by means of apertures with d slits. A successful implementation of the protocol is reported for dimension $d = 6$.

As noisy intermediate-scale quantum computers advance, it becomes useful to develop strategies that estimate a system’s properties with minimal measurements, avoiding the need for full-scale quantum state tomography. For instance, the *classical shadow protocol* creates a classical approximation of an unknown quantum state, which can then be used to simultaneously estimate expectation values for non-commuting observables. The original classical shadow protocol was based on implementing random Pauli measurements on each qubit [198], i.e. three MU bases in $\mathbb{C}^2$. This was later generalised to $(2^n + 1)$ MU bases on an n -qubit system [387]. Another, equally efficient, strategy to simultaneously estimate expectation values of relevant observables implements a *joint measurement* (see Sec. 3.4) of noisy versions of three MU bases on each qubit [281].

Workaround Without knowledge of a complete set, or even if no such set exists, can we

⁵Originally in German: “Die ψ -Funktion als Katalog der Erwartung”, in [330, Sec. 7].

still find an optimal reconstruction procedure for the state in question? Not surprisingly, alternative approaches for state reconstruction exist in arbitrary dimensions. The existence of complete sets—while convenient to have—is not fundamental for optimal quantum tomography.

In the generalisation to arbitrary d -level systems, weighted complex projective 2-designs (defined in Sec. 9.8) play an important role in optimising state reconstruction [322]. It has been shown that a set of bases which constitutes a weighted 2-design forms the orthogonal measurements necessary for optimal quantum tomography.

Explicit examples of weighted 2-designs are constructed in [322] for $d = p^n + 1$ with p prime, where a set of $(d+2)$ orthonormal bases is found. This covers dimension six, in which eight orthonormal bases form a weighted 2-design. Starting with the standard basis $\mathcal{B}_0 = \{|0\rangle, \dots, |5\rangle\}$, the remaining orthonormal bases are given by the states

$$|v_b\rangle = \frac{1}{\sqrt{6}} \sum_{k=0}^5 \omega^{vk} e^{2\pi i b 3^k / 7} |k\rangle, \quad (4.1)$$

where $b = 1 \dots 7$, $v = 0 \dots 5$, and $\omega = e^{2\pi i / 6}$. The overlaps between elements of different bases, given explicitly in [307], are

$$|\langle v_b | v_{b'} \rangle|^2 = \begin{cases} \frac{6}{7} & \text{if } b \neq b', v \neq v', \\ \frac{1}{36} & \text{if } b \neq b', v = v'. \end{cases} \quad (4.2)$$

Surprisingly, by performing the measurements associated with the eight orthonormal bases on the unknown quantum state—the standard basis is measured in the ratio 7 : 6 with respect to each of the remaining bases—optimal state reconstruction can be achieved. In fact, the same minimised statistical error is achieved (hypothetically) by implementing a complete set of seven MU bases.

In higher composite dimensions, when $d \neq p^n - 1$, the minimum number of orthonormal bases needed to construct a weighted 2-design for optimal state reconstruction is not known explicitly, but an upper bound of $\frac{3}{4}(d-1)^2$ is given in [322]. This bound was improved in [279], and weighted 2-designs were found to contain roughly $2(d + \sqrt{d})$ bases when d is odd and $3(d + \sqrt{d})$ for d even.

Another approach to quantum state reconstruction of an arbitrary d -level system is to recast the problem in terms of special types of informationally complete positive operator value

measures (IC-POVM). These are called *tight* rank-one IC-POVMs [332] and are *equivalent* to complex projective 2-designs (see Sec. 5.11). Both SIC-POVMs and complete sets of MU bases are examples of tight rank-one IC-POVMs. It was shown in [332] that these POVMs are optimal for *linear* quantum state tomography. The state reconstruction is “linear” in the sense that it is limited to a simplified state reconstruction procedure.

4.2 Entanglement detection

MU bases provide a simple and efficient criterion for witnessing entanglement in quantum states. An entanglement witness is a Hermitian operator $\mathbf{W}$ that satisfies $\text{Tr}[\mathbf{W}\rho_{\text{sep}}] \geq 0$ for all separable states ρ_{sep} , and $\text{Tr}[\mathbf{W}\rho] < 0$ for at least one entangled state ρ . A negative expectation of the operator $\mathbf{W}$ for a bipartite state indicates the presence of non-classical correlations between its subsystems.

Let us describe the criterion in the case of a bipartite state with both subsystems of dimension d . Given a set of μ MU bases $\mathcal{B}_b = \{|v_b\rangle\}$ of the space $\mathbb{C}^d$, it has been shown in [347] that the operator

$$\mathbf{B}(\mu) := \sum_{b=0}^{\mu-1} \sum_{v=0}^{d-1} |v_b\rangle\langle v_b| \otimes |v_b^*\rangle\langle v_b^*|, \quad (4.3)$$

satisfies, for any separable state,

$$\text{Tr}[\mathbf{B}(\mu) \rho_{\text{sep}}] \leq \frac{d + \mu - 1}{d}. \quad (4.4)$$

Hence, the operator

$$\mathbf{W}(\mu) = \frac{d + \mu - 1}{d} \mathbb{I}_d \otimes \mathbb{I}_d - \mathbf{B}(\mu), \quad (4.5)$$

is an entanglement witness satisfying $\text{Tr}[\mathbf{W}(\mu) \rho_{\text{sep}}] \geq 0$. If a state ρ violates Eq. (4.4), it is necessarily entangled. For example, Eq. (4.4) is violated by all entangled isotropic states—i.e. mixtures of a maximally mixed and maximally entangled state—when $\mu = d + 1$. With fewer measurements, the witness detects a subset of the entangled isotropic states: a pair of MU bases, for example, is enough to detect at least half [347].

A modified witness, constructed in [26], is given by

$$\widetilde{\mathbf{W}}(\mu) = \widetilde{\mathbf{B}}(\mu) - L_\mu \mathbb{I}_d \otimes \mathbb{I}_d, \quad (4.6)$$

for some $L_\mu \geq 0$, where $\tilde{\mathbf{B}}(\mu)$ is identical to Eq. (4.3) but without complex conjugation in the second system. This leads to a lower bound

$$\text{Tr}[\tilde{\mathbf{B}}(\mu) \rho_{\text{sep}}] \geq L_\mu, \quad (4.7)$$

which holds for all separable states. If $\mu = d + 1$, then $L_{d+1} = 1$ and the bound is violated by all entangled Werner states. On the other hand, if $\mu < d + 1$, only numerical values of L_μ are known [26]. Interestingly, the bound depends on the choice of MU bases. For instance, when $d = 4$ and $\mu = 3$, the ability to detect certain entangled states depends on the choice of bases from the infinite family of MU triples [77].

A larger class of entanglement witnesses can be generated by making orthogonal rotations of the basis states on the first Hilbert space [116]. For example, when the measurement basis is permuted, the operator

$$\mathbf{B}_\pi(\mu) = \sum_{b=0}^{\mu-1} \sum_{v=0}^{d-1} |\pi^{(b)}(v)_b\rangle \langle \pi^{(b)}(v)_b| \otimes |v_b^*\rangle \langle v_b^*| \quad (4.8)$$

generates a new class of entanglement witnesses, where $\pi^{(b)}$ is a permutation of the d elements of the basis $\mathcal{B}_b$. For certain permutations, the witness is non-decomposable and detects bound entangled states [25]. In fact, for $\mu > d/2 + 1$, there exist witnesses of this type that are always non-decomposable.

Witnesses have also been derived for MU measurements [106], defined in Sec. 9.9, and more generally 2-designs [168, 209]. Continuous variable systems (cf. Sec. 9.13) admit structurally similar entanglement detection methods [347], as well as more general bipartite systems [386].

4.3 Quantum cryptography...

Measurements on quantum systems tend to disturb the state of the observed system. This fundamental aspect of quantum mechanics has been the springboard to applications in quantum cryptography, a *physics-inspired* means of secret communication [56, 85, 102, 135], fundamentally different from traditional approaches which are based on the difficulty to solve specific mathematical problems. To establish a shared *secret key*, necessary for encrypting a message, the protocols rely on the parties exchanging quantum systems in such a way that outside entities cannot

gain information about it without leaving traces of their interactions. The resulting modifications may subsequently be detected by the legitimate parties, only to reveal that the communication channel is not secure.

... based on pairs of MU bases

The BB84 protocol is one of the earliest examples of quantum key distribution [56]. A secret key, usually a *random* sequence of bits, e.g. 010110, is sent via a series of qubit states to a receiver. The states are taken from two orthonormal bases, $\mathcal{B}_z = \{|0\rangle, |1\rangle\}$ and $\mathcal{B}_x = \{|+\rangle, |-\rangle\}$; given by the eigenstates of the spin operators σ_z and σ_x , respectively, this pair of bases is mutually unbiased. Within each basis, the orthogonal states will represent the bits 0 and 1. The sender *randomly* chooses a basis and sends off the appropriate state corresponding to 0 or 1. The state is transmitted using a quantum channel to the receiver, who then measures the state randomly using either σ_z or σ_x . If the receiver happens to choose the same basis as the sender in a particular run—which will occur in half of all cases—both parties possess the same value for this particular bit.

Once the measurements have been made, both parties publicly reveal the bases used by each individual. The sender and receiver remove all measurement outcomes from their lists in which their choice of bases did not agree. The remaining sequence of bits represents the shared key. To check whether eavesdroppers interfered with the quantum channel, they publicly compare a subset of the key: if they notice discrepancies, quantifiable by an *error rate*, a breach must have occurred.

Other quantum key distribution protocols have since been developed and implemented successfully both experimentally and commercially [328]. The optimal or most robust protocol is one which can tolerate large disturbances (errors) and still result in secure key distribution. The amount of discrepancies caused by the eavesdropper depends on her strategy; considerable effort is invested towards finding the optimal method of attack for each protocol. The optimal eavesdropping strategy for the BB84 protocol is known for *individual* attacks [102]. However, the protocol remains secure even if unlimited resources are available to the eavesdropper. For a correlation-

based cryptographic protocol using pairs of MU bases, see Sec. 3.11.

... based on complete sets of MU bases

Early quantum cryptography protocols based on pairs of MU bases (cf. Sec. 4.3) have been generalised to qutrits [44] exploiting all four MU bases and, subsequently, to d -level systems equipped with a complete set of $(d + 1)$ MU bases [102]. Compared to the approach using a pair of MU bases, individual attacks by means of a quantum cloning machine lead to a slightly higher error rate. Nevertheless, protocols using two bases remain preferable since it is easier to produce longer keys.

In [81] a protocol for an arbitrary d -level systems is given which improves sensitivity to an eavesdropper with respect to the error rate. Here, the secret key is constructed from an alphabet of arbitrary size which is encoded into a basis of the state space $\mathbb{C}^d$. As usual the system is prepared by a sender at A and transported to a receiver at B . The receiver is then set the task of recovering the initial key by performing measurements on the system he has received. The protocol aims to maximise the likelihood of detecting an eavesdropper. Assuming an “intercept-and-resend” attack method, one can calculate the error rates which allow the parties at A and B to detect a breach, with a larger error rate being beneficial for security. The optimal strategy to share the key is found to rely on MU bases.

One disadvantage of this method is the relatively large number of states required to share one bit of information compared to, say, the six-state protocol [85]. At the same time, the protocol is much more sensitive to the eavesdropper since the quantum bit error rate of an attack—proportional to the key elements that contain an error—is much higher. If one considers higher dimensions and uses a complete set of MU bases, this protocol reaches a 100% error rate. However, in this limit one must use *approximate* MU bases (see Sec. 9.6). In the absence of complete sets of MU bases, i.e. for composite dimensions $d \notin \mathbb{PP}$, the protocol is less efficient.

A hybrid security model has been proposed which offers everlasting secure-key agreement rather than the stronger *unconditional* security of standard quantum key distribution methods [379]. The protocol encodes a single bit using

a d -dimensional state chosen from a complete set of $(d + 1)$ MU bases. The basis information is shared between legitimate parties and hidden from Eve under the assumption of short-term computational security (of one-way functions), until her quantum memory has decohered. This hybrid approach has benefits compared to the practicality and implementation issues of traditional quantum key distribution methods.

Mutually unbiased bases also feature in security proofs of cryptographic protocols. For example, measuring a complete set of mutually unbiased bases can ensure statistical security of protocols sharing information [132].

4.4 Quantum secret sharing

Quantum secret sharing involves distributing a secret among multiple parties in a way that access to the secret requires collaboration between a subset of the participants [188]. A quantum secret-sharing scheme based on MU bases in a d -dimensional system has been introduced in [409], with perfect security achievable as d increases. Alternatively, one can set up an efficient protocol using sequential communication of a single quantum d -level system, with $d \in \mathbb{P}$ a prime number [368]. The dimensional restriction is due to its dependence on an algebraic property known at the time only for MU bases in prime dimensions although a generalisation to the case of $d = p^2$, $p \in \mathbb{P}$, has been reported [179].

4.5 Dealing with mean kings

An interesting—but admittedly slightly artificial—application of MU bases is their role in the solution to a measurement problem involving a fictitious “mean” king. The problem arises in a scenario where an observer A prepares a spin- $\frac{1}{2}$ particle in a state of her choice and then performs a control measurement on the system. Between the preparation and measurement, a second observer B measures either σ_x , σ_y or σ_z on the particle state. After the control measurement, observer A is told which spin component observer B measured and is asked to determine the corresponding measurement outcome [377].

The generalisation of this problem is usually told by the following story: a king who lives on a remote island sets a physicist a life or death challenge. He asks the physicist to prepare a d -

state quantum system of her choice and to perform a control measurement on the system. Before her control measurement, she must hand the state over to the king while he secretly performs a measurement. After her control measurement the king reveals his measurement and challenges the opponent to determine his outcome. In this generalisation, the choice of measurement made by the king is restricted to a set of pairwise complementary observables.

The generalised problem was first solved for a system with prime degrees of freedom in [137] and then extended to include prime-powers [19]. Crucially, both solutions rely on the existence of complete sets of MU bases. To resolve the challenge, the physicist must prepare two d -state systems in a maximally entangled state of the space $\mathbb{C}^d \otimes \mathbb{C}^d$. The auxiliary system is kept by the physicist while the king performs a measurement of one of $(d + 1)$ mutually unbiased bases on the object system.

It was shown subsequently that the existence of a complete set of MU bases is, in fact, not the essential factor that allows the physicist to extricate herself [180, 319]. Under the above assumptions, and by restricting the physicist’s measurement to a projection-valued measure (PVM), the mean king’s problem for an arbitrary d -state system has a solution only if the maximum number of $(d - 1)$ mutually orthogonal (MO) Latin squares exist. If d is a prime or prime-power, this maximum is achieved and the solutions agree with those given in [19, 137]. However, in dimension $d = 6$ only three MO Latin squares exist, implying that there is no solution to the problem for this degree of freedom, regardless of whether a complete set of seven MU bases exists. Similarly, this is true for $d = 10$ since no set of nine MO Latin squares exists [192]. However, in these cases, alternative solutions to the mean-king problem can be found (cf. the end of this section).

A Wigner function approach to the mean-king problem for qubits has been developed in [309]. The problem has also been transposed to a setting with continuous variables [70] and the associated MU bases (cf. Sec. 9.13); again, a phase-space approach turns out to be instructive.

Workaround If the physicist is allowed to perform POVM measurements on the space $\mathbb{C}^d \otimes \mathbb{C}^d$, a complete solution to the king’s problem can be

given for arbitrary dimensions $d \in \mathbb{N}$ [226]. Thus, regardless of whether $(d - 1)$ MO Latin squares or complete sets of MU bases exist, the physicist can always determine the king’s measurement outcome.

4.6 Quantum random access codes

A quantum random access code (QRAC), denoted by the symbol $\mu^d \rightarrow 1$, is a communication protocol in which the sender Alice encodes μ classical d -level systems $\mathbf{x} = \{x_1, \dots, x_\mu\}$, with $x_j \in \{1, \dots, d\}$, into a d dimensional quantum state ρ , and the receiver Bob is asked to correctly identify, via a set of μ measurements, one of the d levels $y \in \{x_1, \dots, x_\mu\}$ chosen randomly. In the most common QRAC protocol a μ -bit message is encoded in a qubit [11, 396], rather than the d -level generalisation considered here [367]. For a given strategy (i.e., a state and measurements) one can find the average success probability $p(\mu, d)$ of recovering the correct d -level, which is calculated over all inputs $\mathbf{x}$ and choices y . When $\mu = 2$, the *optimal* average success probability $P(\mu, d)$, maximised over all states and measurements, is given by

$$P(2, d) = \frac{1}{2} \left(1 + \frac{1}{\sqrt{d}} \right), \quad (4.9)$$

and is achieved if and only if Bob measures a pair of MU bases [7, 141]. Consequently, the $2^d \rightarrow 1$ QRAC provides a means for self-testing pairs of MU bases [141, 369].

For larger μ , the optimal strategy does not straightforwardly generalise to measuring μ MU bases. For instance, when $\mu = 3$ and $d = 5$, there exist two inequivalent triples of MU bases and the average success probability for each triple is different. To find optimal measurements for a $\mu^d \rightarrow 1$ QRAC scheme with $d \geq \mu$, MU bases can be extended to “ μ -fold unbiased bases” [142]. However, this approach imposes an additional constraint on the bases that seems overly restrictive, and no examples have been found for $\mu \geq 3$ in any dimension d .

A variant of the QRAC protocol limits the number of classical d level systems addressed by Bob to any ν of the total μ systems. For $\nu = 2 \leq \mu$, the resulting “p-QRAC” protocol $(\mu, \nu)^d \rightarrow 1$ lends itself to characterise MU bases as the measurements of choice for Bob to maximise his success rate [7]. The details are given in

Sec. 5.9 where Equivalence 5.9 establishes a rigorous link between the existence of a complete set of MU bases and the optimal strategy for Bob.

4.7 Other applications

The reconstruction of signals from the magnitudes of vectors in real or complex Hilbert spaces is an important problem in speech recognition. Complete sets of MU bases have been shown to provide a simple approach [28], with the 2-design property of the bases (cf. Sec. 5.11) a central ingredient. MU bases enable the construction of sequences with relatively flat Fourier spectra, an important feature of signals used to efficiently communicate (cf. Sec. 2.1); a complete set of four MU bases has been used to that effect in [404].

5 Equivalences and conjectures

A set of μ MU bases $\mathcal{B}_b, b = 0 \dots \mu - 1$, in the space $\mathbb{C}^d$ is defined by the $d^2\mu^2$ conditions

$$|\langle v_b | v'_{b'} \rangle|^2 = \frac{1}{d}(1 - \delta_{bb'}) + \delta_{vv'}\delta_{bb'}, \quad (5.1)$$

many of which are identical due to the symmetries of exchanging $v \leftrightarrow v'$ and $b \leftrightarrow b'$. Such sets are, as we have seen in the previous two sections, closely related to a number of concepts in seemingly disconnected areas of mathematics and physics. We will now describe many of these and other concepts more rigorously, with the aim to develop alternative perspectives on the original conditions defining MU bases. We will, for example, rephrase Eqs. (5.1) in terms of Hadamard matrices, unitary operator bases, decompositions of Lie algebras, quantum designs and random access codes. The final five reformulations (Secs. 3.2–5.13) are slightly weaker in the sense that they hold only when $\mu = d + 1$, i.e. for a complete set of MU bases. For each “representation”, a *conjecture* will be spelled out which expresses the existence problem in the corresponding mathematical context. Proving or disproving any of these conjectures will solve all others, including the original existence problem.

5.1 MU bases as global minima

Rather than writing down the large number of constraints (5.1) on the vectors defining a set of

μ MU bases, $\mu \in \{2, \dots, d + 1\}$, one can encode them in the global minimum of one *scalar* function $F_d : \mathbb{R}^{p_\mu(d)} \rightarrow \mathbb{R}$ depending on $p_\mu(d) = (d - 1)((\mu - 1)(d - 1) - 1)$ free parameters (cf. Sec. 8.3 for the parameter count).

Equivalence 5.1. *A set of μ orthonormal bases $\{\mathcal{B}_0, \dots, \mathcal{B}_{\mu-1}\}$ in $\mathbb{C}^d$ is mutually unbiased if and only if the non-negative function*

$$F_d(\mathcal{B}_0, \dots, \mathcal{B}_{\mu-1}) = \sum_{b,b'=0}^{\mu-1} \sum_{v,v'=0}^{d-1} \left(|\langle v_b | v'_{b'} \rangle| - \chi_{vv'}^{bb'} \right)^2 \quad (5.2)$$

vanishes; here $\chi_{vv'}^{bb'} = (1 - \delta_{bb'})/\sqrt{d} + \delta_{vv'}\delta_{bb'}$ are the positive real square roots of the right-hand-side of Eq. (5.1).

In this representation of the conditions for a set of $(d + 1)$ bases to form a complete set, Conjecture 1.1 presented in Sec. 1.1 turns into a simple statement about the global minimum of the function $F_d(\mathcal{B}_0, \dots, \mathcal{B}_d)$.

Conjecture 5.1. *For $\mu = d + 1$, the global minimum of the function F_d over all $(d + 1)$ -tuples of orthonormal bases equals zero if and only if d is a prime-power.*

This formulation provides a useful starting point for numerical approaches to the existence problem in composite dimensions, described in Secs. 8.2 and 8.3. It is not excluded that the global minimum of the function $F_d(\mathcal{B}_0, \dots, \mathcal{B}_d)$ is *degenerate* in prime-power dimensions: complete sets of MU bases are not necessarily unique (see Appendix A.8).

5.2 Sets of MU Hadamard matrices

A complex Hadamard matrix of order d is a generalisation of a real Hadamard matrix which is a square, unitary matrix with entries consisting of $\pm 1/\sqrt{d}$ (or just ± 1). The generalisation drops the restriction of real entries to those with modulus $1/\sqrt{d}$. A vector is mutually unbiased to the standard basis if all d components of the vector have modulus $1/\sqrt{d}$ (cf. Eq. (5.7)). It then follows that a basis is MU to the canonical basis if and only if it can be expressed as a complex Hadamard matrix.

This leads to the important observation that any pair of MU bases in $\mathbb{C}^d$ can be represented by a $d \times d$ complex Hadamard matrix. To

see this we simply apply a unitary transformation—which maps the orthonormal basis associated with one of the matrices to the canonical one—to both matrices simultaneously. Since this map preserves the overlap condition of Eq. (5.1), the second matrix maps to a complex Hadamard matrix. Hence, the problem of searching for pairs of MU bases is identical to the problem of finding Hadamard matrices.

A complete classification of Hadamard matrices is known for $d \leq 5$ [174] but it remains an open problem for $d \geq 6$, although a substantial body of knowledge is available. We shall discuss the current efforts to classify Hadamard matrices of order six in Sec. 7.1 and those of higher orders in Sec. 6.1.

The correspondence between pairs of MU bases and Hadamard matrices extends naturally to an equivalence relation between sets of MU bases and sets of Hadamard matrices.

Equivalence 5.2. *A set of μ MU bases $\{\mathcal{B}_0, \dots, \mathcal{B}_{\mu-1}\}$ in $\mathbb{C}^d$ exists if and only if a set of $(\mu-1)$ Hadamard matrices $\{H_1, \dots, H_{\mu-1}\}$ of order d exists such that the products $H_j^\dagger H_{j'}, j \neq j'$, are Hadamard matrices for all values of $j, j' = 1 \dots \mu - 1$.*

Thus, finding a complete set of $(d+1)$ MU bases in dimension d corresponds to identifying a collection of d Hadamard matrices H_j with the property that $H_j^\dagger H_{j'}$ is a Hadamard matrix for all $j \neq j'$. This leads to the following conjecture.

Conjecture 5.2. *A set of d Hadamard matrices H_j of order d such that $H_j^\dagger H_{j'}$ is Hadamard for all $j \neq j'$ exists if and only if d is a prime-power.*

As well as their relation to MU bases, Hadamard matrices play an important role in other areas of mathematics and physics. They arise in the study of quantum groups [34] and have applications in quantum information, e.g. teleportation and dense coding schemes [393]. Their study has also been motivated by the problem of finding bi-unitary sequences and cyclic n -roots [60] (see Sec. 7.3) and they are used in constructing $\ast$ -subalgebras of finite von Neumann algebras [312] and error-correcting codes [6].

5.3 Coupled polynomial equations

Writing out the conditions (5.1) in terms of states relative to a basis of $\mathbb{C}^d$ turns them into a set of

coupled polynomial equations of fourth-order in the expansion coefficients. Although straightforward, this explicit representation is useful to implement computational searches for vectors mutually unbiased to pairs of MU bases (cf. Sec. 7.3) and to prove that certain sets are unextendible (cf. Sec. 7.6).

Let us expand all $d\mu$ states $|v_b\rangle$ forming a hypothetical set of μ MU bases $\mathcal{B}_b, b = 0 \dots \mu - 1$ in the standard basis $\mathcal{B}_z = \{|j\rangle, j = 0 \dots d - 1\}$, i.e. we write

$$|v_b\rangle = \frac{1}{\sqrt{d}} \sum_{j=0}^{d-1} (v_{b,j} + iv_{b,j+d})|j\rangle, \quad (5.3)$$

with expansion coefficients

$$\langle j|v_b\rangle\sqrt{d} = v_{b,j} + iv_{b,j+d} \in \mathbb{C}, \quad (5.4)$$

for $b = 0 \dots \mu - 1$, and $v, j = 0 \dots d - 1$, where $v_{b,j}, v_{b,j+d} \in \mathbb{R}$ are their real and imaginary parts.

Equivalence 5.3. *A set of μ MU bases $\{\mathcal{B}_0, \dots, \mathcal{B}_{\mu-1}\}$ in $\mathbb{C}^d$ exists if and only if the equations*

$$\begin{aligned} & \sum_{j,k=0}^{d-1} (v_{b,j} + iv_{b,j+d})(v'_{b',j} - iv'_{b',j+d}) \times \\ & \times (v_{b,k} - iv_{b,k+d})(v'_{b',k} + iv'_{b',k+d}) = d, \end{aligned} \quad (5.5)$$

with $b \neq b', v, v' = 0 \dots d - 1$ and

$$\sum_{j=0}^{d-1} (v_{b,j} - iv_{b,j+d})(v'_{b',j} + iv'_{b',j+d}) = d\delta_{vv'}, \quad (5.6)$$

with $v, v' = 0 \dots d - 1$, for all b , have a real solution; the equations are a set of coupled fourth-order polynomial equations in $2d^2\mu$ real variables $v_{b,j}, v_{b,j+d}, b = 0 \dots \mu - 1$, and $v, v' = 0 \dots d - 1$.

The set of equations can be simplified since the conditions of Eqs. (5.1) are invariant under a unitary transformation of the bases $\mathcal{B}_b$, so it is natural to choose $\mathcal{B}_0 = \mathcal{B}_z$, or $\langle j|v_0\rangle = \delta_{jv}$. Then, the $d^2(\mu - 1)$ complex expansion coefficients of the remaining $d(\mu - 1)$ vectors must have modulus one, i.e.

$$v_{b,j}^2 + v_{b,j+d}^2 = 1, \quad (5.7)$$

$b = 1 \dots \mu - 1, j = 0 \dots d - 1$ and $v = 0 \dots d - 1$.

A further reduction of parameters is achieved by *dephasing* the second basis (see Sec. 2.1 and

Appendix B). In particular, for the vector $|v = 0_{b=1}\rangle$, i.e. the first vector of the second basis, we can fix the coefficients to be $\text{Re}\langle j|0_1\rangle = 1$ and $\text{Im}\langle j|0_1\rangle = 0$, for all $j = 0 \dots d-1$. Furthermore, in all remaining vectors of the second basis, we can choose $\text{Re}\langle 0|v_1\rangle \equiv v_{1,0} = 1$ and $\text{Im}\langle 0|v_1\rangle \equiv v_{1,d} = 0$, $v = 1 \dots d-1$.

The conjecture associated with Equivalence 5.3 reads as follows.

Conjecture 5.3. *The fourth-order coupled polynomial equations (5.5) and (5.6), with $\mu = d+1$, have real solutions if and only if d is a prime-power.*

Numerical searches for MU bases and smaller constellations (see Sec. 8.3) rely on introducing basis-dependent parameterisations such as Eq. (5.3), especially when formulating the search as an optimisation problem which may use (variants of) the scalar function $F_d(\mathcal{B}_0, \dots, \mathcal{B}_{\mu-1})$ in Eq. (5.2).

5.4 Unitary operator bases

Unitary operator bases, first introduced by Schwinger [331], play an important role in the construction of MU bases. A unitary operator basis is a set of unitary operators which forms an orthonormal basis of the Hilbert-Schmidt space consisting of the linear operators acting on $\mathbb{C}^d$. Let $\mathcal{C} = \{U_1 = \mathbb{I}_d, U_2, \dots, U_{d^2}\}$ be a unitary operator basis for the set of $d \times d$ complex matrices $\mathbb{M}_d(\mathbb{C})$, with any two elements being orthogonal with respect to the Hilbert-Schmidt inner product, $\text{Tr}[U_s^\dagger U_{s'}] = d\delta_{ss'}$, $s, s' = 1 \dots d^2$. The basis $\mathcal{C}$ can be partitioned into $(d+1)$ *maximally commuting operator classes* if $\mathcal{C} = \mathcal{C}_0 \cup \dots \cup \mathcal{C}_d$ such that each class $\mathcal{C}_j$ contains $(d-1)$ commuting matrices from $\mathcal{C}$ together with the identity $\mathbb{I} \in \mathcal{C}_j$, for all j . This partitioning corresponds directly to a complete set of $(d+1)$ MU bases in $\mathbb{C}^d$, as pointed out in Ref. [31]. In particular, such a partitioning exists if and only if a complete set of MU bases exists. Theorems 3.2 and 3.4 of Ref. [31] provide a proof of the underlying equivalence.

Equivalence 5.4. *A set of μ MU bases $\{\mathcal{B}_0, \dots, \mathcal{B}_{\mu-1}\}$ in $\mathbb{C}^d$ exists if and only if there exist μ classes $\mathcal{C}_0, \mathcal{C}_1, \dots, \mathcal{C}_{\mu-1}$, each containing d commuting unitary matrices in $\mathbb{M}_d(\mathbb{C})$ such that all matrices in $\mathcal{C}_0 \cup \mathcal{C}_1 \cup \dots \cup \mathcal{C}_{\mu-1}$ are pairwise orthogonal.*

The crucial property that establishes this equivalence is the fact that the vectors of the MU basis $\mathcal{B}_b$ are given by the common eigenstates of the commuting unitary matrices within class $\mathcal{C}_b$. Since each class $\mathcal{C}_b$ is maximal commuting, their common eigenstates are fixed by the requirement of simultaneous diagonalisation, up to overall phases and ordering. If a set of μ MU bases $\mathcal{B}_b = \{|v_b\rangle\}_{v=1}^d$ exists, with $b = 0 \dots \mu-1$, one can construct the elements of each commuting class $\mathcal{C}_b = \{U_{b,k}\}$ as

$$U_{b,k} = \sum_{v=0}^{d-1} e^{2\pi i k v/d} |v_b\rangle \langle v_b|, \quad (5.8)$$

for $k = 0 \dots d-1$, with $U_{b,0} = \mathbb{I}$. Hence, unitary operator bases with suitable partitions are as unlikely to exist as complete sets of MU bases in composite dimensions $d \notin \mathbb{PP}$.

Conjecture 5.4. *A partition of a unitary operator basis of $\mathbb{M}_d(\mathbb{C})$ into $d+1$ maximally commuting operator classes exists if and only if d is a prime-power.*

We will see that Equivalence 5.4 is useful in relation to *unextendible* MU bases (Sec. 6.10), *nice* MU bases (Sec. 6.5), and *real* MU bases (Sec. 9.1). Further connections between MU bases and maximally commuting operator classes are discussed in [372]. It is found, for example, that non-isomorphic sets of $d+1$ maximally commuting operator classes may not yield inequivalent complete sets of MU bases. It is also shown that a complete set of MU bases generated from maximally commuting operator classes under certain restrictions (such as forming a finite and nilpotent operator group) requires the system size to be a prime-power.

5.5 Decompositions of Lie algebras

The existence problem of complete sets of MU bases is, in fact, equivalent to a problem related to the classical Lie algebras sl_{d+1} which are associated to the Lie groups A_d of invertible linear transformations in $(d+1)$ dimensions. It was posed in 1981 [237] as a response to unsuccessful attempts to construct an “orthogonal decomposition” (see below) of the algebra sl_6 , in contrast to the corresponding algebras of other small values of d .

Problem 5.1 (*Winnie-the-Pooh problem*⁶). *Prove that the Lie algebra of type A_d admits an orthogonal decomposition if and only if $d = p^n - 1$ for some prime p and for some natural number n .*

To grasp the *equivalence* of the existence of MU bases for arbitrary dimension d with orthogonal decompositions shown in [73], we need to briefly review a number of concepts from the theory of Lie algebras. We denote $sl_d(\mathbb{C})$ as the algebra of $d \times d$ matrices over $\mathbb{C}$ of trace zero, with multiplication defined by the commutator $[A, B] = AB - BA$. A *Cartan subalgebra* H of a Lie algebra L is a nilpotent subalgebra which is self-normalising, i.e. if $[A, B] \in H$ for all $A \in H$, then $B \in H$. For the algebra $L = sl_d(\mathbb{C})$, a Cartan subalgebra is a maximal Abelian subalgebra. *Orthogonality* of subalgebras is defined with respect to the *Killing form*, $K(A, B) = \text{tr}(\text{ad}_A \cdot \text{ad}_B)$, where $\text{ad}_A : sl_d \rightarrow sl_d$ is the *adjoint endomorphism*, with $\text{ad}_A(C) = [A, C]$ for all $C \in sl_d(\mathbb{C})$. The Killing form, which for $sl_d(\mathbb{C})$ is given by $K(A, B) = 2d \text{tr}(AB)$, is non-degenerate on the Lie algebra as well as on the restriction to any Cartan subalgebra H . Thus, two Cartan subalgebras H_i and H_j are *orthogonal* if $K(H_i, H_j) = 0$. The algebra $sl_d(\mathbb{C})$ has an orthogonal decomposition if it can be written as a direct sum of orthogonal Cartan subalgebras, i.e.,

$$sl_d(\mathbb{C}) = H_0 \oplus H_1 \oplus \cdots \oplus H_d. \quad (5.9)$$

Now we are in a position to spell out the equivalence between sets of MU bases and orthogonal Cartan subalgebras, first noticed in [73].

Equivalence 5.5. *A set of μ MU bases $\{\mathcal{B}_0, \dots, \mathcal{B}_{\mu-1}\}$ of $\mathbb{C}^d$ exists if and only if a set of μ pairwise orthogonal Cartan subalgebras $\{H_0, \dots, H_{\mu-1}\}$ of $sl_d(\mathbb{C})$ exists, closed under the adjoint operation.*

Here, a Cartan subalgebra is closed under the adjoint operation $\dagger$ (i.e., the conjugate transpose) if $H = H^\dagger$. The equivalence can be understood as follows. One can construct a Cartan subalgebra H from an orthonormal basis $\mathcal{B} = \{|v\rangle\}_{v=1}^d$

if H is defined as the linear subspace of $sl_d(\mathbb{C})$ consisting of all traceless matrices that are diagonal in $\mathcal{B}$. Any element $A \in H$ can be written as $A = \sum_v a_v |v\rangle\langle v|$, with $\sum_v a_v = 0$. By associating each Cartan subalgebra H_i with a mutually unbiased basis $\mathcal{B}_i$ in this way, it is straightforward to show that two Cartan subalgebras H_i and H_j are *orthogonal* with respect to the Killing form.

To construct an orthonormal basis $\mathcal{B}$ from a Cartan subalgebra H , one takes the common eigenvectors of all the matrices in H as the elements of $\mathcal{B}$. To show that two bases $\mathcal{B}_i$ and $\mathcal{B}_j$ which correspond to two orthogonal Cartan subalgebras H_i and H_j are mutually unbiased, one simply assumes the opposite, leading to a contradiction of the orthogonality condition. Note that since any Cartan subalgebra, closed under adjoint operation, has a basis of unitary matrices that is orthogonal with respect to the Killing form, this construction of MU bases is essentially the same as using maximally commuting operator classes (i.e. Equivalence 5.4).

From Equivalence 5.5 it is clear that a complete set of $d+1$ MU bases exists if and only if one can find a set of pairwise orthogonal Cartan subalgebras $H_0, \dots, H_d$ of the Lie algebra $sl_d(\mathbb{C})$. Turning this into a conjecture on MU bases is nothing but a reformulation of the Winnie-the-Pooh problem.

Conjecture 5.5. *The simple Lie algebra $sl_d(\mathbb{C})$ admits an orthogonal decomposition if and only if d is a prime-power.*

In later sections we will see that the correspondence outlined above has useful consequences in relation to monomial MU bases (Sec. 6.6) and the existence of Hadamard matrices (Sec. 7.1). Furthermore, since the automorphism group of a complete set of MU bases is isomorphic to the automorphism group of the associated orthogonal decomposition [3], these can be used to show inequivalences between complete sets (see Appendix A.8).

5.6 Maximal Abelian subalgebras

The one-to-one correspondence between orthonormal bases in $\mathbb{C}^d$ and maximal Abelian subalgebras (MASAs) of $M_d(\mathbb{C})$ mentioned in Sec. 2.1 leads to a natural reformulation of MU bases in terms of the orthogonality relations between collections of MASAs. In particular, an

⁶The unconventional name of the problem is explained in Ref. [238] as a play on words, incomprehensible to the English reader. The pun is based on the pronunciation of the Russian word for “again” being similar to that of “ A_5 ”, leading Kostrikin to adapt a song from A. A. Milne’s “Winnie-the-Pooh” which revolves around the word “again”.

orthonormal basis $\mathcal{B} = \{|v\rangle\}$ generates a MASA,

$$\mathcal{A}(\mathcal{B}) = \left\{ \sum_{v=0}^{d-1} \alpha_v |v\rangle\langle v| \mid \alpha_v \in \mathbb{C} \right\}, \quad (5.10)$$

and, conversely, each MASA defines an orthonormal basis. As shown in [304], given two bases $\mathcal{B}$ and $\mathcal{B}'$, and their corresponding MASAs $\mathcal{A}(\mathcal{B})$ and $\mathcal{A}(\mathcal{B}')$, then $\mathcal{B}$ and $\mathcal{B}'$ are mutually unbiased if and only if $\mathcal{A}(\mathcal{B}) \ominus \mathbb{C}\mathbb{I}$ and $\mathcal{A}(\mathcal{B}') \ominus \mathbb{C}\mathbb{I}$ are mutually orthogonal (in the sense of the Hilbert-Schmidt inner product). Here, $\mathcal{A}(\mathcal{B}) \ominus \mathbb{C}\mathbb{I}$ denotes the orthogonal complement of the subspace $\mathbb{C}\mathbb{I}$ in $\mathcal{A}(\mathcal{B})$, with $\mathbb{C}\mathbb{I} = \{z\mathbb{I} \mid z \in \mathbb{C}\}$. In recent literature, e.g. [310], the orthogonality relation between MASAs is usually called *quasi-orthogonality*. Generalising to larger collections of MASAs, we have the following equivalence [304].

Equivalence 5.6. *A set of μ bases $\{\mathcal{B}_0, \dots, \mathcal{B}_{\mu-1}\}$ of $\mathbb{C}^d$ are mutually unbiased if and only if the MASAs $\mathcal{A}(\mathcal{B}_0), \dots, \mathcal{A}(\mathcal{B}_{\mu-1})$ are quasi-orthogonal.*

This equivalence leads to a conjecture on the existence of MASAs.

Conjecture 5.6. *A set of $(d+1)$ pairwise quasi-orthogonal MASAs of $\mathbb{M}_d(\mathbb{C})$ exists if and only if d is a prime-power.*

Studies on MASAs, from as early as 1983, have provided constructions of complete sets of MU bases in prime dimensions [312] (see Sec. 2.1) which were later rediscovered in the language of MU bases, along with several other results. Since then, MASAs have been relevant for the classification of complex Hadamard matrices of order $d \leq 5$ [174], constructions of strongly unextendible MU bases [358] (Sec. 6.10), as well as to show that d MU bases are sufficient for a complete set (see Sec. 6.3).

5.7 C^* -algebra formulation

Describing a pair of MU bases by their rank-one projectors $P_1(v) = |v_1\rangle\langle v_1|$ and $P_2(v) = |v_2\rangle\langle v_2|$ for $v = 0 \dots d-1$, it is easy to check that the following conditions hold: (i) $P_1(v)P_1(v') = \delta_{vv'}P_1(v)$; (ii) $\sum_v P_1(v) = \mathbb{I}$; (iii) $P_1(v)P_2(v')P_1(v) = P_1(v)/d$; (iv) $[P_1(v)UP_1(v), P_1(v)VP_1(v)] = 0$, for all $v, v' = 0, \dots, d-1$ and $U, V \in \mathbb{C}^{d \times d}$. Relaxing the condition that the projectors are $d \times d$ matrices, a

special type of C^* -algebra can be defined called a (d, μ) -MUB algebra [297].

Definition 5.1. A C^* -algebra $\mathcal{A}$ is called a (d, μ) -MUB algebra if it contains Hermitian elements $X_{v,b}$ for all $v = 0 \dots d-1$ and $b = 1 \dots \mu$, which satisfy the following conditions:

- (i) $X_{v,b}X_{v',b} = \delta_{v,v'}X_{v,b}$ for all $v, v' = 0 \dots d-1$ and $b = 1 \dots \mu$;
- (ii) $\sum_{v=0}^{d-1} X_{v,b} = I$ for all $b = 1 \dots \mu$;
- (iii) $X_{v,b} = dX_{v,b}X_{v',b'}X_{v,b}$ for all $v, v' = 0 \dots d-1$ and $b, b' = 1 \dots \mu$ with $b \neq b'$;
- (iv) $[X_{v,b}UX_{v,b}, X_{v,b}VX_{v,b}] = 0$ for all $v = 0 \dots d-1$ and $b = 1 \dots \mu$, and $U, V \in \langle \mathbf{X} \rangle$, where $\langle \mathbf{X} \rangle$ denotes the set of monomials in $X_{v,b}$.

If $X_{v,b}$ form the rank-one projectors associated with μ MU bases of $\mathbb{C}^d$, then the conditions (i-iv) are clearly satisfied, with $U, V \in \mathbb{C}^{d \times d}$. Thus, μ MU bases give rise to a (d, μ) -MUB algebra. The converse, proved in [297], is also true, i.e., the existence of a (d, μ) -MUB algebra with $I \neq 0$, implies the existence of μ MU bases in $\mathbb{C}^d$. Thus, the existence of MU bases can be reformulated in terms of a C^* -algebra [297].

Equivalence 5.7. *A set of μ MU bases $\{\mathcal{B}_0, \dots, \mathcal{B}_{\mu-1}\}$ in $\mathbb{C}^d$ exists if and only if there exist a (d, μ) -MUB algebra with $I \neq 0$.*

The equivalence implies a conjecture about MUB-algebras corresponding to *complete* sets of MU bases.

Conjecture 5.7. *A $(d, d+1)$ -MUB algebra exists if and only if d is a prime-power.*

Formulating the existence question in this manner yields a non-commutative polynomial optimisation problem [170]. Upon exploiting existing symmetries, a tractable hierarchy of semidefinite programs is constructed, leading to numerical sum-of-squares certificates for the non-existence of $(d+2)$ MU bases for $d \leq 8$.

5.8 Quantum designs

In this section we discuss Zauner's definition of quantum designs and show how they relate to MU bases and complex projective 2-designs.

A *quantum design* of order d is a set $\mathcal{D} = \{P_1, \dots, P_n\}$ of complex orthogonal $d \times d$ projection matrices; it is called k -coherent if for each unitary U , we have

$$\sum_{i=1}^n P_i^{\otimes k} = \sum_{i=1}^n (UP_i U^{-1})^{\otimes k}. \quad (5.11)$$

The set $\mathcal{D}$ is a *quantum t -design* if it is a k -coherent quantum design for all $1 \leq k \leq t$ [412]. In the particular case that $\mathcal{D}$ is a finite subset of the complex projective space, i.e. $\mathcal{D} \subset \mathbb{C}P^{d-1}$, as discussed in Sec. 5.11, the condition of k -coherence is equivalent to the definition of a complex projective k -design, i.e.,

$$\frac{1}{|\mathcal{D}|} \sum_{x \in \mathcal{D}} P(x)^{\otimes k} = \int_{\mathbb{C}P^{d-1}} P(x)^{\otimes k} d\nu(x), \quad (5.12)$$

where the points $x \in \mathcal{D}$ can be represented as unit vectors $|x\rangle \in \mathbb{C}^d$ or rank-one projectors $P(x) = |x\rangle\langle x|$, and ν is the unitarily invariant Haar measure on $\mathbb{C}P^{d-1}$.

The focus of Zauner's 1999 PhD thesis was on so-called *regular affine* quantum designs [412] (see [413] for an English translation). A *regular* quantum design is a set $\mathcal{D} = \{P_1, \dots, P_n\}$ of $d \times d$ projection matrices such that $\text{Tr}[P_i] = r$ for all $i = 1 \dots n$. The degree of a quantum design is defined as the number of distinct elements in the set $\{\text{Tr}[P_i P_j] : 1 \leq i \neq j \leq n\}$. A quantum design is called *resolvable* if the n projections can be partitioned into μ subclasses, where each subclass contains n/μ pairwise orthogonal projections summing to the identity. An *affine* quantum design is resolvable and has degree two. When affine designs are regular, i.e. $r = 1$, the elements of $\mathcal{D}$ form a set of MU bases, and the following equivalence holds [413].

Equivalence 5.8. *A set of μ MU bases $\{\mathcal{B}_0, \dots, \mathcal{B}_{\mu-1}\}$ of $\mathbb{C}^d$ exists if and only if an affine quantum design of order d and $r = 1$ exists with μ orthogonal subclasses.*

Unaware of this equivalence, Zauner found that regular affine quantum designs have $(d+1)$ orthogonal classes when d is a prime or prime-power. The solution generalises to $r \geq 1$, where the existence of $r^2(d^2 - 1)(d - r)$ orthogonal classes is shown. He also suggests that “*Presumably a complex, affine quantum design with $d = 6$, $r = 1$ and $\mu = 4$ does not exist*” [413]. This appears to be

the first statement conjecturing the non-existence of *four* MU bases in $\mathbb{C}^6$; Winnie-the-Pooh's formulation of the problem in the Lie algebraic setting (see Sec. 5.5) was silent with regards to this question. Zauner's statement is easily generalised to the case of complete sets of MU bases in composite dimensions $d \notin \mathbb{P}\mathbb{P}$.

Conjecture 5.8. *An affine quantum design of order d with $r = 1$ and $(d + 1)$ orthogonal subclasses exists if and only if d is a prime-power.*

In Sec. 7.2 we describe an infinite family of triples of MU bases in $\mathbb{C}^6$ which were first constructed as affine quantum designs.

5.9 Quantum random access codes

As already mentioned in Sec. 4.6, the QRAC $\mu^d \rightarrow 1$ protocol can be modified by giving Alice an extra piece of information about Bob's actions: Alice is told that Bob will only be questioned on a certain subset of the d levels. In particular, let S_ν be the set of all possible subsets of $\{1, \dots, \mu\}$ of size $\nu \leq \mu$, and suppose Alice receives an input $s \in S_\nu$ with the promise that $y \in s$. This setting defines a “p-QRAC protocol” (with “p” for “promise”) of type $(\mu, \nu)^d \rightarrow 1$. The average success probability, $p(\mu, \nu, d)$, is then calculated over all $\mathbf{x}_s$, $y \in s$, and $s \in S_\nu$, where $\mathbf{x}_s = \{x_{j_1}, \dots, x_{j_\nu}\}$ such that $\{j_1, \dots, j_\nu\} = s$. When $\nu = 2$, the *optimal* average success probability $P(\mu, 2, d)$, maximised over all states and measurements, is intimately connected to MU bases [7].

Equivalence 5.9. *For a p-QRAC of the type $(\mu, 2)^d \rightarrow 1$, the optimal average success probability satisfies*

$$P(\mu, 2, d) \leq \frac{1}{2} \left(1 + \frac{1}{\sqrt{d}} \right), \quad (5.13)$$

and achieves equality if and only if Bob's measurement bases are a set of μ MU bases $\{\mathcal{B}_0, \dots, \mathcal{B}_{\mu-1}\}$ of $\mathbb{C}^d$.

In other words, sets of μ MU bases in dimension d exist if and only if the optimal average success probability saturates the bound in Eq. (5.13). It follows that the optimal average success probability with $\mu = d + 1$ cannot reach this bound in composite dimensions if no complete set of MU bases exists.

Conjecture 5.9. *A p -QRAC of the type $(d + 1, 2)^d \rightarrow 1$ achieves the optimal average success probability given by the RHS of Eq. (5.13) if and only if d is a prime-power.*

Equivalence 5.9 leads naturally to an *operational* measure of mutual unbiasedness for a set of μ bases, given by the average success probability $p(\mu, \nu, d)$ of the $(\mu, 2)^d \rightarrow 1$ p -QRAC protocol, when the μ bases are measured by Bob. Numerical calculations of this measure provide additional evidence that only three MU bases exist in dimension six (cf. Sec. 8.2).

The equivalence relation also provides a strategy to prove the conjecture that no set of four MU bases exists in $d = 6$ (cf. Sec. 10.2). Using semidefinite programming methods derived in [298] to find an upper bound on $P(4, 2, d)$ for the $(4, 2)^6 \rightarrow 1$ p -QRAC, one can conclude that four MU bases do not exist if the bound falls below the optimal value in Eq. (5.13).

5.10 Geometry of MU bases

A complete set of MU bases for a qubit consists of six states in Hilbert space $\mathbb{C}^2$. They form three orthogonal pairs while states taken from different pairs have constant overlap of modulus $1/\sqrt{2}$. The rank-one projectors onto these states can be pictured as points on the surface of the three-dimensional *Bloch ball* used to represent both pure and mixed qubit states in the space $\mathbb{R}^3$. The convex combinations associated with the orthogonal quantum states within a pair form three line segments, each contained in a one-dimensional subspace of $\mathbb{R}^3$. The line segments are pairwise perpendicular in terms of the standard Euclidian geometry of $\mathbb{R}^3$, and the distance between endpoints belonging to different segments is constant. Forming the convex hull of the six states of the complete set, one obtains an *octahedron* contained entirely within the Bloch ball, known as the *complementarity polytope* associated with a qubit [50, 53].

Interestingly, polytopes with these characteristics exist in any Euclidean space of dimension $\mathbb{R}^{d^2-1}$, $d \in \mathbb{N}$, used to represent the state space of a qudit. The one-dimensional line segments with two endpoints each generalise to *regular simplices* with $(d - 1)$ equidistant vertices. In total, $(d + 1)$ such simplices exist in the space $\mathbb{R}^{d^2-1}$. They are orthogonal to each in the Euclidean sense, i.e.

they have no point in common except for the origin, just as the three line segments. Here, the expression

$$D^2(A, A') = \frac{1}{2} \text{Tr}(A - A')^2 \quad (5.14)$$

defines the (Hilbert-Schmidt) distance in the $(d^2 - 1)$ -dimensional Euclidean space of Hermitian matrices A, A' , with unit trace. Using the inner product

$$(A, A') = \frac{1}{2} \left(\text{Tr}(AA') - \frac{1}{d} \right) \quad (5.15)$$

results in a vector space $\mathbb{R}^{d^2-1}$, with the maximally mixed state $\mathbb{I}/d$ taken as its origin.

The density matrices of a qudit define a convex set of points in $\mathbb{R}^{d^2-1}$, generalising the Bloch ball for a qubit in $\mathbb{R}^3$. While complementarity polytopes exist for every dimension d , they do not necessarily fit inside the body of density matrices: inscribing the polytope requires its vertices to correspond to rank-one projectors.

Equivalence 5.10. *The $d(d + 1)$ vertices of the complementarity polytope are given by rank-one projectors if and only if they correspond to the states of a complete set of MU bases in $\mathbb{C}^d$.*

In the space $\mathbb{R}^{d^2-1}$, it is difficult to geometrically identify suitable rotations ensuring this property although each construction of a complete sets of MU bases for $d \in \mathbb{PP}$ guarantees the existence of such a rotation.

Conjecture 5.10. *For a qudit, the $(d^2 - 1)$ -dimensional complementarity polytope fits inside the body of density matrices if and only if d is a prime-power.*

5.11 Complex projective 2-designs

Loosely speaking, a complex projective t -design is a finite set of points on the unit sphere which can be used to calculate integrals of functions over the entire unit sphere. More precisely, it is a finite subset $\mathcal{D}$ of the complex projective space $\mathbb{CP}^{d-1}$ of lines passing through the origin, such that the expectation of every polynomial of degree at most t over the points (defined as the intersections of the lines with the unit sphere) is the same irrespective of the distribution being the Haar measure or the t -design.

It is often convenient to represent these points $x \in \mathcal{D} \subset \mathbb{C}P^{d-1}$ as a collection of unit vectors $|x\rangle \in \mathbb{C}^d$ or, alternatively, by rank-one projectors $P(x) = |x\rangle\langle x|$. For a unit vector $|x\rangle = \sum_{j=1}^d x_j |j\rangle$, with $x_j \in \mathbb{C}$, we define $f : \mathbb{C}P^{d-1} \rightarrow \mathbb{R}$ to be a homogenous polynomial $f(x) = f(x_1, \dots, x_d, x_1^*, \dots, x_d^*)$ of degree at most t in the coefficients x_j , and of degree at most t in x_j^* . Polynomials of this type are denoted as $f \in \text{Hom}(t, t)$. The identity

$$\frac{1}{|\mathcal{D}|} \sum_{x \in \mathcal{D}} f(x) = \int_{\mathbb{C}P^{d-1}} f(x) d\nu(x), \quad (5.16)$$

holds for all $f \in \text{Hom}(t, t)$, if and only if $\mathcal{D}$ is a complex projective t -design, where the integral is evaluated over the unitarily invariant Haar measure ν on the unit sphere in $\mathbb{C}^d$. This type of identity, which equates an integral of a function over a domain with a sum of the function values evaluated at specific points of the domain, is known as a *cubature* (formula). It represents a convenient starting point to evaluate integrals by numerical methods.

The definition of a complex projective t -design implies that it is also a t' -design for every $t' \leq t$. In particular, any t -design with $t \geq 1$ is a projective 1-design, which in the language of frame theory is equivalent to a finite unit-norm tight frame. Consequently, rescaling the rank-one operators $|x\rangle\langle x|d/|\mathcal{D}|$ by the factor $d/|\mathcal{D}|$ generates a POVM.

Designs of this type are known to exist in every dimension d and for any t [337]. An example of a 1-design is an orthonormal basis of the space $\mathbb{C}^d$. The smallest set of vectors which constitute a 2-design is formed by d^2 complex equiangular lines which correspond to the elements of a SIC-POVM [320], as described in Sec. 3.9. The set of qubit stabilizer states form a 3-design [241].

It can be convenient to define a complex-projective t -design (cf. Eq. (5.16)) via an equivalent expression. For example, a t -design is a set $\mathcal{D}$ such that

$$\begin{aligned} \frac{1}{|\mathcal{D}|} \sum_{x \in \mathcal{D}} P(x)^{\otimes t} &= \int_{\mathbb{C}P^{d-1}} P(x)^{\otimes t} d\nu(x) \\ &= \binom{d+t-1}{t}^{-1} \Pi_{\text{sym}}^{(t)}, \end{aligned} \quad (5.17)$$

where $\Pi_{\text{sym}}^{(t)}$ is the projector onto the symmetric subspace of $(\mathbb{C}^d)^{\otimes t}$ and $P(x) = |x\rangle\langle x|$ is the

projection operator associated with $x \in \mathbb{C}P^{d-1}$. The equivalence between Eqs. (5.16) and (5.17) is shown in Ref. [320].

Barnum [36] appears to have been among the first to point out—in the context of information-disturbance tradeoffs—that the uniform ensemble supported on a complete set of MU bases forms a complex projective 2-design. Klappe-necker and Rötteler [230] subsequently related Zauner’s notion of quantum designs (see Sec. 5.8) to MU bases, showing that a set of $(d+1)$ MU bases forms a complex projective 2-design containing $d(d+1)$ elements. If the elements of a design $\mathcal{D}$ are restricted to a set of μ orthonormal bases, then $\mathcal{D}$ is a 2-design only when $\mu \geq d+1$, with equality if and only if the bases are mutually unbiased [322]. This observation leads to an equivalence between complex projective 2-designs and MU bases [322].

Equivalence 5.11. *Suppose $\mathcal{D}$ is a set of $(d+1)$ orthonormal bases in $\mathbb{C}^d$. Then $\mathcal{D}$ is a complex projective 2-design if and only if $\mathcal{D}$ is a set of MU bases.*

Thus, any set of $(d+1)$ MU bases $\mathcal{B}_b = \{|v_b\rangle\}_{v=0}^{d-1}$, satisfies the condition

$$\sum_{b=0}^d \sum_{v=0}^{d-1} P_b(v)^{\otimes 2} = 2\Pi_{\text{sym}}^{(2)}, \quad (5.18)$$

where $P_b(v) = |v_b\rangle\langle v_b|$. With this equivalence in mind we formulate a conjecture on the existence of complex projective 2-designs.

Conjecture 5.11. *A complex-projective 2-design formed from $(d+1)$ orthonormal bases in $\mathbb{C}^d$ exists if and only if d is a prime-power.*

We note that an equivalence relation also exists between a projective toric 2-design [244] and a complete set of MU bases, as shown in Refs. [201, 202]. In particular, a set of d complex Hadamard matrices of order d is mutually unbiased if and only if their columns form a projective toric 2-design. A projective toric 2-design is a finite set of points in $P(T^d)$ that satisfies a condition similar to Eq. (5.16), replacing the polynomials with monomials on T^d of a specific degree. Here, T^d denotes the d -dimensional torus $T = \mathbb{R}/2\pi\mathbb{Z}$, and $P(T^d)$ consists of the set of points on T^d identified up to a constant additive factor (i.e. without the global phase redundancy).

Interestingly, a projective toric 2-design can be used to construct a complex projective 2-design with $d(d+1)$ elements that does not form complete sets of MU bases [201], disproving a conjecture by Zhu [420].

In Secs. 4.1 and 4.2 we discussed applications of MU bases which included quantum state tomography and entanglement detection, respectively. However, these applications are not restricted to MU bases—other complex projective 2-designs [26, 322] may be used instead. Furthermore, in composite dimensions $d \notin \mathbb{PP}$, the 2-design property of the $(d+1)$ MU bases plays an important role in restricting their entanglement content (cf. Sec. 6.8). In Sec. 7.5 we will see that a search for projective toric 2-designs that form groups reveals a clear distinction between complete sets in dimension six and those in prime (or prime-powered) dimensions. Finally, Sec. 9 deals with modifications of Eq. (5.16) which extend the definition of complex projective 2-designs to *approximate* (Sec. 9.7), *weighted* (Sec. 9.8), and *conical* (Sec. 9.9) 2-designs.

5.12 Welch bounds

Sets of points in the complex projective space $\mathbb{CP}^{d-1}$ are not only related to designs but also come with bounds on the moduli of overlaps between the states associated with them. The *Welch bounds* [392]

$$\frac{1}{|\mathcal{X}|^2} \sum_{x,y \in \mathcal{X}} |\langle x|y \rangle|^{2k} \geq \binom{d+k-1}{k}^{-1}, \quad (5.19)$$

$k \in \mathbb{N}_0$, apply to any finite set $\mathcal{X} = \{x : x \in \mathbb{CP}^{d-1}\}$ with $|\mathcal{X}| > 0$ elements. Equality holds for all integer values of k up to t , i.e. $0 \leq k \leq t$, if and only if the set $\mathcal{X}$ is a complex projective t -design [230]. Thus, if the set $\mathcal{X}$ consists of $(d+1)$ MU bases—which form a complex projective 2-design according to Sec. 5.11—then we have the two identities

$$\sum_{x,y \in \mathcal{X}} |\langle x|y \rangle|^2 = d(d+1)^2, \quad (5.20)$$

and

$$\sum_{x,y \in \mathcal{X}} |\langle x|y \rangle|^4 = 2d(d+1), \quad (5.21)$$

for $k=1$ and $k=2$, respectively. The equality for $k=0$ simply counts the number of ordered pairs of vectors from the set $\mathcal{X}$, and the $k=1$

identity reduces to the normalisation condition. Hence, the Welch bounds can be used to reformulate the existence problem of MU bases.

Equivalence 5.12. *Suppose that $\mathcal{X}$ is a set of $(d+1)$ orthonormal bases in $\mathbb{C}^d$. Then $\mathcal{X}$ saturates the Welch bounds in Eq. (5.19) for $0 \leq k \leq 2$ if and only if $\mathcal{X}$ is a set of $(d+1)$ MU bases.*

The proof can be found in [322]. It relies on the observation in [230] that $\mathcal{X}$ saturates the Welch bound for $0 \leq k \leq 2$ if and only if $\mathcal{X}$ is a 2-design. It then follows from Equivalence 5.11 that $\mathcal{X}$ constitutes a complete set of MU bases. Thus, the existence problem for MU bases in composite dimensions turns into an open problem for bases saturating Welch bounds.

Conjecture 5.12. *A set of $(d+1)$ orthogonal bases in $\mathbb{C}^d$ saturating the Welch bound of Eq. (5.19) for $k=0,1,2$ exists if and only if d is a prime-power.*

Using Welch bounds, it is also possible recast the existence question of MU bases as one involving only orthogonal vectors. Suppose that A and B are matrices of order d , and let $A \circ B$ denote the Hadamard product, i.e., $(A \circ B)_{jk} = A_{jk} \times B_{jk}$, and $A^{(\ell)}$ the ℓ -th Hadamard power of A , with matrix elements $A^{(\ell)}_{jk} = A_{jk}^\ell$. For a suitable matrix, the following proposition demonstrates an equivalence between its columns saturating a Welch bound and its rows satisfying a set of orthogonality conditions [45].

Proposition 5.1. *Let B be a $d \times n$ matrix and denote its sets of columns and rows by $\mathcal{C} = \{c_1, \dots, c_n\} \subset \mathbb{C}^d$ and $\mathcal{R} = \{r_1, r_2, \dots, r_d\} \subset \mathbb{C}^n$, respectively. Then the column vectors $\mathcal{C}$ saturate the Welch bound for $k=2$ if and only if all vectors from the set $\{r_j^{(2)}\} \cup \{\sqrt{2}r_j \circ r_k | 1 \leq j < k \leq d\}$ are pairwise orthogonal and of equal length.*

If the columns of B are given by the columns of d Hadamard matrices of order d , the row vectors of B form a set of d vectors in $\mathbb{C}^{d^2}$. Subsequently, via a Hadamard product, every pair of these d row vectors maps to a new vector in $\mathbb{C}^{d^2}$. It follows from the above proposition that the d Hadamard matrices are MU if and only if the latter vectors in $\mathbb{C}^{d^2}$ are pairwise orthogonal. This gives rise to yet another characterisation of complete sets of MU bases.

Equivalence 5.13. *Let $\{H_1, \dots, H_d\}$ be a set of Hadamard matrices of order d , and let matrix B be the $d \times d^2$ matrix formed from the set of normalised column vectors of each Hadamard matrix. The set of columns and rows of B are given by $\mathcal{C} = \{c_1, \dots, c_{d^2}\} \subset \mathbb{C}^d$ and $\mathcal{R} = \{r_1, r_2, \dots, r_d\} \subset \mathbb{C}^{d^2}$, respectively. Then $\{H_1, \dots, H_d\}$ are pairwise mutually unbiased if and only if all vectors from the set $\{r_j \circ r_k | 1 \leq j \leq k \leq d\}$ are pairwise orthogonal.*

With this equivalence in mind, the existence problem of a complete set of MU bases leads to a conjecture about the orthogonality of a set of vectors in $\mathbb{C}^{d^2}$.

Conjecture 5.13. *A set of pairwise orthogonal vectors $\{r_j \circ r_k | 1 \leq j \leq k \leq d\}$ in $\mathbb{C}^{d^2}$ with the properties defined in Equivalence 5.13 exists if and only if d is a prime-power.*

5.13 Rigidity of MU bases

The existence problem of complete sets of MU bases can be reformulated in terms of the overlap constraints on a set of vectors, without reference to orthonormal bases [275].

Equivalence 5.14. *Let $\mathcal{S}_d = \{|\phi_i\rangle | i = 1, \dots, d(d+1)\}$ be a collection of $d(d+1)$ unit vectors in $\mathbb{C}^d$. A set of $(d+1)$ MU bases in $\mathbb{C}^d$ exists if and only if $|\langle\phi_i|\phi_j\rangle|^2 \in \{0, 1/d\}$ for all $i \neq j$.*

Clearly, the existence of a complete set of MU bases implies all $d(d+1)$ vectors are either orthogonal or mutually unbiased. The converse is less obvious: for example, as many as $(d-1)^2$ unit vectors in $\mathbb{C}^d$ exist which are pairwise unbiased. The proof of the equivalence [275] relies on graph theoretic methods. Consequently, we have the following conjecture on the existence of a collection of vectors that can be pairwise orthogonal or mutually unbiased.

Conjecture 5.14. *A set $\mathcal{S}_d$ of $d(d+1)$ unit vectors satisfying the conditions $|\langle\phi_i|\phi_j\rangle|^2 \in \{0, 1/d\}$ for all $i \neq j$ exists if and only if d is a prime-power.*

6 Rigorous results: Composite dimensions

This section collects rigorous existence and non-existence results relating to MU bases in non-

prime-power dimensions. We start with the problem of identifying all pairs of MU bases, which is equivalent to listing all complex Hadamard matrices. Moving on to the existence of larger sets of MU bases, we review various construction techniques and discuss their limitations. Most constructions (in Sec. 6.5–6.9) impose additional constraints on the bases (e.g. niceness, monomiality, separability and entanglement) which help simplify the problem, leading to larger sets of MU bases or proofs of unextendibility (cf. Sec. 6.10). Finally, in Sections 6.11 and 6.12, we review some mathematical techniques that shed light on the structure of complete sets, and may be useful in a solution to the existence problem. In Sec. 7, we will make explicit the consequences of these results for $d = 6$ and summarise additional ones specific to this dimension.

6.1 Pairs of MU bases

Any pair of mutually unbiased bases $\{\mathcal{B}_0, \mathcal{B}_1\}$ of the space $\mathbb{C}^d$ is equivalent to the existence of a complex Hadamard matrix of order d (see Equivalence 5.2). Thus, listing all $d \times d$ Hadamard matrices provides a full characterisation of pairs of MU bases in dimension d . While every Hadamard matrix is known up to and including dimension five [174, 239], there is no exhaustive list for dimensions six and above.

The study of real and complex Hadamard matrices has been an active research area for several centuries, and continues to be so. Instead of describing all constructions, which is beyond the scope of this review, we will summarise results which are relevant in our context. For standard definitions such as the equivalence between Hadamard matrices, their defects, isolated Hadamard matrices as well as affine and non-affine families, see Appendix B.

An early construction of a complex Hadamard matrix dates back to Sylvester (see Sec. 2.1) who described the $d \times d$ Fourier matrices F_d in prime dimensions $d \in \mathbb{P}$, with matrix elements,

$$F_{jk} = \frac{1}{\sqrt{d}} e^{2\pi i jk/d}, \quad j, k = 0 \dots d-1. \quad (6.1)$$

For every prime-power dimension $d = p^n$, with $n > 1$, there exists an affine Fourier family with the number of free parameters given by

$$\text{def}(F_d) = \sum_{n=1}^{d-1} (\gcd(n, d) - 1). \quad (6.2)$$

The value $\text{def}(F_d)$ is known as the *defect* of the Fourier matrix [38, 361] and, in general, gives an upper bound on the number of free parameters of any smooth dephased Hadamard family stemming from F_d (see Appendix B). When d is a prime-power, there exist simple constructions of families saturating this bound. However, for *composite* dimensions $d \in (7, 100]$, the number of free parameters is strictly *less* than Eq. (6.2) [38].

Hadamard matrices derive their name from a 1893 paper by Hadamard in which he studies the maximal determinant of matrices with entries having modulus at most one [176]. However, already in 1867 Sylvester constructed $2^k \times 2^k$ Hadamard matrices using tensor products [354]. In 1933, Paley uses quadratic residues in $GF(p^k)$ to construct Hadamard matrices of order $(p^k + 1)$ for $p^k + 1 \equiv 0 \pmod{4}$ [303].

The set of Butson-Hadamard matrices $BH(d, r)$ consists of $d \times d$ matrices, the elements of which are r -th roots of unity [90] (see Sec. 9.2). When $r = 2$, the class $BH(d, 2)$ equates to *real* Hadamard matrices of order d , famously conjectured to exist when $d = 4k$, for every $k \in \mathbb{N}$. More generally, Hadamard matrices with real entries give rise to real MU bases, discussed in Sec. 9.1. Whether matrices of type $BH(d, r)$ exist for arbitrary r is still an open problem. For instance, if $p \in \mathbb{P}$, there exist $p \times p$ Butson-Hadamard matrices $BH(p, 2^j p^k)$ for all $0 \leq j \leq k$ [90].

For many other constructions of $d \times d$ complex Hadamard matrices we refer the reader to the compendia [6, 191, 361] and the 400-page “Invitation to Hadamard matrices” [35], as well as the *online catalogue* [84]. In Sec. 7.1 all known complex Hadamard matrices for $d = 6$ are described.

6.2 Larger sets of MU bases

It is well-known that up to $(d + 1)$ MU bases in total may be found (see Appendix A) when aiming to go beyond *pairs* of MU bases in a complex vector space $\mathbb{C}^d$. The following theorem by Klappenecker and Rötteler [229] establishes the minimal number of MU bases that are guaranteed to exist in any given finite-dimensional Hilbert space.

Theorem 6.1. *Let $d = p_1^{n_1} \dots p_r^{n_r}$ be a factorisation of d into distinct primes p_i and let $N(d)$ denote the number of mutually un-*

biased bases in dimension d . Then $N(d) \geq \min\{N(p_1^{n_1}), N(p_2^{n_2}), \dots, N(p_r^{n_r})\}$.

To see this, denote the smallest number of MU bases by $\mu = \min_i N(p_i^{n_i})$ and choose for every prime-power factor (i.e. $\mathbb{C}^{p_i^{n_i}}$) a set of μ MU bases labeled by $\mathcal{B}_1^{(i)}, \dots, \mathcal{B}_\mu^{(i)}$. A set of μ MU bases of the space $\mathbb{C}^d$ is then given by the product bases $\mathcal{B}_k^{(1)} \otimes \dots \otimes \mathcal{B}_k^{(r)}$, where $k = 1, \dots, \mu$.

Since we know that every prime-power dimension $p_i^{n_i}$ has $(p_i^{n_i} + 1)$ MU bases, it follows that $N(d) \geq 3$ for $d \geq 2$, i.e., at least three MU bases exist in any finite dimension. The existence of triples of MU bases in dimension six is an obvious consequence.

Corollary 6.1. *In dimension six there exist at least three MU bases.*

This statement is contained in Zauner’s PhD thesis (cf. Proposition 2.20 of [413]), expressed in the language of affine quantum designs (see Sec. 5.8). The triple in dimension $d = 2$ and the $(p + 1)$ -tuples in prime dimensions were known since 1960 (cf. Sec. 2.1).

6.3 Sets of d MU bases are sufficient

There is a general result which makes the search for complete sets a little less challenging [391].

Theorem 6.2. *Suppose that $\{\mathcal{B}_0, \dots, \mathcal{B}_{d-1}\}$ is a collection of d MU bases in $\mathbb{C}^d$. Then there exists a basis $\mathcal{B}_d$ such that $\{\mathcal{B}_0, \dots, \mathcal{B}_{d-1}, \mathcal{B}_d\}$ is a complete collection of $(d + 1)$ MU bases.*

The proof makes use of the connection between MU bases and maximal Abelian subalgebras (see Equivalence 5.6). In particular, the proof shows that, given a set of d quasi-orthogonal MASAs, one can always find a MASA quasi-orthogonal to all of them. An alternative proof was later given in [95].

Interestingly, the property observed in Thm. 6.2 mirrors an analogous result on mutually orthogonal Latin squares, adding a further connection between the two related structures (cf. Appendices A.5 and C). In particular, a collection of $(d - 2)$ mutually orthogonal Latin squares can always be completed to $(d - 1)$ mutually orthogonal Latin squares.

Theorem 6.2 implies that any collection of six MU bases in $\mathbb{C}^6$ leads to the existence of a full set

of seven MU bases. If two bases are missing from a complete set, however, then it is not necessarily possible to “complete” the set (see Sec. 6.10 for an example). Thus, five MU bases in dimension six would not prove the existence of seven MU bases in $\mathbb{C}^6$.

6.4 Biunimodular sequences

First considered by Björck in 1985 [62], a *biunimodular sequence* is defined as a vector⁷ $x = (x_0, x_1, \dots, x_{d-1}) \in \mathbb{C}^d$ such that $|x_j| = |\hat{x}_j| = 1$ for all j , where $\hat{x} = (\hat{x}_0, \hat{x}_1, \dots, \hat{x}_{d-1})$ is the Fourier transform $\hat{x}_j = \frac{1}{\sqrt{d}} \sum_{k=0}^{d-1} \omega^{jk} x_k$ of the vector x , and $\omega = e^{2\pi i/d}$ is a d -th root of unity. In other words, biunimodularity requires both x and $\hat{x} = F_d x$ to be unimodular, where F_d is the Fourier matrix.

A unimodular sequence x is biunimodular if and only if its cyclic translations are all orthogonal. It follows that finding a biunimodular sequence can be translated into solving the set of equations

$$\begin{aligned} z_0 + z_1 + \dots + z_{d-1} &= 0, \\ z_0 z_1 + z_1 z_2 + \dots + z_{d-2} z_{d-1} + z_{d-1} z_0 &= 0, \\ z_0 z_1 z_2 + z_1 z_2 z_3 + \dots + z_{d-1} z_0 z_1 &= 0, \\ &\vdots \\ z_0 z_1 \dots z_{d-2} + \dots + z_{d-1} z_0 \dots z_{d-3} &= 0, \\ z_0 z_1 \dots z_{d-1} &= 0, \end{aligned} \quad (6.3)$$

defining the *cyclic d -roots problem* (the mathematical literature usually speaks of “cyclic n -roots”) [60, 61]. A solution $z = (z_0, z_1, \dots, z_{d-1})$ is known as a cyclic d -root. Imposing the additional constraint $|z_j| = 1$ gives rise to a biunimodular sequence x , where $z_j = x_{j+1}/x_j$.

Finding all biunimodular sequences, or solving the cyclic d -roots problem, corresponds to finding all vectors mutually unbiased to the standard and Fourier basis. Solutions are known for $d \leq 14$ (see [151] for a summary). There are 156 cyclic 6-roots and 48 biunimodular sequences among them (see Sec. 7.3 for details). The next non-prime-power dimension contains 34,940 cyclic 10-roots [143]. For prime p there are $\binom{2p-2}{p-1}$ cyclic p -roots, if counted with multiplicities [175].

⁷In this section, we will not distinguish between a vector x and its transpose x^T , for notational simplicity.

For d divisible by a square, the number of cyclic d -roots is infinite [24]. The same statement is also true for biunimodular sequences [61].

Theorem 6.3. *For d divisible by a square, the number of biunimodular sequences (with leading entry 1) is infinite. Equivalently, the number of vectors MU to $\{\mathbb{I}, F_d\}$ is infinite.*

Since all cyclic translations of a biunimodular sequence x are orthogonal, one can construct a $d \times d$ circulant Hadamard matrix from x , defined by the matrix elements $H_{jk} = x_{j-k}$ [61].

Theorem 6.4. *A Hadamard matrix H of order d is circulant if and only if $H_{jk} = x_{j-k}$ for a biunimodular sequence $x = (x_0, x_1, \dots, x_{d-1})$.*

This result imposes an interesting restriction on the type of basis mutually unbiased to the Fourier matrix [61].

Corollary 6.2. *Any Hadamard matrix whose columns are mutually unbiased to the pair $\{\mathbb{I}, F_d\}$ is equivalent to a circulant Hadamard matrix.*

Here, equivalence is understood up to diagonal phase matrices and permutations of rows and columns, as defined in Appendix B. Combining Thms. 6.3 and 6.4 with Cor. 6.2 implies that the space $\mathbb{C}^d$ supports infinitely many triples of MU bases containing both the Fourier matrix and a circulant Hadamard matrix if the dimension d is divisible by a square.

A more general type of biunimodular sequence x can be considered by requiring both x and Ax to be unimodular, with the freedom to choose A from the set of unitary matrices rather than the Fourier matrix [151]. The existence of these sequences, for an arbitrary unitary A , is known indirectly from other results, e.g. [59, 114, 199].

Theorem 6.5. *For any unitary matrix A of order d , there exists a sequence $x = (x_0, x_1, \dots, x_{d-1})$ such that both x and Ax are unimodular.*

If A is a Hadamard matrix, a biunimodular sequence corresponds to a vector which is mutually unbiased to both the standard basis and A . Therefore, we have the following observation [13, 199, 236, 259].

Corollary 6.3. *There exists at least one vector mutually unbiased to any pair of MU bases in $\mathbb{C}^d$.*

6.5 Nice error bases

A set of μ MU bases in the space $\mathbb{C}^d$ is equivalent to partitioning a subset of a unitary operator basis into μ commuting classes, as was described in Sec. 5.4. Here we will require, in addition, that the elements of the unitary operator basis generate a certain group, resulting in a *nice error basis* [73]. Under this assumption there is a limit on the number of MU bases we can construct from any partitioning of the basis [21].

Definition 6.1. Let $\mathcal{G}$ be a group of order d^2 with identity element e , and let $\mathcal{N} = \{U_g : g \in \mathcal{G}\} \subset \mathbb{C}^{d \times d}$ be a set of unitary matrices which are traceless (except for the identity), i.e. $\text{Tr}[U_g] = 0$ for all $g \in \mathcal{G} \setminus \{e\}$. The set $\mathcal{N}$ is a *nice error basis* if its elements satisfy $U_g U_h = \omega(g, h) U_{gh}$ for all $g, h \in \mathcal{G}$, where $\omega(g, h) \in \mathbb{C}$ has modulus one.

In other words, the unitaries must form a faithful projective (or ray) representation of the group $\mathcal{G}$. As a simple example, consider $d = p^n \in \mathbb{PP}$ and take the index group as $\mathcal{G} = \mathbb{Z}_p^n \times \mathbb{Z}_p^n$ where $\mathbb{Z}_p = \{0, \dots, p-1\}$ such that $(k, \ell) = (k_1, \dots, k_n, \ell_1, \dots, \ell_n) \in \mathbb{Z}_p^n \times \mathbb{Z}_p^n$. A nice error basis $\mathcal{N}$ can be constructed from the Heisenberg-Weyl operators X and Z , defined in Eq. (A.7), by taking

$$\mathcal{N} = \{U(k, \ell) \mid (k, \ell) \in \mathbb{Z}_d^n \times \mathbb{Z}_d^n\}, \quad (6.4)$$

with

$$U(k, \ell) := X^{k_1} Z^{\ell_1} \otimes \dots \otimes X^{k_n} Z^{\ell_n}. \quad (6.5)$$

Definition 6.2. The MU bases associated with partitioning a subset of a nice error basis into maximally commuting operator classes (via Equivalence 5.4) are called *nice* MU bases.

Aschbacher *et al.* [21] showed that there is a limit on the number of nice MU bases one can construct from partitioning the nice error basis into maximally commuting classes.

Theorem 6.6. For dimension $d = p_1^{n_1} \dots p_r^{n_r} \notin \mathbb{PP}$, where $p_i \in \mathbb{P}$ and $n_i \in \mathbb{N}$, no more than $\min_i (p_i^{n_i} + 1)$ nice MU bases exist.

The proof establishes a connection between the index group $\mathcal{G}$ of a nice error basis $\mathcal{N}$ and Abelian subgroups of $\mathcal{G}$ constructed from the commuting classes of $\mathcal{N}$. Then, the known upper bound on

the number of trivially intersecting Abelian subgroups of $\mathcal{G}$ provides the bound in Thm. 6.6.

It is easy to see that the bound is tight for arbitrary d . For $d = p^n \in \mathbb{PP}$, the nice error basis of Eqs. (6.4) and (6.5) can be partitioned into $(d+1)$ maximally commuting classes, leading to a complete set of $(d+1)$ nice MU bases. An obvious consequence of Thm. 6.6 for dimension six is the following.

Corollary 6.4. In dimension six, no more than three nice MU bases exist.

This does not rule out the existence of additional bases which are mutually unbiased to a set of three nice MU bases, although a different construction would be required.

However, as shown by Nieter *et al.* [300], a sufficiently large set of nice MU bases extends to a complete set in exactly one way. This observation, based on a connection between MU bases and combinatorial designs called k -nets, leads to Thm. 6.13 (Sec. 6.10) which shows that some sets of nice MU bases do not extend (by *any* methods) to a complete set.

6.6 Monomial bases

It was pointed out in Ref. [157] that every known complete set of MU bases is *monomial* in the following sense.

Definition 6.3. A set of MU bases is monomial if the unitary operator basis from which it is constructed contains only monomial matrices, i.e. matrices that have only one non-zero element in each row and column.

Furthermore, every known complete set of MU bases can be obtained by partitioning a nice error basis into commuting classes. For $d = p^n \in \mathbb{PP}$, every nice error basis that partitions into maximally commuting classes is equivalent to the monomial basis defined in Eqs. (6.4) and (6.5) [21, 73]. Thus, complete sets of nice MU bases are always monomial. In general, however, MU bases need not be “nice” and monomial simultaneously. For example, the “incomplete” sets of MU bases constructed in square dimensions from Latin squares (Thm. 6.11, Sec. 6.9) are monomial but cannot be obtained by partitioning a nice error basis.

Given that all known complete sets of MU bases are monomial, the following theorem

provides quite a severe restriction on our ability to find complete sets in dimension six.

Theorem 6.7. *In dimension six, no more than three monomial MU bases exist.*

This result, shown in [73], is a consequence of the equivalence of MU bases in $\mathbb{C}^d$ and orthogonal decompositions of $sl_d(\mathbb{C})$, described in Sec. 5.5. It follows directly from a result proved in [238] which shows that no more than three monomial and pairwise orthogonal Cartan subalgebras of $sl_6(\mathbb{C})$ exist. It remains unknown whether complete sets of monomial MU bases exist only in prime-power dimensions [73].

6.7 MU product bases

As discussed in Sec. 6.2, product bases provide a simple yet effective means to construct MU bases in composite dimensions $d \notin \mathbb{PP}$. It is natural, therefore, to ask whether an exhaustive classification of MU product bases is possible, or whether a tight upper bound on their number can be found. In dimension six both questions have been answered positively (Sec. 7.4). For arbitrary multipartite systems, tight upper bounds are also known, but a classification of MU product bases has been obtained only in specific cases.

An orthonormal basis $\mathcal{B}$ of the space $\mathbb{C}^d$ with dimension $d = d_1 d_2 \cdots d_n$ is a product basis if each basis vector takes the form $|v^1, \dots, v^n\rangle \equiv |v^1\rangle \otimes |v^2\rangle \otimes \dots \otimes |v^n\rangle \in \mathbb{C}^d$, with states $|v^r\rangle \in \mathbb{C}^{d_r}$, $r = 1, \dots, n$. The following result places an upper bound on the maximum number of MU product bases in arbitrary composite dimensions.

Theorem 6.8. *If $d = d_1 d_2 \cdots d_n \notin \mathbb{PP}$ then there exist at most $(d_m + 1)$ MU product bases in $\mathbb{C}^d$, where d_m is the dimension of the subsystem with the least number of MU bases.*

The proof for $d_1 = 2, 3$ was given in Ref. [282], and the general case was solved in [96] using Thm. 6.10. We note that the bound is tight by applying the construction from Thm. 6.1. For dimensions $d = d_1 d_2 \cdots d_n$, with $d_1 = 2$ or $d_1 = 3$, a classification of maximal sets of MU product bases is also possible. For example, when $d = 2^n$ and $d = 3^n$, there exists a unique triple and a unique quadruple of MU product bases, respectively, up to equivalence [282]. Furthermore, a vector which is mutually unbiased to a set of $(d_1 + 1)$ MU product

bases must have a particular entanglement structure.

Lemma 6.1. *Let $d = d_1 \cdots d_n$ with $d_r = p_r^{k_r}$, $p_r \in \mathbb{P}$ and $k_r \in \mathbb{N}$, $r = 1 \dots n$, such that $d_1 \leq \dots \leq d_n$. A vector, mutually unbiased to a set of $(d_1 + 1)$ MU product bases (where the product bases of $\mathbb{C}^d$ contain at least one orthogonal set of d_1 vectors in the subsystem $\mathbb{C}^{d_1}$), is maximally entangled across $\mathbb{C}^{d_1} \otimes \mathbb{C}^{d_2 \cdots d_n}$.*

For dimensions $d = 2d_2$ and $d = 3d_2$, where d_2 is prime and $d_2 \geq d_1$, Lemma 6.1 implies that any vector mutually unbiased to a set of $(d_1 + 1)$ MU product bases in $\mathbb{C}^d$ is maximally entangled. For the special case $d = d_1 \cdots d_n = p^n$, with $d_r = p$ and $r = 1 \dots n$, it follows that any vector MU to a set of $(p + 1)$ MU product bases (where the product bases of $\mathbb{C}^d$ contain at least one orthogonal set of d_r vectors in each subsystem $\mathbb{C}^{d_r}$), is maximally entangled across *all* bipartitions $\mathbb{C}^p \otimes \mathbb{C}^{p^{n-1}}$.

The inconvenient requirement in Lemma 6.1—namely that the product bases of $\mathbb{C}^d$ contain at least one orthogonal set of d_1 vectors in the subsystem $\mathbb{C}^{d_1}$ —is an unfortunate consequence of our inability to fully characterise the structure of product bases. It also limits our ability to classify smaller sets of MU product bases (except when $d = 6$). The characterisation of product bases in terms of their orthogonality relations is particularly difficult and remains an open problem, although it is expected that the following simple structure holds.

Conjecture 6.1. *If $\mathcal{B} = \{|v^1, v^2\rangle\}_{v=0}^{d-1}$ is an orthonormal product basis of the space $\mathbb{C}^d$, with $d = d_1 d_2$, then the d vectors $\{|v^1\rangle \in \mathbb{C}^{d_1}\}_{v=0}^{d-1}$ and the d vectors $\{|v^2\rangle \in \mathbb{C}^{d_2}\}_{v=0}^{d-1}$ can be grouped into d_2 orthonormal bases $\mathcal{B}_j^{(d_1)}$, $j = 1 \dots d_2$, and d_1 orthonormal bases $\mathcal{B}_k^{(d_2)}$, $k = 1 \dots d_1$, respectively.*

A similar problem was considered for n -qubit orthogonal product bases, with their construction reducing to a purely combinatorial problem [109]. For the 4-qubit case, 33 multiparameter families were found such that any orthogonal product basis of four qubits is equivalent (under local unitaries and qubit permutations) to a basis in at least one of these families.

We note that MU product bases play a useful role in constructing a special class of *isol-*

ated Hadamard matrices (see Appendix B), as described in [284].

6.8 Entanglement in MU bases

One way to learn more about the properties of MU bases in composite dimensions $d \notin \mathbb{P}$ is to treat the Hilbert space $\mathbb{C}^d$ as a tensor product of its factors, e.g. $\mathbb{C}^d \cong \mathbb{C}^{d_1} \otimes \mathbb{C}^{d_2}$ in a bipartite system of dimension $d = d_1 d_2$. As seen in Thm. 6.1, the product structure provides a convenient way to construct MU bases in composite dimensions. This approach opens up the possibility of investigating quantum correlations in MU bases, leading to novel insights on their entanglement structure. For example, it has been noticed that a complete set of MU bases in dimension $d = p^n \times p^n$, $p \in \mathbb{P}$ and $n \in \mathbb{N}$, can be expressed in terms of product states and maximally entangled states of the space $\mathbb{C}^{p^n} \otimes \mathbb{C}^{p^n}$ [171].

Another observation concerns bipartite quantum systems of dimension $d = d_1 d_2$, with $d_1 \leq d_2$: a complete set of MU bases necessarily has a fixed average entanglement (equivalently, a fixed average purity of the reduced states) [397].

Theorem 6.9. *Suppose $\{|\psi_i\rangle\}_{i=1}^{d(d+1)}$ is a complete set of $(d+1)$ MU bases in dimension $d = d_1 d_2$ and let $\mathcal{P}(\rho_i) \equiv \text{Tr}[\rho_{1|i}^2]$ denote the purity of the reduced density operator of the state $\rho_i = |\psi_i\rangle\langle\psi_i|$, given by $\rho_{1|i} = \text{Tr}_2[|\psi_i\rangle\langle\psi_i|]$. Then a complete set of $(d+1)$ MU bases contains a fixed total purity (entanglement) content of*

$$\sum_{i=1}^{d(d+1)} \mathcal{P}(\rho_i) = d_1 d_2 (d_1 + d_2). \quad (6.6)$$

The proof follows by first observing that the average purity of a bipartite state is $(d_1 + d_2)/(d+1)$ [261]. Since the purity $\mathcal{P}(\rho_i)$ is a polynomial of degree two, we can use the 2-design property of MU bases (cf. Sec. 5.11) to show that the average purity over all pure states is equal to the average purity over the 2-design. This implies that the average purity of a state in the 2-design is $(d_1 + d_2)/(d+1)$ and, hence, summing over all $d(d+1)$ states gives Eq. (6.6).

The purity of a state achieves its minimum value of $1/d_1$ when the state is maximally entangled, and its maximum of unity when separable. Consequently, complete sets must include both entangled and product states (provided we

take the first basis as the canonical one). In other words, the fixed average entanglement makes it impossible for a complete set to contain only maximally entangled states or product states. Related entanglement constraints hold for multipartite tight informationally complete measurements, which include complete sets of MU bases as a special case [122]. Such measurements cannot consist entirely of separable states or entirely of maximally entangled states.

The distribution of entanglement within a complete set is arbitrary. For example, suppose that for a bipartite quantum system of dimension $d = d_1 d_2$ with $d_1 \leq d_2$, we have a set of $(d_1 + 1)$ MU product bases. Then the remaining bases of a (hypothetical) complete set of $(d+1)$ bases must contain only maximally entangled states.

For composite systems of two, three and four qubits, a detailed analysis of the entanglement structure of a complete set can be found in [321]. Two-qubit systems are special in the sense that there exists an *iso-entangled* complete set of five MU bases, i.e. all states come with exactly the same amount of entanglement [121]. As mentioned before, the standard construction of a complete set in the space $\mathbb{C}^{p^n} \otimes \mathbb{C}^{p^n}$ yields only product bases and maximally entangled bases [171].

In dimension six, where $d_1 = 2$ and $d_2 = 3$, the purity (or entanglement) content of any complete set equals 30. For example, a set of three MU product bases can be constructed from the tensor product of three MU bases of the space $\mathbb{C}^2$ with three MU bases of the space $\mathbb{C}^3$ (see Eq. (7.22)). However, due to the fixed average entanglement, the remaining four bases must contain entangled states only. In Sec. 7.4 we will discuss some stronger results relating to MU product bases in dimension six.

Thm. 6.9 can be adapted to sets of μ MU bases, for $\mu \leq d+1$, in bipartite system $d = d_1 d_2$, with $d_1 \leq d_2$ [96].

Theorem 6.10. *Suppose $\{|\psi_i\rangle\}_{i=1}^{d\mu}$ is the set of vectors in a collection of μ MU bases in dimension $d = d_1 d_2$ and let $\mathcal{P}(\rho_i) \equiv \text{Tr}[\rho_{1|i}^2]$ denote the purity of the reduced density operator of the state $\rho_i = |\psi_i\rangle\langle\psi_i|$, given by $\rho_{1|i} = \text{Tr}_2[|\psi_i\rangle\langle\psi_i|]$. The purity content of the set of μ MU bases satisfies*

$$\sum_{i=1}^{d\mu} \mathcal{P}(\rho_i) \leq (d_1^2 + \mu - 1)d_2. \quad (6.7)$$

The proof, in analogy with Thm. 6.9, relies on properties of 2-designs. By requiring that the vectors in a set of μ MU bases have Schmidt rank less than or equal to k , an immediate consequence of Thm. 6.10 is an upper limit on the number of MU bases.

Corollary 6.5. *Suppose there exists a set of μ MU bases in $\mathbb{C}^d$, with $d = d_1 d_2$, such that the Schmidt rank of each vector is at most k , and $k < d_1 \leq d_2$. Then*

$$\mu \leq k \left(\frac{d_1^2 - 1}{d_1 - k} \right). \quad (6.8)$$

Notice that when $k = 1$, the bases contain only separable states, and the bound implies at most $(d_1 + 1)$ MU product bases exist. Additional results on product bases can be found in Sec. 6.7. A bound similar to Eq. (6.8) also applies for MU bases in a real vector space (see Sec. 9.1).

Entangled bases with a fixed Schmidt rank are considered in [172]. In the next section we focus on bases with maximal Schmidt rank, i.e. maximally entangled bases.

6.9 Maximally entangled bases

As we have just seen, the simplest construction of MU bases in bipartite systems $d = d_1 d_2$ starts from $(d_1 + 1)$ MU bases in each subsystem $\mathbb{C}^{d_1}$ and $\mathbb{C}^{d_2}$ (provided they exist). Tensoring pairs of these bases (one from each subsystem) produces a set of $(d_1 + 1)$ MU product bases. Due to the fixed average entanglement condition (cf. Sec. 6.8), the remaining states in a hypothetical complete set of $(d + 1)$ MU bases must be maximally entangled, i.e. of the form $|\psi\rangle = \frac{1}{\sqrt{d}} \sum_{i=0}^{d-1} |i\rangle |i'\rangle$ for orthonormal bases $\{|i\rangle\}$ and $\{|i'\rangle\}$ of $\mathbb{C}^{d_1}$ and $\mathbb{C}^{d_2}$, respectively.

This motivates the study of maximally entangled bases and, in particular, to find bounds on the number of maximally entangled MU bases that exist. In this section we summarise several methods to construct MU bases consisting of maximally entangled states.

Mutually unbiased unitary bases—To simplify the problem we initially consider $d_1 = d_2$. In this case, there is a one-to-one correspondence between maximally entangled states in $\mathbb{C}^d \otimes \mathbb{C}^d$ and $d \times d$ unitary matrices. Furthermore, a unitary operator basis of $\mathbb{M}_d(\mathbb{C})$ —i.e. a set of d^2 unitary matrices U_i such that $\text{Tr}[U_i^\dagger U_j] = d\delta_{ij}$ (see

Sec. 5.4)—is equivalent to a maximally entangled basis. In particular, a basis of orthogonal unitary operators $\{U^{(i)}\}$, $i = 0, \dots, d^2 - 1$, corresponds to a set of orthogonal states

$$|U^{(i)}\rangle = \frac{1}{\sqrt{d}} \sum_{j,k=0}^{d-1} U_{jk}^{(i)} |j\rangle |k\rangle, \quad (6.9)$$

forming a maximally entangled basis, where $U_{jk}^{(i)}$ are the matrix elements of $U^{(i)}$. Consequently, finding maximally entangled bases is equivalent to constructing unitary operator bases, which is a well studied topic [233, 393].

Mutually unbiased unitary operator bases—defined by the condition that the Hilbert-Schmidt inner product between pairs of unitaries from different bases is constant—were first introduced by Scott [333] in relation to optimal quantum process tomography. Later, Shaari *et al.* [338] pointed out that these bases translate into mutually unbiased maximally entangled bases. In particular, any pair of *mutually unbiased* unitary operator bases of $\mathbb{M}_d(\mathbb{C})$ gives rise to a pair of maximally entangled MU bases in $\mathbb{C}^d \otimes \mathbb{C}^d$. For arbitrary d , the maximal number of pairwise MU unitary operator bases is $d^2 - 1$, although a construction which saturates this bound is known only for the primes $d = 2, 3, 5, 7$, and 11 [333]. Some lower bounds on the number of maximally entangled MU bases (and hence, lower bounds on the number of MU unitary operator bases) are presented at the end of this section.

Is a classification of unitary operator bases (and hence maximally entangled MU bases) possible? Unfortunately, this seems unlikely. For example, one of the simplest constructions, called the *shift and multiply* method, involves a Latin square (see Appendix A.5) and a family of Hadamard matrices. For example, as shown in [52, 388], by taking the Latin square

$$\begin{array}{ccc} 0 & 1 & 2 \\ 1 & 2 & 0 \\ 2 & 0 & 1 \end{array} \quad (6.10)$$

of order three, we can easily find three orthogonal entangled states in $\mathbb{C}^3 \otimes \mathbb{C}^3$,

$$|\psi_0\rangle = \frac{1}{\sqrt{3}}(|0\rangle|0\rangle + |1\rangle|1\rangle + |2\rangle|2\rangle), \quad (6.11)$$

$$|\psi_1\rangle = \frac{1}{\sqrt{3}}(|0\rangle|1\rangle + |1\rangle|2\rangle + |2\rangle|0\rangle), \quad (6.12)$$

$$|\psi_2\rangle = \frac{1}{\sqrt{3}}(|0\rangle|2\rangle + |1\rangle|0\rangle + |2\rangle|1\rangle). \quad (6.13)$$

Now choosing a Hadamard matrix H with matrix elements H_{ij} , each of the states $|\psi_k\rangle$ can be mapped into three additional orthogonal states. The first state $|\psi_0\rangle$, for example, becomes

$$|\psi_{0j}\rangle = \frac{1}{\sqrt{3}}(H_{j0}|0\rangle|0\rangle + H_{j1}|1\rangle|1\rangle + H_{j2}|2\rangle|2\rangle), \quad (6.14)$$

$j = 0, 1, 2$. This leads to a maximally entangled basis of states $\{|\psi_{ij}\rangle\}$ for $i, j = 0, 1, 2$, from a Latin square and Hadamard matrix. More generally in $\mathbb{C}^d \otimes \mathbb{C}^d$, a maximally entangled basis of this form has basis elements

$$|\psi_{ij}\rangle = \frac{1}{\sqrt{d}} \sum_{k=0}^{d-1} H_{jk}|k\rangle|L_{ik}\rangle, \quad (6.15)$$

for $i, j = 0, \dots, d-1$, where H_{jk} are the elements of a $d \times d$ Hadamard matrix and L_{ik} is the (i, k) -th component of a Latin square L of order d . Note that the corresponding unitary operator basis of the shift and multiply method is always a monomial basis (see Sec. 6.6).

Even the classification of unitary operator bases from this simple construction—dependent on a Latin square and a Hadamard matrix—becomes unfeasible as the dimension increases. Equivalence classes of Hadamard matrices have been described in Appendix B (see Definition B.1), and we refer the reader to [147] for more details on equivalences between Latin squares. In dimensions $d \leq 5$, the situation is just about manageable since all Hadamard matrices and Latin squares are known [147, 174]. For example, in dimension $d = 5$ there is only one Hadamard matrix up to equivalence, and two Latin squares exist. For $d = 6$, although the number of inequivalent Latin squares is 22, there are infinitely many Hadamard matrices, and their classification remains an open problem. In higher dimensions the number of Latin squares starts to increase significantly, and it becomes ever harder to list Hadamard matrices.

While there are several known constructions of unitary operator bases (e.g. nice error bases [233], see Sec. 6.5), two approaches yield maximally entangled MU bases in composite dimensions other than prime-powers. These are based on Latin and quantum Latin squares, as summarised below.

Latin squares—One construction of maximally entangled MU bases, which provides a simple and effective way to build MU bases in square dimensions, is based on Latin squares [400]. In particular, a pair of maximally entangled bases is constructed from two Latin squares L and L' of order d and a single $d \times d$ Hadamard matrix H . A first set of d vectors stemming from the Latin square L is defined as

$$|\psi_{0j}\rangle = \frac{1}{\sqrt{d}} \sum_{i,k=0}^{d-1} E_{ik}^L(j)|i\rangle|k\rangle, \quad (6.16)$$

$k = 0, \dots, d-1$, where $E_{ik}^L(j) = 1$ if $L_{ik} = j$ and zero otherwise, and L_{ik} the (i, k) -th entry of L [388, 400]. Next, each of these vectors is mapped to d vectors by means of the Hadamard matrix H , using the method from Eq. (6.14), which, taken together, form orthonormal bases $\{|\psi_{ij}\rangle\}$, $i, j = 0, \dots, d-1$. Repeating this construction with a second Latin square L' , orthogonal to L , the resulting bases are mutually unbiased [400].

Theorem 6.11. *Given a set of μ mutually orthogonal Latin squares of order d , there exists a set of $(\mu + 2)$ MU bases in $\mathbb{C}^d \otimes \mathbb{C}^d$.*

The additional two MU bases follow from extending the set of orthogonal Latin squares to an *augmented* set (see Appendix A.5).

Rather surprisingly, this approach leads—in specific dimensions—to *more* MU bases than the standard method based on product bases. The smallest known dimension with an increased number of MU bases in $\mathbb{C}^d$ is $d = 26^2$. The known number of MO Latin squares in this case is four, leading to *six* MU bases rather than the *five* MU bases established in Thm. 6.1 in Sec. 6.2, which arise from the factor of four in the prime decomposition of $d = 2^2 \times 13^2$. Although this method offers some hope that larger sets of MU bases exist, it yields at most $(d+1)$ MU bases in the space $\mathbb{C}^d \otimes \mathbb{C}^d$ since at most $(d-1)$ MO Latin squares of order d exist. While the maximum number of MO Latin squares exist when d is a prime or a prime-power, in most dimensions—except in special cases—the number is unknown. More details

on MO Latin squares and their role in constructing complete sets of MU bases are described in Appendix A.5.

Quantum Latin squares—The shift and multiply approach for constructing unitary operator bases has been generalised to a *quantum shift and multiply* method using *quantum* Latin squares. A quantum Latin square is a $d \times d$ array of elements in the space $\mathbb{C}^d$ such that every row and column is an orthonormal basis [291]. Suppose Q is a quantum Latin square of order d and H_j labels a $d \times d$ Hadamard matrix, then

$$|\psi_{ij}\rangle = \frac{1}{\sqrt{d}} \sum_{k=0}^{d-1} |k\rangle |Q_{kj}\rangle \langle k|H_j|i\rangle, \quad (6.17)$$

for $i, j = 0, \dots, d-1$, forms a set of d^2 orthogonal maximally entangled states. Here, $|Q_{kj}\rangle$ is the vector from the (k, j) -th components of Q . Although the quantum shift and multiply method reproduces all unitary operator bases from the non-quantum version, it also yields unitary operator bases which are not monomial [291].

A generalisation of the construction of MU bases from Latin squares to quantum Latin squares follows rather straightforwardly after defining orthogonality. A pair of quantum Latin squares Q and Q' are weakly orthogonal if, for all vector entries $|Q_{ij}\rangle$ and $|Q'_{ij}\rangle$, there exists a fixed $t \in \{0, \dots, d-1\}$ such that

$$\sum_{k=0}^{d-1} |k\rangle \langle Q_{ki}|Q'_{kj}\rangle = |t\rangle, \quad (6.18)$$

for all $i, j = 0, \dots, d-1$. A set of maximally entangled MU bases is then constructed from a set of weakly orthogonal quantum Latin squares [292].

Theorem 6.12. *Let Q and Q' be a pair of weakly orthogonal quantum Latin squares of order d , and let H_i and H'_i denote Hadamard matrices of order d . Then the pair of maximally entangled bases from Eq. (6.17) using $\{Q, H_i\}$ and $\{Q', H'_i\}$ are mutually unbiased.*

When the quantum Latin squares reduce to Latin squares, this result reproduces the set of $(\mu + 2)$ MU bases of Thm. 6.11. In general, very little is known about weakly orthogonal quantum Latin squares, as well as their potential for constructing larger sets of MU bases.

Other related results—Ad hoc construction methods of maximally entangled bases in the space $\mathbb{C}^d \otimes \mathbb{C}^{d'}$, and their relation to MU bases, can be found in [112, 260, 263, 363, 406, 410], some of which are reviewed in Ref. [340]. For instance, in the space $\mathbb{C}^d \otimes \mathbb{C}^{kd}$, the set of kd^2 states

$$|\phi_{n,m}^j(U)\rangle = \frac{1}{\sqrt{d}} \sum_{\ell=0}^{d-1} \omega^{n\ell} |\ell \oplus m\rangle \otimes U|\ell + dj\rangle \quad (6.19)$$

with $m, n = 0, 1, \dots, d-1$, and $j = 0, 1, \dots, k-1$, forms a maximally entangled basis for any unitary U , and can be used to construct sets of five and three maximally entangled MU bases in $\mathbb{C}^2 \otimes \mathbb{C}^4$ and $\mathbb{C}^2 \otimes \mathbb{C}^6$, respectively [363]. Here $\ell \oplus m = (\ell + m) \bmod d$ is addition modulo d , and $\omega = e^{2\pi i/d}$.

A pair of maximally entangled MU bases in the space $\mathbb{C}^2 \otimes \mathbb{C}^3$ is presented in [340]. This generates—by a recursive construction—pairs of maximally entangled MU bases in $\mathbb{C}^d \otimes \mathbb{C}^{d'}$, for infinitely many d and d' , provided d is not a divisor of d' .

A summary of *lower bounds* on the number $N(d, d')$ of maximally entangled MU in a bipartite setting with Hilbert space $\mathbb{C}^d \otimes \mathbb{C}^{d'}$ is presented in [340]. For example, if $d = p_1^{n_1} \dots p_r^{n_r}$ is even, the bases of Eq. (6.19) provide a lower bound $N(d, d) \geq \min_i (p_i^{n_i} - 1)$ [260]. For odd $d = p_1^{n_1} \dots p_r^{n_r}$, this bound increases to $N(d, d) \geq \min_i 2(p_i^{n_i} - 1)$ [112] while for $d = p^n$ with any prime number p , one finds $N(d, d) \geq 2(d - 1)$ [406]. Also, when $d = p^n$, the canonical construction of a complete set of $(d^2 + 1)$ MU bases in $\mathbb{C}^d \otimes \mathbb{C}^d$ yields $(d^2 - d)$ maximally entangled bases and $(d + 1)$ product bases, hence $N(d, d) \geq d^2 - d$ [171].

A more exotic basis, namely an *unextendible maximally entangled* (UME) basis has been introduced in [76]. This is an orthogonal basis of $\mathbb{C}^d \otimes \mathbb{C}^{d'}$ which contains $n < dd'$ maximally entangled states $|\psi_i\rangle \in \mathbb{C}^d \otimes \mathbb{C}^{d'}$ such that no additional maximally entangled vector $|\psi\rangle$ satisfies $\langle \psi_i | \psi \rangle = 0$. For a two-qubit system, these bases do not exist. Constructions are known, however, for $\mathbb{C}^d \otimes \mathbb{C}^d$ when $d = 3, 4$ [76], and in $\mathbb{C}^d \otimes \mathbb{C}^{d'}$, for $\frac{d'}{2} < d < d'$, containing d^2 maximally entangled states [105]. For example, in $\mathbb{C}^2 \otimes \mathbb{C}^3$ there exist two UME bases which are mutually unbiased. Similar examples of mutually unbiased UME bases have been found in

[294, 301, 346, 417]. Furthermore, by taking a single UME basis and a maximally entangled basis, other pairs of MU bases can be constructed [416].

Finally, Shi *et al.* [340] presented a construction of MU bases with fixed Schmidt rank, and derived upper bounds on the maximal number of these bases, complementing the upper bound (6.8) in Cor. 6.5.

6.10 Unextendible sets of MU bases

Given the difficulty to construct complete sets of MU bases in spaces of composite dimension, it is instructive to investigate the possibility to extend particular sets of MU bases by individual vectors or bases. We have already discussed several positive results, including the observation in Sec. 6.4 that a vector mutually unbiased to a given pair of MU bases always exists.

It is also interesting to ponder whether *any* pair of MU bases extends to a *triple*. The answer is negative: while every MU pair extends to a triple in dimensions $d \leq 5$, the specific pair $\{\mathbb{I}, S_6\}$ in dimension $d = 6$ violates this property [79] (cf. Sec. 7.6). In fact, numerical searches suggest that most pairs do not extend to a triple for $d = 6$ (see Sec. 8.1). On the other hand, no unextendible pair is known for larger d [165].

More generally, a set of μ MU bases is called *extendible* if it can be enlarged by adding at least one further MU basis, and *unextendible* otherwise. To distinguish between different types of unextendibility we will use the following terminology.

Definition 6.4. A set of μ MU bases in $\mathbb{C}^d$ is *strongly unextendible* if there exists no additional vector unbiased to any of the μ bases. A set of μ MU bases in $\mathbb{C}^d$, constructed by partitioning a unitary operator basis $\mathcal{C}$ (see Sec. 5.4) into μ commuting classes, is *weakly unextendible* if none of the remaining elements of $\mathcal{C}$ form an additional commuting class containing d elements.

We have already discussed (indirectly) weakly unextendible MU bases in the form of nice MU bases when $d \notin \mathbb{PP}$ (see Thm. 6.6 of Sec. 6.5). For prime and prime-power dimensions, several constructions of weakly and strongly unextendible MU bases are known. For example, the Heisenberg-Weyl group, which forms a nice error basis (cf. Sec. 6.5), is partitioned by Mandayam

et al. [270] (and later by Garcia and López [153]) into unextendible maximally commuting classes (i.e., classes for which no other commuting class can be constructed from the remaining group elements), resulting in sets of weakly unextendible MU bases for n -qubit systems, with $n = 2, 3, 4, 5$.

More generally, for an even number of $n = 2m$ qubits, Grassl [167] shows there exists a weakly unextendible set of $(2^m + 1)$ MU bases. This observation is based on a connection between weakly unextendible MU bases and maximal symplectic partial spreads [371]. Other examples of maximal symplectic partial spreads, and therefore weakly unextendible MU bases, for various even and odd prime-power dimensions are listed in [167, 215]. Thas [371] uses symplectic partial spreads to find sets of weakly unextendible MU bases for all dimensions $d = p^2$, with $p \in \mathbb{P}$.

Nietert *et al.* [300] have shown that Thas' set of weakly unextendible MU bases [371] cannot be enlarged to a complete set of $(d + 1)$ MU bases. This follows from a connection between MU bases and combinatorial designs called k -nets [300] (cf. Sec. 6.5):

Theorem 6.13. *A weakly unextendible set of at least $(d + 1 - \sqrt{d})$ nice MU bases in $\mathbb{C}^d$ cannot be enlarged to $(d + 1)$ MU bases.*

A construction of $(p^2 - p + 2)$ strongly unextendible MU bases for $d = p^2$ and $p \equiv 3 \pmod{4}$, based on complementary decompositions and MASAs (Sec. 5.6), is found by Szántó [358]; the special Galois MU bases in dimensions $d = p^2$, with $p = 2, 3, 5, 7, 11$, also form a set of $(d - 1)$ strongly unextendible bases [358]. A recent construction in [207] finds smaller sets of only $(2^{2n-1} + 1)$ strongly unextendible MU bases for $d = 2^{2n}$ and $n \geq 1$.

What is the minimum number of MU bases in an unextendible set? Table 1 provides a summary up to dimension 16 [165]. While minimal sets are known for $d = 2, \dots, 6$ (although for dimensions $d = 3, 5$ these are actually complete sets), the upper bound is equal to three for $d = 7, \dots, 16$. As already mentioned, the smallest set of unextendible MU bases for $d = 6$ has cardinality two, however, no *strongly* unextendible pair exists.

Corollary 6.6. *In finite dimensions $d \geq 2$, no pair of strongly unextendible MU bases exists.*

This is a direct consequence of Cor. 6.3 in Sec. 6.4: any pair of orthonormal bases has at least one additional vector unbiased to both.

In the infinite-dimensional Hilbert space $L^2(\mathbb{T}_1)$ associated with the continuous variables (see Sec. 9.13) of a particle moving on a one-dimensional torus $\mathbb{T}_1$, however, a pair of *strongly* unextendible MU bases is known: not even a single quantum state exists which is MU to both the continuous position and the discrete momentum basis.

dimension	$\aleph(d)$
2	3
3	4
4	3
5	6
6	3
7 to 16	≤ 3
∞	2

Table 1: The cardinality $\aleph(d)$ of the smallest set of unextendible MU bases for $d = 2, \dots, 16$, and $d = \infty$. The minimal sets for $d = 3$ and $d = 5$ form complete sets of MU bases. For $d = 6$ the pair $\{\mathbb{I}, S_6\}$ is unextendible, and for dimensions $7 \leq d \leq 16$ the minimal set contains at most three bases. For $d = \infty$, see Sec. 9.13.

For non-prime-power dimensions $d = p_1^{n_1} p_2^{n_2} \dots p_r^{n_r}$, one can construct $\mu = \min_i (p_i + 1)$ weakly unextendible MU bases from the eigenbases of the Heisenberg-Weyl operators $Z, X, XZ, XZ^2, \dots, XZ^{\mu-2}$ [21, 165]. For even dimensions $d = 10, 12, 14$, the eigenbases of X, Z and XZ are strongly unextendible [165]. For $d = 9, 15$, the eigenbases of Z, X, XZ , and XZ^2 lead to four unextendible MU bases, although smaller unextendible sets of cardinality three have also been found. It is expected that similar results holds for other composite dimensions, leading to a conjectured systematic behaviour.

Conjecture 6.2. *For all composite dimensions $d = p_1^{n_1} \dots p_r^{n_r}$, and $\mu = 1 + \min_i p_i$, the eigenbases of the Heisenberg-Weyl operators $Z, X, XZ, XZ^2, \dots, XZ^{\mu-2}$ form a set of μ unextendible MU bases.*

Secs. 7.3–7.6 describe additional results on sets of unextendible MU bases valid for dimension $d = 6$.

6.11 Positive definite functions

We now summarise an approach in which certain positive definite functions provide upper bounds on the maximum cardinality of a set of MU bases [235, 276]. The method applies a generalised version of Delsarte’s linear programming bound in the non-commutative setting [125, 422]. Suppose that G is a compact group with multiplication as the group operation. Let $A = A^{-1} \subset G$ be a symmetric subset, called the “forbidden” set, containing the identity element $e \in A$. The aim is to determine the maximum cardinality of a set $B = \{b_1, \dots, b_k\} \subset G$ such that $b_i^{-1} b_j \in A^c$ for all $i \neq j$, i.e. all pairwise differences avoid the forbidden set A . Here, $A^c = G \setminus A$ denotes the complement of A . Bounding the cardinality of B involves finding a positive definite function on G satisfying certain conditions.

Definition 6.5. For a compact group G , a continuous function $h : G \rightarrow \mathbb{C}$ is positive definite if for all $t \geq 1$, $g_1, \dots, g_t \in G$ and $c_1, \dots, c_t \in \mathbb{C}$, then

$$\sum_{i,j=1}^t h(g_i^{-1} g_j) c_i^* c_j \geq 0. \quad (6.20)$$

The following result specifies a class of positive definite functions relevant for bounding the cardinality of B [235].

Theorem 6.14. *Let G be a compact group and $A = A^{-1} \subset G$ a symmetric subset with identity $e \in A$. Suppose there exists a positive definite function $h : G \rightarrow \mathbb{R}$ such that $h(x) \leq 0$ for all $x \in A^c$ and $\int h d\nu > 0$, where ν is the normalised Haar measure. For any $B = \{b_1, \dots, b_k\} \subset G$ such that $b_i^{-1} b_j \in A^c$ for all $i \neq j$, the cardinality of B is bounded by $|B| \leq h(e) / \int h d\nu$.*

Matolcsi [276] first made the connection to MU bases in the commutative setting by taking $G = \mathbb{T}^d$, where $\mathbb{T}$ is the complex unit circle (see Sec. 6.12). Later, once the extension of Delsarte’s bound to non-commutative groups was established, Kolountzakis *et al.* [235] formalised a simpler relation by taking $G = U(d)$ as the group of unitaries, and $A^c = H(d)$ as the set of complex Hadamard matrices. Since the maximum number of MU bases in $\mathbb{C}^d$ is equivalent to the maximum cardinality of $B = \{U_1, \dots, U_k\} \subset G$, where the differences $U_i^{-1} U_j$ are elements of $H(d)$ (cf. Sec. 5.2), Thm. 6.14 leads to the following result.

Corollary 6.7. *Let $G = U(d)$ and $A^c = H(d)$, and let $h : G \rightarrow \mathbb{R}$ be any positive definite function satisfying the conditions of Thm 6.15. The maximum number μ of MU bases in $\mathbb{C}^d$ satisfies $\mu \leq h(e) / \int h d\nu$.*

Consider, for example, the polynomial

$$h_0(U) = -1 + \sum_{i,j=1}^d |U_{ij}|^4, \quad (6.21)$$

where $U = (U_{i,j})_{i,j=1}^d \in U(d)$, which is positive definite on $U(d)$ and takes the value zero whenever $U \in H(d)$. Since $h_0(e) = d - 1$ and $\int h_0 d\nu = (d - 1)/(d + 1)$, Cor. 6.7 yields the well known upper bound $\mu \leq d + 1$.

The ultimate aim is to construct a positive definite function for a non-prime-power d to show $\mu < d + 1$. While h_0 is one function that vanishes on the set of Hadamard matrices, other possible examples arise for $d = 6$ in the following way. Consider,

$$f_1(U) = \sum_{\sigma \in S_6} \sum_{j=1}^3 \prod_{i=1}^3 U_{\sigma(i),j} U_{\sigma(i+3),j}^*, \quad (6.22)$$

and $f_2(U) = f_1(U^*)$, with S_6 the permutation group of the set of 6 elements. Both functions are real-valued and expected to vanish for every $U \in H(d)$ (see Conjecture 6.4). Furthermore, the three functions $f(U) = (f_1(U) + f_2(U))^2$, $f(U) = f_1^2(U) + f_2^2(U)$ and $f(U) = f_1^2(U)f_2^2(U)$, satisfy $f(e) = 0$ and $\int_{U \in U(d)} f(U) d\nu > 0$. If one can show that for any $\epsilon > 0$, $h_1(U) = h_0(U) + \epsilon f(U)$ is positive definite, then the upper bound on the cardinality of B will fall below $(d + 1)$, i.e., $|B| \leq \frac{h_1(e)}{\int h_1 d\nu} < d + 1$.

A recent result suggests the method based on positive definite functions may not be a suitable strategy to tackle the existence problem. By considering positive definite polynomials in the entries of $U \in U(d)$ and their conjugates, with degree at most 6, Bandeira *et al.* [30] showed the following.

Theorem 6.15. *The method of positive definite polynomials of degree at most 6 cannot be used to show that fewer than seven MU bases exist in $\mathbb{C}^6$.*

The proof involves a convex duality argument with computer-aided symbolic calculations. The

techniques could also be applied for larger values of d and polynomials of degree q , but the calculations become computationally intractable beyond $d = q = 6$. Instead, the construction of a dual certificate is presented that, if verified, would prove the following claim for arbitrary system sizes [30].

Conjecture 6.3. *The method of positive definite functions cannot be used to show that fewer than $(d + 1)$ MU bases exist in $\mathbb{C}^d$, for all $d > 1$.*

6.12 Linear constraints

By considering the group $G = \mathbb{T}^d$, where $\mathbb{T}$ is the complex unit circle, Matolcsi's original application of positive definite functions in [276] applied a more restricted version of Theorem 6.14 to bound the cardinality of $B \subset G$, where the elements of B are no longer unitary matrices but the *columns* of mutually unbiased Hadamard matrices. In related work [272], Fourier analytic arguments were applied to reduce the MU conditions to linear constraints, leading to two important consequences. First, the constraints reveal several interesting structural features about sets of MU bases. Second, one can attempt to demonstrate that the constraints do not hold, providing a strategy to prove that complete sets do not exist in composite dimensions.

The dual group of $G = \mathbb{T}^d$ is given by $\hat{G} = \mathbb{Z}^d$, and the action of a character $\gamma = (n_1, n_2, \dots, n_d) \in \mathbb{Z}^d$ on an element $\mathbf{u} = (u_1, u_2, \dots, u_d) \in \mathbb{T}^d$ is $\gamma(\mathbf{u}) = \mathbf{u}^\gamma = u_1^{n_1} u_2^{n_2} \dots u_d^{n_d}$. For a set $S \subset G$ the Fourier transform is denoted by $\hat{S} = \sum_{\mathbf{s} \in S} \mathbf{s}^\gamma$. Thus, given a complete set of MU bases $\{\mathbb{I}, H_1, \dots, H_d\}$, where $H_j \subset G$ is represented as a d element set $\{\mathbf{c}_{j1}, \dots, \mathbf{c}_{jd}\}$ of its columns, the Fourier transform of H_j is

$$g_j(\gamma) \equiv \hat{H}_j(\gamma) = \sum_{k=1}^d \mathbf{c}_{jk}^\gamma, \quad (6.23)$$

for each $\gamma \in \mathbb{Z}^d$. Two functions, $E(\gamma)$ and $F(\gamma)$, that prove essential in this framework are defined as

$$E(\gamma) \equiv \sum_{j=1}^d E_j(\gamma), \quad (6.24)$$

where $E_j(\gamma) \equiv |g_j(\gamma)|^2$, and

$$F(\gamma) \equiv |f(\gamma)|^2, \quad (6.25)$$

with $f(\gamma) \equiv \sum_{j=1}^d g_j(\gamma)$ for each $\gamma \in \mathbb{Z}^d$. The orthogonality and unbiasedness relations can then be expressed as *linear* constraints on the functions E and F . In other words, the polynomial relations from the orthogonality and unbiasedness conditions are transformed into linear relations using Fourier transforms, and one should expect that these constraints are simpler to deal with.

Explicitly, the orthogonality conditions for each basis are

$$\sum_{r=1}^d E_j(\gamma + \pi_r) = d^2, \quad (6.26)$$

for each $\gamma \in \mathbb{Z}^d$, which imply

$$\sum_{r=1}^d E(\gamma + \pi_r) = d^3, \quad (6.27)$$

where $\pi_r = (0, \dots, 0, 1, 0, \dots, 0) \in \mathbb{Z}^d$ denotes the vector with its r -th coordinate equal to one. The constant overlap constraint simplifies to

$$dE(\gamma) + \sum_{r \neq t} F(\gamma + \pi_r - \pi_t) = d^4. \quad (6.28)$$

The functions exhibit additional trivial constraints such as $F(0) = d^4$ and $E(0) = d^3$, and satisfy inequalities

$$0 \leq F(\gamma) \leq d^4, \quad 0 \leq E(\gamma) \leq d^3, \quad (6.29)$$

and

$$F(\gamma) \leq dE(\gamma), \quad (6.30)$$

for each $\gamma \in \mathbb{Z}^d$.

For $d \leq 5$ the derivations of several known results on MU bases follow simply from the linear constraints of Eqs. (6.26–6.30). For example, Eqs. (6.26–6.30) imply that the matrix elements of all d Hadamard matrices in a complete set are d -th roots of unity; which in turn provides a simple means to classify complete sets in these dimensions.

When $d = 5$ the constraints imply that any Hadamard matrix of order five is equivalent to the Fourier matrix, which was first observed by Haagerup [174]. To prove this using the constraints above, the function $E_1(\gamma) = |\hat{H}_1(\gamma)|^2$, where H_1 is a Hadamard of order five, is treated as a *variable* for each $\gamma \in \mathbb{Z}^5$. The function $E_1(\gamma)$ satisfies Eq. (6.27), $E_1(0) = 25$ and $0 \leq E_1(\gamma) \leq 25$, for all $\gamma \in \mathbb{Z}^5$. By choosing $\sigma \in \mathbb{Z}^5$ as any permutation of $(5, -5, 0, 0, 0)$ one can show via a

linear programming code that $E_1(\sigma) = 25$. This condition implies that all elements of H_1 are fifth roots of unity, whence H_1 is the Fourier matrix.

In higher dimensions, if one can show that $F(\rho) = d^4$, where ρ is a permutation of $(d, -d, 0, \dots, 0)$, then the set of d Hadamard matrices contain only d -th roots of unity. Imposing this structure on a set of bases in $d = 6$ is incompatible with the existence of a complete set of MU bases (see Thm. 7.15 of Sec. 7.6), and would prove Zauner’s conjecture. Alas, the linear constraints of Eqs. (6.27)–(6.30) do not appear to imply $F(\rho) = d^4$, and hence the matrix entries cannot be restricted to roots of unity [272].

One of the main consequences of the above approach is a limitation on the number of real Hadamard matrices in a complete set [272].

Theorem 6.16. *Let $\{\mathbb{I}, H_1, \dots, H_d\}$ be a complete system of MU bases, in matrix form, and suppose that H_1 is a real Hadamard matrix. Then there is no further purely real column in any of the matrices $H_2, \dots, H_d$. In particular it is impossible to have two real Hadamard matrices in a complete set of MU bases.*

An additional consequence is that no complete set of MU bases in dimension six contains the pair $\{\mathbb{I}, F_6\}$, a result we will see in Sec. 7.3. The original proof uses a computer algebraic method, whereas the method here relies only on Fourier analytic arguments. Furthermore, a stronger result excluding the existence of a complete set containing the family of pairs $\{\mathbb{I}, F_6^{(2)}\}$, namely Thm. 7.7, can be proved using similar arguments if the following is true [272]:

Conjecture 6.4. *Let H be any complex Hadamard matrix of order 6, not equivalent to the isolated matrix S_6 and let σ be any permutation of the vector $(1, 1, 1, -1, -1, -1)$. Then the function $g_j(\sigma)$ defined in Eq. (6.23) cannot vanish everywhere.*

We note, however, that the conjecture is not necessary to prove Thm. 7.7. A computer search first confirmed this result [205], and later an analytic proof based on improvements to the Delstarte-type linear programming bound [274].

Some progress towards proving Conjecture 6.4 was achieved in [278], but only by restricting the class of matrices to the three-parameter Karlsson family $K_6^{(3)}$, described in Eq. (7.3). It has been

predicted that Conjecture 6.4, by offering an additional linear constraint on the function E , may be useful in a proof of the non-existence of a complete set in dimension six.

7 Rigorous results: Dimension six

With $d = 6$ being the smallest dimension where the existence problem manifests itself, quite a few studies have focussed on this specific case, in the hope of conclusive insights. First, we will summarise all known pairs and triples of MU bases for dimension six, as well as the properties of sets which contain the Fourier family of 6×6 Hadamard matrices. Then, we review a number of results that exploit the tensor product structure of dimension six. Finally, we describe non-existence results which show that certain pairs and triples do not extend to larger collections of MU bases. Numerical results will be summarised in the subsequent section.

7.1 Pairs of MU bases

In Sec. 6.1 some well-known examples of $d \times d$ complex Hadamard matrices were discussed. We now focus on *classifying* complex Hadamard matrices of order six since each such matrix guarantees the existence of a *pair* of MU bases in $\mathbb{C}^6$ when combined with the identity matrix. An early review was provided in Ref. [49], and an up-to-date summary can be found online [84].

We begin by summarising the currently known 6×6 complex Hadamard matrices in terms of a theorem.

Theorem 7.1. *All currently known 6×6 complex Hadamard matrices belong to one of the three classes: (i) an isolated matrix S_6 ; (ii) a three-parameter family $K_6^{(3)}$; and (iii) a four-parameter family $G_6^{(4)}$.*

Let us describe what is known about the classes of matrices listed in the theorem. To simplify notation, we will occasionally suppress the normalisation factor $1/\sqrt{d}$ in this subsection and the next one; in other words, the entries of the Hadamard matrices we consider may have modulus 1.

The isolated matrix S_6

A Hadamard matrix is *isolated* if it does not belong to any continuous family of Hadamard matrices. In particular, a Hadamard matrix with zero *defect* must be isolated (cf. Appendix B). The only known isolated matrix of order six can be traced back to a construction by Butson [90] in 1962 of order $2p$ matrices which contain only p -th roots of unity, when p is prime. For $p = 3$, the construction leads to a matrix consisting of third roots of unity only, namely

$$S_6 = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & \omega & \omega & \omega^2 & \omega^2 \\ 1 & \omega & 1 & \omega^2 & \omega^2 & \omega \\ 1 & \omega & \omega^2 & 1 & \omega & \omega^2 \\ 1 & \omega^2 & \omega^2 & \omega & 1 & \omega \\ 1 & \omega^2 & \omega & \omega^2 & \omega & 1 \end{pmatrix}, \quad (7.1)$$

where $\omega = e^{2\pi i/3}$. The matrix S_6 is also known as *Tao's matrix*, displayed explicitly for the first time in a paper from 2004 [362]. Other independent derivations of S_6 are based on symmetry conditions [273] and or use product bases [284] (see Sec. 7.4).

The three-parameter family $K_6^{(3)}$

The three-parameter family $K_6^{(3)}$ has been discovered by Karlsson in 2011 [220]. Before describing its construction, it is instructive to summarise the derivations of various one- and two-parameter families which are contained in the larger set $K_6^{(3)}$. In general, constructions have been quite haphazard, with individual examples found and later extended or connected to one- and two-parameter families.

The simplest examples of Hadamard matrices are affine families (see Appendix B). The only known affine families are the two-parameter Fourier family $F_6^{(2)}$ (and its transpose), and the one-parameter Diţă family $D_6^{(1)}$ [130]. The Diţă family provides a full characterisation of *regular* Hadamard matrices of order six [33]. The classification of all *self-adjoint complex* Hadamard matrices of order six yields a non-affine one-parameter family $B_6^{(1)}$ found in [43]. Another non-affine example, derived in [273], is the one-parameter family of symmetric matrices $M_6^{(1)}$. More general non-affine two-parameter families $X_6^{(2)}$ and $K_6^{(2)}$ were later discovered by Szöllősi

[356] and Karlsson [218], respectively, each containing previously discovered one-parameter families, with the inclusions $D_6^{(1)} \subset X_6^{(2)}, B_6^{(1)} \subset X_6^{(2)}$ and $D_6^{(1)} \subset K_6^{(2)}, M_6^{(1)} \subset K_6^{(2)}$.

The Karlsson family $K_6^{(3)}$, which encompasses *all* previously known one- and two-parameter families, was found by investigating matrices that are H_2 -reducible; a property demanding that all 2×2 blocks of a 6×6 matrix be complex Hadamard matrices themselves [219].

Theorem 7.2. *Every Hadamard matrix of order six is equivalent to a matrix where all or none of the nine (non-overlapping) 2×2 blocks are (proportional to) Hadamard matrices.*

It is simple to check the H_2 -reducibility property since a matrix of order six is H_2 -reducible if and only if its dephased form (cf. Appendix B) contains an element equal to (-1) .

To construct $K_6^{(3)}$, one starts with a general dephased block matrix of nine 2×2 submatrices. Requiring the matrix of order six to be H_2 -reducible and using the unitary and unimodularity constraints on its elements, a complete classification of all H_2 -reducible Hadamard matrices is given by the set

$$K_6^{(3)} \equiv K_6(\theta, \phi, \lambda) = \begin{pmatrix} F_2 & Z_1 & Z_2 \\ Z_3 & \frac{1}{2}Z_3AZ_1 & \frac{1}{2}Z_3BZ_2 \\ Z_4 & \frac{1}{2}Z_4BZ_1 & \frac{1}{2}Z_4AZ_2 \end{pmatrix} \quad (7.2)$$

as described in [220]. Three parameters enter this expression in the following way. The 2×2 matrix

$$A = \begin{pmatrix} A_{11} & A_{12} \\ A_{12} & -A_{11} \end{pmatrix} \quad (7.3)$$

has elements

$$A_{11} = \frac{1}{2} + i\frac{\sqrt{3}}{2}(\cos\theta + e^{-i\phi}\sin\theta), \quad (7.4)$$

$$A_{12} = -\frac{1}{2} + i\frac{\sqrt{3}}{2}(-\cos\theta + e^{i\phi}\sin\theta), \quad (7.5)$$

with $\theta, \phi \in [0, \pi)$, while the matrix B is defined as $B = -F_2 - A$, with F_2 the Fourier matrix. The submatrices

$$Z_j = \begin{pmatrix} 1 & 1 \\ z_j & -z_j \end{pmatrix}, \quad Z_k = \begin{pmatrix} 1 & z_k \\ 1 & -z_k \end{pmatrix}, \quad (7.6)$$

with the left and right versions defined for $j = 1, 2$ and $k = 3, 4$, respectively, depend on unimodular

parameters, i.e. $|z_j| = |z_k| = 1$, which are related by Möbius transformations $\mathcal{M}(z) = \frac{\alpha z - \beta}{\beta z - \alpha}$. In particular, one has $z_3^2 = \mathcal{M}_A(z_1^2)$, $z_3^2 = \mathcal{M}_B(z_2^2)$, $z_4^2 = \mathcal{M}_A(z_2^2)$ and $z_4^2 = \mathcal{M}_B(z_1^2)$, where $\alpha_A = A_{12}^2$, $\beta_A = A_{11}^2$, $\alpha_B = B_{12}^2$ and $\beta_B = B_{11}^2$. By choosing $z_1 = e^{i\lambda}$, say, the remaining three z -parameters are uniquely determined through the Möbius transformations, resulting in the three-parameter family $K_6(\theta, \phi, \lambda)$.

The parameterisation used to describe $K_6^{(3)}$ differs from those of the smaller one- and two-parameter families, so connections between $K_6^{(3)}$ and its subfamilies are difficult to spot. Exceptions occur when θ and ϕ are constant: for example, $D_6^{(1)}$ is recovered when $\theta = \arccos(1/\sqrt{3})$ and $\phi = \pi/4$. The Fourier family $F_6^{(2)}$ is recovered in the limit of $\theta = 0$, taking z_1 and ϕ as the free parameters [220].

The four-parameter family $G_6^{(4)}$

Evidence of the existence of a four-parameter family was first provided by numerical calculations in Ref. [345]. Performing infinitesimal shifts of phases in the Fourier matrix was found to preserve the unitary condition of the Hadamard matrix while moving away along four independent directions. This property was, in fact, expected already in 2005 since the *defect*—an upper bound on the dimensionality of a set of Hadamard matrices (see Appendix B)—equals four for many Hadamard matrices of order six [53].

The construction of a proposed four-parameter family was first presented by Szöllősi in 2012 [357], but a rigorous proof of its existence appeared only later by Bondal and Zhdanovskiy [67]. The result, using methods from algebraic geometry, is formulated in terms of orthogonal pairs of Cartan subalgebras in $sl_d(\mathbb{C})$.

Theorem 7.3. *There exists a four-parameter family of orthogonal pairs of Cartan subalgebras in $sl_6(\mathbb{C})$.*

Combining this result with Equivalence 5.5 immediately implies the existence of a four-parameter family of 6×6 complex Hadamard matrices.

The proof of Thm. 7.3 is not constructive; instead we review the construction of the four-parameter set $G_6^{(4)}$ proposed in [357]. The general technique aims to embed a “well-behaved”

3×3 submatrix $E(a, b, c, d)$ into a larger complex Hadamard matrix, viz.

$$G_6(a, b, c, d) = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & a & b & e & s_1 & s_2 \\ 1 & c & d & f & s_3 & s_4 \\ 1 & g & h & * & * & * \\ 1 & t_1 & t_3 & * & * & * \\ 1 & t_2 & t_4 & * & * & * \end{pmatrix} \equiv \begin{pmatrix} E & B \\ C & D \end{pmatrix}, \quad (7.7)$$

where B, C and D are also 3×3 submatrices. First, the unimodular entries of B and C are determined by the orthogonality requirements from the first three rows and columns of $G_6^{(4)}$. Once e, f, g, h, s_i and t_i —all of which depend on a, b, c and d —have been calculated, the entries of D are then evaluated. These are fixed by $D = -CE^\dagger(B^{-1})^\dagger$, where $\dagger$ denotes the conjugate transpose; if the entries are unimodular, $G_6^{(4)}$ is a complex Hadamard matrix. It is conjectured that E can be chosen to ensure a *finite* number of candidate submatrices B and C , so that it is feasible to check whether the resulting matrix is a Hadamard matrix.

The explicit algorithm which generates $G_6^{(4)}$ is presented in [357]. The entries of $G_6^{(4)}$ are given by algebraic functions of roots of sextic polynomials, without known closed expressions. A Mathematica script which provides random matrices according to the above construction is available online [84].

Unfortunately, the relation between $G_6^{(4)}$ and $K_6^{(3)}$ is not fully understood. According to [357, Prop. 2.16], if a Hadamard matrix H is not equivalent to either S_6 or a member of $K_6^{(3)}$, then it contains a well-behaved submatrix E , and consequently there is the possibility to reconstruct H from the above method. On the other hand, it is not known if $K_6^{(3)}$ contains a suitable 3×3 submatrix that would result in $K_6^{(3)} \subset G_6^{(4)}$.

Taken together, the sets of 6×6 complex Hadamard matrices listed in Thm. 7.1 are expected to exhaust all such matrices [357].

Conjecture 7.1. *Every complex Hadamard matrix of order six is equivalent to a member of either $K_6^{(3)}$ or $G_6^{(4)}$, or to Tao’s matrix S_6 .*

If true, this result would open up a feasible approach to decide how many MU bases the space

$\mathbb{C}^6$ can accommodate. One could attempt an exhaustive computer search in analogy to the proof which excludes both the Fourier family $F_6^{(2)}$ and its transpose from appearing in a hypothetical set of seven MU bases [205].

Examples of non- H_2 -reducible 6×6 Hadamard matrices—which one expects to be members of $G_6^{(4)}$ —appear in [255]. Further properties of Hadamard matrices of order six can be found, for example, in [254, 255].

7.2 Triples of MU bases

Given the different pairs of MU bases that result from Thm. 7.1, it is natural to wonder if they extend to triples of MU bases. Does every pair of MU bases extend to at least one triple? In other words, given a Hadamard matrix H does there exist another one, say K , such that their product $H^\dagger K$ is also a Hadamard matrix?

An extensive *numerical* search of matrices K unbiased to $\{\mathbb{I}, H\}$, for every affine and non-affine family (known before 2009), is given in [79]. For each family, a search was conducted both at regular intervals along the parameter space as well as at random. When H belongs to an affine family, i.e. the Fourier family $F_6^{(2)}$ or the Diță family $D_6^{(1)}$, a triple of the form $\{\mathbb{I}, H, K\}$ is *always* found. In particular, the number of vectors MU to the Diță family fluctuates between 48, 72 and 120 vectors, depending on the value of the parameter. Meanwhile, 48 vector are found to be mutually unbiased to the Fourier family, for each sampled parameter value. In contrast, the isolated matrix S_6 of Eq. (7.1) does not extend to a triple (see Sec. 7.6).

When H belongs to a non-affine family, direct calculations become more complicated, necessitating certain approximations. Results pertaining to these cases are discussed further in the section on numerics (Sec. 8.1). Numerical methods from several studies suggest extensions to MU triples are not always possible [163, 271]. The extendibility properties of all known pairs of MU bases are summarised in Table 2 of Sec. 7.6, combining rigorous results and numerical evidence discussed in Sec. 8.1.

Finding *closed-form* expressions of MU triples appears to be difficult: we are, in fact, aware of only three infinite families in dimension six. A one-parameter family was first presented by Za-

uner [411, 413], and the method was later used to generate a two-parameter family by Szöllősi [356]. Another one-parameter family was found by Jaming *et al.* [205], containing a subset of the family $F_6^{(2)}$.

Let us spell out the closed-form expressions of these examples. The first two use a result obtained by Zauner [411] (see also [356]).

Theorem 7.4. *If T is a $2n \times 2n$ Hadamard matrix with $n \times n$ circulant blocks, then there exist $2n \times 2n$ Hadamard matrices E_1 and E_2 such that $T = E_1^{-1}E_2$.*

This theorem implies that a triple of MU bases $\{\mathbb{I}, E_1, E_2\}$ exists given a Hadamard matrix T consisting of circulant blocks. Zauner considers an explicit construction of T , E_1 and E_2 in the space $\mathbb{C}^6$, with T a one-parameter family of Hadamard matrices.

Let T be a 6×6 matrix of the form

$$T = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}, \quad (7.8)$$

where A_{ij} are circulant matrices of order three. Since A_{ij} are circulant they may be written in the form $A_{ij} = F_3^{-1} \bar{A}_{ij} F_3$, where F_3 is the 3×3 Fourier matrix and $\bar{A}_{ij} = \text{diag}(a_{ij}^1, a_{ij}^2, a_{ij}^3)$. If T is unitary then the matrices

$$S_k = \begin{pmatrix} a_{11}^k & a_{12}^k \\ a_{21}^k & a_{22}^k \end{pmatrix}, \quad k = 1, 2, 3, \quad (7.9)$$

are unitary. For each of these 2×2 unitary matrices there exist parameters $b_\ell^k \in [0, 2\pi)$, $\ell = 1 \dots 4$, such that

$$S_k = \frac{1}{2} \begin{pmatrix} (e^{ib_1^k} + e^{ib_2^k}) & e^{ib_4^k}(e^{ib_1^k} - e^{ib_2^k}) \\ e^{-ib_3^k}(e^{ib_1^k} - e^{ib_2^k}) & e^{-ib_3^k}e^{ib_4^k}(e^{ib_1^k} + e^{ib_2^k}) \end{pmatrix}. \quad (7.10)$$

We can then write $T = E_1^{-1}E_2$ where

$$E_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} F_3 & U_3 F_3 \\ F_3 & -U_3 F_3 \end{pmatrix} \quad (7.11)$$

and

$$E_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} U_1 F_3 & U_1 U_4 F_3 \\ U_2 F_3 & -U_2 U_4 F_3 \end{pmatrix}, \quad (7.12)$$

with diagonal unitaries $U_\ell = \text{diag}(e^{ib_\ell^1}, e^{ib_\ell^2}, e^{ib_\ell^3})$, $\ell = 1 \dots 4$. Now, since E_1 and E_2 are Hadamard matrices and by requiring that T has entries of

constant modulus, the columns of E_1 and E_2 form a pair of MU bases. Finally, taking

$$T = \begin{pmatrix} 1 & e^{-ix} & e^{ix} & -1 & ie^{-ix} & ie^{ix} \\ e^{ix} & 1 & -e^{-ix} & ie^{ix} & -1 & ie^{-ix} \\ -e^{-ix} & e^{ix} & 1 & ie^{-ix} & ie^{ix} & -1 \\ 1 & ie^{-ix} & ie^{ix} & 1 & e^{-ix} & -e^{ix} \\ ie^{ix} & 1 & ie^{-ix} & -e^{ix} & 1 & e^{-ix} \\ ie^{-ix} & ie^{ix} & 1 & e^{-ix} & -e^{ix} & 1 \end{pmatrix} \quad (7.13)$$

with $x \in [0, 2\pi)$, the triple $\{\mathbb{I}, E_1, E_2\}$ can be shown to form a set of three MU bases containing one free parameter.

Szöllősi's two-parameter family of Hadamard matrices $X_6^{(2)} \equiv X_6(\alpha) \equiv X_6((x, y), (u, v))$ also contains 3×3 circulant blocks for all parameter values [356], and is therefore a suitable candidate for Thm. 7.4. Written in dephased form,

$$X_6^{(2)} = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & x^2 y & xy^2 & \frac{xy}{uv} & uxy & vxy \\ 1 & \frac{x}{y} & x^2 y & \frac{x}{u} & \frac{x}{v} & uvx \\ 1 & uvx & uxy & -1 & -uxy & -uvx \\ 1 & \frac{x}{u} & vxy & -\frac{x}{u} & -1 & -vxy \\ 1 & \frac{x}{v} & \frac{xy}{uv} & -\frac{xy}{uv} & -\frac{x}{v} & -1 \end{pmatrix}, \quad (7.14)$$

where (x, y) and (u, v) are determined by the roots of $f_\alpha(z)$ and $f_{-\alpha}(z)$, respectively, where $f_\alpha(z) = z^3 - \alpha z^2 + \alpha^* z - 1 = 0$, and $\alpha \in \mathbb{D}$. Here, $\mathbb{D}$ is a region defined by the intersection of two deltoids, as described in [356]. For this choice of matrix, Thm. 7.4 leads to a two-parameter family of MU triples.

Theorem 7.5. *There exists a two-parameter family of MU triples $\{\mathbb{I}, E_1(\alpha), E_2(\alpha)\}$ in dimension six, where $X_6(\alpha) = E_1^{-1}(\alpha)E_2(\alpha)$ is the two-parameter Szöllősi family of Hadamard matrices.*

Recall that the Diță family $D_6^{(1)}$ and the self-adjoint family $B_6^{(1)}$ are both included in the set $X_6^{(2)}$. Consequently, they both extend to sets of three MU bases.

A one-parameter family of triples was found by Jaming *et al.* [205]. It consists of the standard basis, the Fourier family $F_6^{(2)} \equiv F_6(a, b)$, which

can be written in dephased form as

$$F_6^{(2)} = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & -\omega^2 x & \omega & -x & \omega^2 & -\omega x \\ 1 & \omega y & \omega^2 & y & \omega & \omega^2 y \\ 1 & -1 & 1 & -1 & 1 & -1 \\ 1 & \omega^2 x & \omega & x & \omega^2 & \omega x \\ 1 & -\omega y & \omega^2 & -y & \omega & -\omega^2 y \end{pmatrix}, \quad (7.15)$$

with $x = e^{2\pi ia}$, $y = e^{2\pi ib}$ and $\omega = e^{2\pi i/3}$, and the matrix $C(t)$ defined in Appendix A of [205]. The one-parameter family of three MU bases consists of the standard basis combined with $F_6(0, b(t))$ and $C(t)$, where $\frac{1}{2} \arcsin \frac{\sqrt{5}}{3} \leq t \leq \frac{\pi}{2} - \frac{1}{2} \arcsin \frac{\sqrt{5}}{3}$.

A simple characterisation of the complex Hadamard matrices appearing in the known families of MU triples can be found in [277]. In particular, if at least three columns of a complex Hadamard matrix of order six (in dephased form) contains a -1 entry, then it belongs to the transposed Fourier family $(F_6^{(2)})^T$ or the Szöllősi family $X_6^{(2)}$. Furthermore, these two families can be easily distinguished by properties of their submatrices [277].

In view of these constructions, together with the unextendibility results summarised in Table 2, the options to extend pairs $\{\mathbb{I}, H\}$ appear to be limited.

7.3 Sets containing the Fourier family

Pairs of MU bases involving the Fourier family have been widely studied in dimension six. As discussed in the preceding section, there exists a one-parameter family of MU triples involving $F_6(0, b)$. Furthermore, the existence of MU triples containing each member of $F_6(a, b)$ is supported by strong numerical evidence [205], but no rigorous proof is known. Let us now attempt a chronological description of *non-existence results* related to the Fourier family, starting with the cyclic d -roots problem, solved in 1991 by Björck and Fröberg [60].

Searching for vectors mutually unbiased to $\{\mathbb{I}, F_6\}$ is, according to Sec. 6.4 on biunimodular sequences, equivalent to finding biunimodular vectors $x \in \mathbb{C}^6$. In turn, finding these biunimodular sequences means solving the cyclic 6-roots problem defined by the set of equations (6.3), with the added constraints $|z_i| = 1$ for each i . Without the unimodular condition on

z , a computer-aided search found the full set of 156 cyclic 6-roots [60]. In 1997, Haagerup showed that 48 of these vectors are unimodular, including twelve classical solutions of the type $(\alpha, \alpha^3, \alpha^5, \alpha^7, \alpha^9, \alpha^{11})$ where α is a twelfth root of unity [174]. He expressed the remaining 36 vectors as

$$z = \left(\omega^k z_{j-\ell}^{(0)} \right)_{j \in \mathbb{Z}_6}, \quad k, \ell \in \mathbb{Z}_6, \quad (7.16)$$

where $\omega = e^{2\pi i/6}$,

$$z^{(0)} = (1/a, i, ia, -ia, -i, -i/a), \quad (7.17)$$

and $a = \frac{1-\sqrt{3}}{2} + i \left(\frac{\sqrt{3}}{2} \right)^{1/2}$. The corresponding biunimodular sequences take the form

$$x = c \left(\omega^{kj} x_{j-\ell}^{(0)} \right)_{j \in \mathbb{Z}_6}, \quad k, \ell \in \mathbb{Z}_6, c \in \mathbb{T}, \quad (7.18)$$

with $x_j^{(0)} = (1, i/a, -1/a, -i, -a, ia)$. In 2004, Grassl rediscovered these 48 biunimodular sequences in the language of MU bases [166]. Furthermore, he showed that the pair $\{\mathbb{I}, F_6\}$ does not extend to a complete set of MU bases.

Theorem 7.6. *There exist only 48 vectors mutually unbiased to the pair $\{\mathbb{I}, F_6\}$. One can arrange these vectors into 16 different orthonormal bases $\mathcal{B}_k$, $k = 1 \dots 16$, to produce 16 MU triples $\{\mathbb{I}, F_6, B_k\}$, but no remaining vector is mutually unbiased to any of them.*

The proof involves solving a set of polynomial equations obtained by expressing candidate vectors of $\mathbb{C}^6$ in the form

$$|\psi\rangle = \frac{1}{\sqrt{6}}(1, x_1 + ix_6, x_2 + ix_7, \dots, x_5 + ix_{10})^T, \quad (7.19)$$

where the variables x_j are real and $x_j^2 + x_{j+5}^2 = 1$, $j = 1 \dots 5$. By requiring that $|\psi\rangle$ is MU to the columns of F_6 , the computer algebra system MAGMA finds 48 real solutions for the set of variables x_j , which are listed explicitly in the updated preprint of [166]. Later, in 2012, an independent analytic proof of the unextendibility of $\{\mathbb{I}, F_6\}$ to a complete set was found [272], based on Fourier analytic techniques (see Sec. 6.12).

Further analysis of the structure of these 48 vectors and the corresponding 16 orthonormal bases has been carried out in [49] and later in [163]. Of the 16 orthonormal bases, two are Fourier matrices enphased with 12th roots of

unity, two are equivalent to $F^T(1/6, 0)$, six are Björck matrices [61] and six are Fourier matrices enphasized with Björck's number a defined in Eq. (7.17).

As described in [163], the vectors group into three sets, each corresponding to one orbit under the Heisenberg-Weyl group, whose elements are the displacement operators $D_{jk} = \tau^{jk} X^j Z^k$ with $\tau = -e^{\pi i/d}$, $j, k = 0, \dots, \bar{d} - 1$, expressed in terms of the shift and phase operators X, Z defined in Eq. (A.7). The order of τ depends on the parity of d : we have $\bar{d} = d$ if d is odd, and $\bar{d} = 2d$ if d is even. The three vectors generating the orbits are $v_1 = (1, i, \omega^4, i, 1, i\omega^4)$, $v_2 = (1, -i, \omega^2, -i, 1, -i\omega^2)$ and $v_3 = (1, ia, a^2, -ia^2, -a, -i)$, with $\omega = e^{2\pi i/6}$. The vectors v_1 and v_2 are eigenvectors of $D_{\ell, \ell}$ and $D_{\ell, 5\ell}$, respectively, for every $\ell = 0, \dots, \bar{d} - 1$, resulting in orbits of six elements each; they are, in fact, product states after a suitable permutation of elements. Every eigenvector of XZ is a member of the orbit generated by v_1 , while the second orbit is obtained from complex conjugation of the elements of the first orbit. The vector v_3 is not an eigenvector of any displacement operator and gives rise to an orbit of 36 states. Shifting the elements of v_3 two places to the right yields the vector $-ax_j^{(0)}$, in agreement with the biunimodular sequences of Björck, Fröberg and Haagerup.

Jaming *et al.* [205] obtain unextendibility results which apply to the entire two-parameter Fourier family.

Theorem 7.7. *The family of MU pairs $\{\mathbb{I}, F_6(a, b)\}$ does not extend to a quadruple of MU bases.*

The proof of Thm. 7.7 relies on a discretisation scheme and a computational search similar to the one described in Sec. 8.2, but the result is rigorous due to exact bounds on the error terms. The search for candidate MU vectors involves finding *approximate* MU vectors by estimating the phases of the vector components using N -th roots of unity. Each vector component is evaluated at regular intervals of $2\pi j/N$, with $j = 1, \dots, N$, and a computer-aided search calculates N^ν states, where ν denotes the number of free variables (phases) for the candidate MU vectors. By choosing a sufficiently large positive integer N , rigorous bounds of the errors given by

the inner products of the approximated states can be established. If the errors from these approximated states are too large, no such MU vectors exist. Importantly, this method can be generalised and could therefore lead to a proof of the conjectured non-existence of complete sets in dimension six (or any other composite dimension $d \notin \mathbb{PP}$), even without an exhaustive classification of 6×6 complex Hadamard matrices [206].

The computational search over the parameter values (a, b) finds the number of vectors MU to the pair $\{\mathbb{I}, F_6(a, b)\}$ is 48. In most cases these 48 vectors produce 8 orthonormal bases $C_1(a, b), \dots, C_8(a, b)$, but in exceptional cases one can construct additional orthonormal bases. For example, there exist 16 and 70 orthonormal bases when $(a, b) = (0, 0)$ and $(a, b) = (1/6, 0)$, respectively.

A proof of Thm. 7.7—not dependent on a computer search—was later found by Matolcsi and Weiner [274] by improving the Delsarte linear-programming bound (see Secs. 6.11 and 6.12).

7.4 MU product bases

We have discussed MU *product* bases for multipartite systems in Sec. 6.7 and found that their classification is, in arbitrary composite dimensions, quite difficult. However, if we limit ourselves to product bases in $\mathbb{C}^2 \otimes \mathbb{C}^3$, an exhaustive list of MU product bases can be given. What is more, we can find tight upper bounds on maximal sets of MU product bases, and show that any such set is strongly unextendible.

Let us denote product bases of the space $\mathbb{C}^6$ by

$$\{|v^1, v^2\rangle, v = 0, \dots, 5\} \subset \mathbb{C}^2 \otimes \mathbb{C}^3, \quad (7.20)$$

with qubit states $|v^1\rangle \in \mathbb{C}^2$ and qutrit states $|v^2\rangle \in \mathbb{C}^3$, respectively. It was shown in [283], via a classification of all product bases of the form (7.20), that a pair of bases $\mathcal{B} = \{|v^1, v^2\rangle\}_{v=0}^5$ and $\mathcal{B}' = \{|u^1, u^2\rangle\}_{u=0}^5$ is MU if and only if $|v^1\rangle$ is MU to $|u^1\rangle$, and $|v^2\rangle$ is MU to $|u^2\rangle$, for all $v, u = 0, \dots, 5$. We note that this statement has not been extended to arbitrary composite dimensions (cf. Sec. 6.7) due to our inability to classify product bases in general.

The unbiasedness condition on the states in $\mathbb{C}^2$ and $\mathbb{C}^3$ is essential for the classification of all MU product bases in dimension six. In [283] an exhaustive list of pairs and triples of MU product

bases is constructed, up to local “equivalence” transformations. We say that sets of MU product bases are “equivalent” if we can transform one set into another by some local (anti-) unitary transformations. These include, for example, a local unitary transformation mapping one set to another, permutations of states, and complex conjugation operations.

To express the exhaustive list we use complete sets of MU bases in dimensions two and three. We denote the complete set in dimension two by $\{|v_a\rangle\}$, $a = z, x, y$, where $v = 0, 1$, indicate the orthonormal vectors which are eigenstates of the Pauli operators σ_a . In dimension three, the eigenstates of the four Heisenberg-Weyl operators Z , X , $Y = XZ$ and $W = XZ^2$ (defined in Appendix A.4) form the four MU bases and are denoted by $\{|V_b\rangle\}$, $b = z, x, y, w$, and $V = 0, 1, 2$.

For example, consider a basis of $\mathbb{C}^6$ given by $\{|0_z, V_z\rangle, |1_z, V_y\rangle\}$: it consists of three states from the tensor product of $|0_z\rangle \in \mathbb{C}^2$ with the eigenstates of the Heisenberg-Weyl operator Z , and three states resulting from tensoring the states $|1_z\rangle \in \mathbb{C}^2$ with the eigenstates of Y . The states $|0_z\rangle$ and $|1_z\rangle$ form the canonical basis in dimension two. This construction is an example of an *indirect product* basis: all the states are product states of the bi-partite system but they are obtained by tensoring the elements of *three* bases rather than two, namely the standard basis of the space $\mathbb{C}^2$ and a *pair* of different bases, $\{|V_y\rangle\}$ and $\{|V_z\rangle\}$, of $\mathbb{C}^3$.

The complete list of MU product pairs comes in four different flavours according to the following theorem.

Theorem 7.8. *Any pair of MU product bases in the space $\mathbb{C}^2 \otimes \mathbb{C}^3$ is equivalent to a member of the families*

$$\begin{aligned}\mathcal{P}_0 &= \{|v_z, V_z\rangle; |v_x, V_x\rangle\}, \\ \mathcal{P}_1 &= \{|v_z, V_z\rangle; |0_x, V_x\rangle, |1_x, \hat{R}_{\xi, \eta} V_x\rangle\}, \\ \mathcal{P}_2 &= \{|0_z, V_z\rangle, |1_z, V_y\rangle; |0_x, V_x\rangle, |1_x, V_w\rangle\}, \\ \mathcal{P}_3 &= \{|0_z, V_z\rangle, |1_z, \hat{S}_{\zeta, \chi} V_z\rangle; \\ &\quad |v_x, 0_x\rangle, |\hat{r}_\sigma v_x, 1_x\rangle, |\hat{r}_\tau v_x, 2_x\rangle\}, \quad (7.21)\end{aligned}$$

with $v = 0, 1$, and $V = 0, 1, 2$. The unitary operator $\hat{R}_{\xi, \eta}$ is defined as $\hat{R}_{\xi, \eta} = |0_z\rangle\langle 0_z| + e^{i\xi}|1_z\rangle\langle 1_z| + e^{i\eta}|2_z\rangle\langle 2_z|$, for $\eta, \xi \in [0, 2\pi)$, and $\hat{S}_{\zeta, \chi}$ is defined analogously with respect to the x -basis; the unitary operators $\hat{r}_\sigma$ and $\hat{r}_\tau$ act on

the basis $\{|v_x\rangle\} \equiv \{|\pm\rangle\}$ according to $\hat{r}_\sigma|v_x\rangle = (|0_z\rangle \pm e^{i\sigma}|1_z\rangle)/\sqrt{2}$ for $\sigma \in (0, \pi)$, etc.

The pairs $\mathcal{P}_0$ and $\mathcal{P}_2$ have no parameter dependence, the pair $\mathcal{P}_1$ depends on two parameters, while $\mathcal{P}_3$ is a four-parameter family. The ranges of the parameters are assumed to be such that no MU product pair occurs more than once in the list.

If we consider *triples* of MU product bases, there exists only one example in addition to the expected Heisenberg-Weyl triple:

Theorem 7.9. *Any triple of MU product bases in the space $\mathbb{C}^2 \otimes \mathbb{C}^3$ is equivalent to either*

$$\begin{aligned}\mathcal{T}_0 &= \{|v_z, V_z\rangle; |v_x, V_x\rangle; |v_y, V_y\rangle\}, \\ \text{or } \mathcal{T}_1 &= \{|v_z, V_z\rangle; |v_x, V_x\rangle; |0_y, V_y\rangle, |1_y, V_w\rangle\}.\end{aligned}\quad (7.22)$$

A consequence of exhaustively enumerating MU product bases in dimension six is a bound on their number in a hypothetical complete set. It is straightforward to see that no single *product* state can be MU to the two triples $\mathcal{T}_0$ and $\mathcal{T}_1$. However, a stronger result is within reach: it is impossible to complement either $\mathcal{T}_0$ or $\mathcal{T}_1$ by *any* MU vector [285]. Thus, *a complete set of MU bases in dimension six cannot contain a product triple*. This is in marked contrast to the prime-power dimension p^2 where a complete set of MU bases includes $(p+1)$ MU product bases constructed from the tensor products of Heisenberg-Weyl operators [248].

By further investigating the set of MU product pairs given in Thm. 7.8, a stronger statement on the non-existence of MU product bases can be derived [286].

Theorem 7.10. *If a complete set of seven MU bases in dimension six exists, it contains at most one product basis.*

In other words, six of the seven MU bases contain entangled states. The proof of Thm. 7.10 relies on Theorems 7.7, 7.8 and 7.14. It is shown in [286] that the four pairs in Thm. 7.8 are equivalent, under non-local equivalence transformations, to either $\{\mathbb{I}, S_6\}$ or $\{\mathbb{I}, F_6(a, b)\}$. But since neither pair extends to a complete set (Theorems 7.7 and 7.14), no pair of product bases appears in a complete set. It is clear from the proof that the following result is also true.

Corollary 7.1. *If a set of four MU bases in dimension six exists, it contains at most one product basis.*

The refined concept of MU product *constellations* (cf. Sec. 8.3) rather than entire bases has been considered to find further limitations on the number of product states in a complete set [107].

Theorem 7.11. *Let H be a 6×6 Hadamard matrix in which three of its columns are product vectors of $\mathbb{C}^2 \otimes \mathbb{C}^3$. Then the pair $\{\mathbb{I}, H\}$ does not extend to a set of four MU bases.*

The proof is based on considering all possible orthogonality relations between the three product vectors which form the product columns of H , and on showing that H is equivalent to a matrix containing a 3×3 submatrix proportional to a unitary. Then the following lemma can be applied [107].

Lemma 7.1. *Let H be a 6×6 Hadamard matrix containing a 3×3 submatrix U , which is proportional to a unitary matrix. Then the pair $\{\mathbb{I}, H\}$ does not extend to a set of four MU bases.*

To prove this result, one rewrites the matrix H in block form as

$$H' = \begin{pmatrix} U & A \\ B & C \end{pmatrix}, \quad (7.23)$$

where the rows and columns of H have been permuted such that U is now in the top left block of H' . One can easily check that if H' is unitary, then both $\sqrt{2}U$ and $\sqrt{2}B$ are unitaries. Thus, the pair $\{\mathbb{I}, H'\}$ can be mapped to

$$\left\{ \sqrt{2} \begin{pmatrix} U^\dagger & 0 \\ 0 & B^\dagger \end{pmatrix}, \sqrt{2} \begin{pmatrix} \mathbb{I}/2 & U^\dagger A \\ \mathbb{I}/2 & B^\dagger C \end{pmatrix} \right\}, \quad (7.24)$$

and, since the latter matrix is unitary, we also have $U^\dagger A = -B^\dagger C$. Therefore, the columns of both matrices are product vectors in the space $\mathbb{C}^2 \otimes \mathbb{C}^3$. Corollary 7.1 is then applied to show that these bases cannot exist in a set of four MU bases.

We note that a result similar to Thm. 7.11 has been derived in [108] which places a limit on the number of product states in a set of four MU bases in $\mathbb{C}^2 \otimes \mathbb{C}^3$, by assuming that the first basis is an arbitrary product basis rather than the canonical one.

Finally, let us mention an unextendibility result for Hadamard matrices of order six and low Schmidt rank. Given an operator P acting on the space $\mathbb{C}^{d_1} \otimes \mathbb{C}^{d_2}$, its operator-Schmidt decomposition reads $P = \sum_j s_j A_j \otimes B_j$, where A_j and B_j are operators acting on $\mathbb{C}^{d_1}$ and $\mathbb{C}^{d_2}$ respectively, and $s_j \geq 0$. The *Schmidt rank* of P is the number of non-zero coefficients s_j in this decomposition. Investigating this quantity for Hadamard matrices of order six leads to the following result [107].

Theorem 7.12. *Let H be a 6×6 Hadamard matrix with Schmidt rank $r \leq 2$. Then the pair $\{\mathbb{I}, H\}$ does not extend to a set of four MU bases.*

The proof relies on an exhaustive classification of 6×6 Hadamard matrices with Schmidt rank one and two. Any pair $\{\mathbb{I}, H\}$, where H has Schmidt rank at most two, is equivalent to a pair of MU product bases. Since no set of four MU bases contains a pair of product bases (see Corollary 7.1) the proof is complete.

Although a classification of Hadamard matrices with Schmidt rank three is known [195], a statement analogous to Thm. 7.12 is not. Further properties of such matrices are discussed in [110].

7.5 Group theory of complete sets

Some restrictions on the structure of a hypothetical complete set are known which relate to group theory. We have seen in Sec. 6.5 that no complete set in dimension six exists that consists entirely of nice MU bases. In particular, if seven MU bases exist, they cannot be constructed from partitioning a nice error basis into maximally commuting classes. Instead, the MU bases must come from a unitary operator basis without the appropriate group structure (cf. Thm. 6.6).

Another restriction arises from the connection between MU bases and projective toric 2-designs. As described in Sec. 5.11, a set of d complex Hadamard matrices of order d is mutually unbiased if and only if the columns form a projective toric 2-design of $P(T^d)$. For $d = 6$, an exhaustive computational search confirmed that such a design, formed from d Hadamard matrices, cannot be a subgroup of $P(T^6)$ [201].

Theorem 7.13. *A set of six Hadamard matrices of order six are pairwise mutually unbiased if and only if their columns form a projective toric 2-design which is not a subgroup of $P(T^6)$.*

This is markedly distinct from prime and prime-power dimensions, where all (known) complete sets relate to projective toric 2-designs that are groups [201]. If, as predicted, a complete set for $d = 6$ does not exist, Thm. 7.13 implies that toric non-group designs do not exist. More generally, it is conjectured that for any d , complete sets of MU bases originate only from group projective toric 2-designs [201].

7.6 Unextendible MU bases

According to Thm. 7.7, any triple of MU bases that includes the Fourier family $F_6(a, b)$ is *unextendible*, as is any triple which contains multiple product bases (Corollary 7.1). In this section, we summarise further results on (un-) extendibility of pairs of MU bases valid in dimension $d = 6$ (cf. Table 2). The table also contains numerical results on unextendibility discussed in Sec. 8, including evidence that certain families of MU pairs do not extend to triples (Sec. 8.1) or quadruples (Sec. 8.2).

Generalising Grassl’s computer-algebraic calculation for the Heisenberg-Weyl pair (Thm. 7.6) to pairs of the form $\{\mathbb{I}, H\}$, with a 6×6 complex Hadamard matrix H , was considered in Ref. [79]. Using Buchberger’s algorithm [86], the original set of polynomials was mapped to another, easier to solve “tri-diagonal” set of coupled polynomial equations, the so-called Gröbner basis. In this way, all vectors mutually unbiased to a particular pair $\{\mathbb{I}, H\}$ were constructed.

The number of vectors MU to $\{\mathbb{I}, H\}$, where H is the Diţă-matrix $D_6(0)$, the circulant matrix C_6 [61] (which is a member of the self-adjoint family $B_6^{(1)}$) and the isolated matrix S_6 equal 120, 56 and 90, respectively. Ten triples exist containing the pair $\{\mathbb{I}, D_6(0)\}$, but none extend to four MU bases. Similarly, no four MU bases exist containing $\{\mathbb{I}, C_6\}$, and no orthonormal basis can be constructed from the 90 vectors MU to $\{\mathbb{I}, S_6\}$.

Theorem 7.14. *The pairs $\{\mathbb{I}, C_6\}$ and $\{\mathbb{I}, D_6(0)\}$, which have an additional 56 and 120 unbiased vectors respectively, do not extend to four MU bases. The pair $\{\mathbb{I}, S_6\}$ has 90 unbiased vectors and does not extend to an MU triple.*

The calculations were also carried out for regularly spaced values of the parameter x in the Diţă family $D_6(x)$ and a grid of points of the two-parameter Fourier family $F_6(a, b)$. For the pair

$\{\mathbb{I}, D_6(x)\}$, the number of MU vectors appears to be piecewise constant, dropping from 120 to 72 and then to 48 at the end points of the parameter range. For the Fourier family, there exist 48 MU vectors at each of the tested parameter values. In both cases, no set of four MU bases can be formed. This result was later shown to be valid for all members of the Fourier family, as stated in Thm. 7.7.

While these results provide rigorous limits on the number of vectors MU to pairs $\{\mathbb{I}, H\}$, no definite results were obtained for non-affine complex Hadamard matrices H . For the symmetric, Hermitian and Szöllösi non-affine families, i.e. $M_6^{(1)}$, $B_6^{(1)}$ and $X_6^{(2)}$, the available computational memory was insufficient to produce the relevant Gröbner basis, making certain approximations necessary. Thus, no rigorous conclusion regarding the existence of a fourth MU basis containing these families could be drawn.

In Hadamard form, all known complete sets of MU bases (cf. Appendix A) are of Butson-type, with matrix elements consisting of either d or $2d$ roots of unity depending on whether the dimension of the Hilbert space d is odd or even, respectively. Motivated by this observation, a search was carried out in Ref. [49] for mutually unbiased Butson-type Hadamard matrices $B(6, 12)$ (cf. Sec. 9.2), whose entries consist only of twelfth roots of unity. The search confirmed that a Butson-type matrix $B(6, 12)$ does not appear in any MU quadruple.

Theorem 7.15. *If a set of four MU bases in dimension six exists, it contains no Butson-type Hadamard matrix $BH(6, 12)$.*

Non-existence theorems of this type, i.e. for specific *quadruples* of MU bases, are of considerable interest since they would help rule out complete sets. A series of papers [111, 256, 257] leads to the statement that no set of four MU bases in dimension six contains a pair of type $\{\mathbb{I}, D_6^{(1)}\}$, $\{\mathbb{I}, B_6^{(1)}\}$, $\{\mathbb{I}, M_6^{(1)}\}$, or $\{\mathbb{I}, X_6^{(2)}\}$. Unfortunately, the derivation of this result builds on a lemma in Ref. [107] which is erroneous [287]. Thus, numerical evidence (cf. Sec. 8.1) remains the main argument against the presence of these families in quadruples of MU bases, as shown in Table 2.

$\{\mathbb{I}, \cdot\}$	type	defined in	triples exists?	source	no quadruple	source
S_6	isolated	[362]	no	[79]	✓	implied
$F_6^{(2)}$	affine	[239]	(✓)	[205]	✓	[205, 274]
$D_6^{(1)}$	affine	[130]	✓	[356]	(✓)	[79]
$B_6^{(1)}$	not affine	[43]	✓	[356]	?	
$M_6^{(1)}$	not affine	[273]	(some)	[79, 163]	?	
$X_6^{(2)}$	not affine	[356]	✓	[356]	?	
$K_6^{(2)}$	not affine	[218]	(some)	[163]	(✓)	[163, 271]
$K_6^{(3)}$	not affine	[220]	(some)	[163]	(✓)	[163, 271]
$G_6^{(4)}$	not affine	[67, 357]	?		?	

Table 2: Extendability of pairs of MU bases $\{\mathbb{I}, \cdot\}$ in dimension six to triples and quadruples, collecting results described in Secs. 7.2, 7.6 and 8.1. Checkmarks “✓” either confirm that the pairs in question *do* extend to an MU triple, or that they *do not* extend to quadruples; brackets “(·)” indicate the statement is based on numerical evidence. The rigorous (non-) existence proofs of *triples* follow from Thms. 7.5 and 7.14, while the non-existence result of *quadruples* is a consequence of Thm. 7.7. Numerical evidence in [205] supports the existence of a triple containing $\{\mathbb{I}, F_6(a, b)\}$ for all a and b , but a rigorous proof is only known for the pairs $\{\mathbb{I}, F_6(0, b)\}$ (cf. Sec. 7.2).

8 Numerical results: Dimension six

This section reports numerical evidence which overwhelmingly points towards the non-existence of four mutually unbiased bases in dimension six. Even the existence of a single vector mutually unbiased to any triple of MU bases seems unlikely.

8.1 Triples of MU bases

According to Thm. 7.14, the pair $\{\mathbb{I}, S_6\}$, defined by the *isolated* Hadamard matrix of Eq. (7.1), does not extend to an MU triple. We now describe numerical evidence (see Table 2 in Sec. 7.6) suggesting that many other pairs of MU bases do not extend to triples.

Goyeneche [163] carried out a comprehensive computational search for MU triples based on an iterative procedure which constructs approximations of vectors MU to pairs $\{\mathbb{I}, H\}$, where H is a 6×6 complex Hadamard matrix. The solutions (MU vectors) are attractive fixed points of a “physical imposition operator”. The operator is used to transform a state $|\Psi\rangle$, chosen at random, into $|\Psi'\rangle$, which solves the set of equations $|\langle\psi_i|\Psi'\rangle| = |\langle\phi_j|\Psi'\rangle| = 1/d$, where $|\psi_i\rangle$ and $|\phi_j\rangle$ are vectors from the MU pair $\{\mathbb{I}, H\}$.

The method successfully confirmed the results of several previously studied cases (e.g. Thms. 7.5 and 7.14). It outputs, for example, all 90 vectors MU to the pair $\{\mathbb{I}, S_6\}$, all 48 vectors MU to the

pair $\{\mathbb{I}, F_6\}$, and a triple containing $\{\mathbb{I}, F_6(a, b)\}$ for all sampled a and b . It does not find a single vector MU to a triple containing the pair $\{\mathbb{I}, F_6(a, b)\}$. Furthermore, the iterative method confirms the existence of an MU triple for *each* sampled element of the non-affine family $B_6^{(1)}$, in agreement with the search in [79] and Thm. 7.5. The theorem confirms that any matrix from $D_6^{(1)}$ or $B_6^{(1)}$ is contained in an MU triple because both one-parameter families are subsets of $X_6^{(2)}$.

The search [163] finds MU triples containing a member of the non-affine family $M_6^{(1)} \equiv M_6(t)$ for some but not all values of the parameter space. In particular, pairs $\{\mathbb{I}, M_6(t)\}$ were not found to extend to triples in small regions around the values $t = \pi/2, \pi, 3\pi/2, 2\pi$. “Approximate” triples containing $M_6^{(1)}$ were found in an earlier search [79].

For the Karlsson families $K_6^{(2)}$ and $K_6^{(3)}$, the search identified triples in only a limited region of the parameter space. An analysis of the numerical results reveals that certain “symmetries” exist within these families. The Fourier matrix F_6 and the Diţă family $D_6^{(1)}$ appear as centres of symmetry in the parameter space of $K_6^{(2)}$. Reflection symmetries are observed in $K_6^{(3)}$, as illustrated pictorially in Ref. [163].

An independent numerical search provides further evidence of widespread unextendibility

among pairs of MU bases [271]. The idea is to search for three unitary matrices U_1, U_2 , and U_3 such that their transition matrices $U_i^\dagger U_j$ are Hadamard matrices, ensuring that the triple gives rise to three MU bases. The numerical evidence suggests that the transition matrices must belong to the Fourier family $F_6^{(2)}$, its transpose, or the Szöllősi family $X_6^{(2)}$, leading to a restrictive conjecture concerning the existence of MU triples.

Conjecture 8.1. *In dimension six, a pair $\{\mathbb{I}, H\}$ can be extended to an MU triple if and only if H is equivalent to a member of the families of Hadamard matrices $F_6^{(2)}$, $(F_6^{(2)})^T$ or $X_6^{(2)}$.*

If true, the construction from Thm. 7.5 is likely to describe all MU triples [271]. It is important to realise that a proof of Conjecture 8.1 would be a major step towards confirming Zauner’s conjecture that a set of four MU bases does not exist. Since Thm. 7.7 states that an MU quadruple cannot contain any member of the families $F_6^{(2)}$ or $(F_6^{(2)})^T$, it would be sufficient to prove that no member of $X_6^{(2)}$ is contained in a quadruple.

The findings that predict Conjecture 8.1 are consistent with the evidence in Table 2 due to known relations between families of Hadamard matrices discussed in Sec. 7.1, such as the inclusions $D_6^{(1)} \subset X_6^{(2)}$ and $B_6^{(1)} \subset X_6^{(2)}$. In addition, it seems necessary that the family $K_6^{(2)}$ must overlap in yet unknown ways with $X_6^{(2)}$; in particular one expects at least a subset of $M_6^{(1)}$ to be contained in the set $X_6^{(2)}$. The numerical evidence resulting in Conjecture 8.1 also rules out the possibility that *all* members of the three-parameter families $K_6^{(3)}$ and $G_6^{(4)}$ figure in an MU triple.

8.2 Non-existence of MU quadruples

The search for MU bases can be recast as an optimisation problem of a function over a set of orthonormal bases whose maximum (or minimum) is achieved if and only if the bases are mutually unbiased (see Sec. 5.1). A slightly modified version of the function considered in Eq. (5.2) was derived in [49] as a measure of the squared distance between pairs of orthonormal bases,

$$D_{b,b'} = 1 - \frac{1}{d-1} \sum_{v', v=0}^{d-1} \left(|\langle v_b | v'_{b'} \rangle|^2 - \frac{1}{d} \right)^2, \quad (8.1)$$

which takes the maximum value of $D_{b,b'} = 1$ if and only if the bases $\mathcal{B}_b$ and $\mathcal{B}_{b'}$ are mutually unbiased. This measure of “unbiasedness” is quite natural when viewing the basis vectors of the space $\mathbb{C}^d$ as density matrices in a real vector space of dimension $d^2 - 1$. In this representation, a d -dimensional Hilbert space spans a $(d-1)$ -plane in a real vector space of dimension $d^2 - 1$, and two MU bases correspond to two orthogonal $(d-1)$ -planes.

The degree of unbiasedness for a set of μ bases can be quantified by the average squared distance between all pairs of bases, i.e.,

$$\overline{D}_\mu = \frac{2}{\mu(\mu-1)} \sum_{0 \leq b < b' \leq \mu-1} D_{b,b'}, \quad (8.2)$$

which achieves the value $\overline{D}_\mu = 1$ if and only if all μ bases $\{\mathcal{B}_0, \dots, \mathcal{B}_{\mu-1}\}$ are mutually unbiased. In [91], a numerical search for the minimum of the expression $1 - \overline{D}_\mu$ was carried out for dimensions $d \leq 7$, producing strong evidence in support of the conjecture that only three MU bases exist in the space $\mathbb{C}^6$. The minimisation, which is a non-linear least squares problem, was approached by means of the Levenberg-Marquadt algorithm. While this finds only *local* minima, the algorithm was run repeatedly from different starting points, in an attempt to identify the global minimum. In all dimension below $d = 6$, almost all test runs (i.e. $\geq 99.98\%$) converge to $\overline{D}_{d+1} = 1$, implying the existence of a complete set of MU bases. However, in dimension $d = 6$, searching over sets of four and seven orthonormal bases found maximal values of only $\overline{D}_4 = 0.9982917$ and $\overline{D}_7 = 0.9849098$, respectively. In the case $d = 7$, complete sets of MU bases were found, but only in 3 of the 250 test runs.

Further analysis in [318], using the steepest ascent method to maximise the average distance square function of Eq. (8.2), also supports the earlier numerical result that only three MU bases exist in dimension six. Furthermore, a set of four “most distant” bases with $\overline{D}_4 = 0.9982917$ is identified. In particular, a two-parameter family of three orthonormal bases is explicitly derived which, together with the canonical basis, achieve the numerically determined maximum of $\overline{D}_4$ for certain parameter values. Of the four bases, three are equidistant and the remaining basis is mutually unbiased to the others. Thus, the set can be written as the identity matrix together with

three complex Hadamard matrices containing two parameters. All three Hadamard matrices have the same determinant and are members of the transposed Fourier family. For their explicit parameterisation we refer the reader to the original paper [318].

A relation between MU bases and the average success probability of quantum random access codes (QRACs), as described in Equivalence 5.9 of Sec. 5.9, provides an alternative way to measure the unbiasedness of a set of μ orthonormal bases [7]. For μ bases $\mathcal{B}_b = \{|v_b\rangle\}_{v=0}^{d-1}$ in dimension d , the maximum attainable average success probability of a $(\mu, 2)^d \rightarrow 1$ p-QRAC is given by

$$\bar{P}_\mu = \frac{2}{\mu(\mu-1)} \sum_{\{b,b'\} \in S_2} \left(\frac{1}{2} + \frac{1}{2d^2} \sum_{v,v'=0}^{d-1} |\langle v_b | v_{b'} \rangle| \right), \quad (8.3)$$

where the bracketed quantity is averaged over all pairs of bases $\mathcal{B}_b$ and $\mathcal{B}_{b'}$ from the set of μ bases, and S_2 is the set of all possible subsets of $\{1, \dots, \mu\}$ of size 2. As shown in Sec. 5.9, this saturates the upper bound in Eq. (5.13) if and only if the bases are mutually unbiased. Normalising this function provides a new measure of unbiasedness such that the upper bound of one is reached for MU bases and the zero lower bound when the bases are identical.

While semidefinite programming techniques may be used to find this upper bound—and possibly prove non-existence by finding an upper bound smaller than Eq. (5.13)—so far only indirect numerical calculations have been applied [7]. In particular, the $(4, 2)^6 \rightarrow 1$ protocol is optimised using the see-saw method, involving an iterative process which alternates between optimising Alice’s state and Bob’s measurement to find the global maximum. Using these techniques the $(4, 2)^6 \rightarrow 1$ protocol yields a maximum guessing probability of $\bar{P}_4 = 0.703888$, with an average squared distance $\bar{D}_4 = 0.9982839$. This falls just short of the optimal value of $\bar{D}_4 = 0.9982917$ calculated in [91]. If one applies the $(4, 2)^6 \rightarrow 1$ pQRAC to the four bases which are maximally unbiased with respect to $\bar{D}$, the protocol has an optimal average success probability of $\bar{P}_4 = 0.703887$. This implies that the two measures of unbiasedness are inequivalent and have different partial orderings on the set of μ bases.

Another numerical search relies on Bell inequalities (see Sec. 3.11) which are maximally vi-

olated if and only if a set of μ MU bases exists in $\mathbb{C}^d$ [120]. In analogy with the methods described above, i.e. quantifying unbiasedness and QRACs, the search can be recast as an optimisation of the function that gives rise to the Bell inequality. Numerical approaches to the optimisation problem included a see-saw optimisation, a non-linear SDP and Monte Carlo techniques. Each approach failed to find a fourth MU basis in dimension six, and the bases which optimised the function are close to the four “most distant” bases given in [318]. The Monte Carlo approach also suggests that no fourth basis exists in dimension ten.

8.3 Non-existence of MU constellations

Extensive numerical searches for mutually unbiased *constellations*, fleetingly mentioned in Sec. 7.4, were carried out in Ref. [78]. The findings provide further substantial evidence that any three MU bases in dimension six are *strongly* unextendible (cf. Sec. 6.10): not even a single vector is MU to three MU bases.

A mutually unbiased *constellation* is a set of vectors, partitioned into sets of orthonormal states, such that the states within each set are MU to all others not in the set. Constellations are denoted by $\{x_1, \dots, x_n\}_d$, where x_j is the number of orthonormal vectors in the j -th set, and d is the dimension of the vector space. The constellation $\{6, 6, 4\}_6$, for example, contains two sets of six orthogonal states, i.e. two MU bases, and a set of four orthogonal states MU to all members of the first two bases. We will abbreviate this notation to $\{6^2, 4\}_6$ where 6^2 denotes the two sets of six orthonormal states. Since $(d-1)$ orthonormal states already determine an orthonormal basis of the space $\mathbb{C}^d$ uniquely, one can leave out one vector from each basis, hence denoting the MU constellation $\{6^2, 4\}_6$ by $\{5^2, 4\}_6$ instead.

The idea underlying a search for constellations is simple. If a complete set of seven MU bases exists, any MU constellation also exists by suppressing a suitable set of states. Hence, the non-existence of *any* MU constellation between a triple and a complete set implies the non-existence of any larger constellation, including the complete set. The obvious advantage of using constellations rather than entire sets of MU bases is a substantial reduction in the number of free parameters.

$d = 6$	Parameters p_C					Success rate				
x, y	z					z				
	1	2	3	4	5	1	2	3	4	5
1,1	10					100.00				
2,1	15					100.00				
2,2	20	25				100.00	100.00			
3,1	20					100.00				
3,2	25	30				99.95	100.00			
3,3	30	35	40			99.42	39.03	0.00		
4,1	25					100.00				
4,2	30	35				92.92	44.84			
4,3	35	40	45			12.97	0.00	0.00		
4,4	40	45	50	55		0.74	0.00	0.00	0.00	
5,1	30					95.40				
5,2	35	40				76.71	10.96			
5,3	40	45	50			1.47	0.00	0.00		
5,4	45	50	55	60		0.00	0.00	0.00	0.00	
5,5	50	55	60	65	70	0.00	0.00	0.00	0.00	0.00

Table 3: Success rates for searches of MU constellations $\mathcal{C} = \{5, x, y, z\}_6$ in dimension six, each based on 10,000 randomly chosen initial points. The number of free parameters p_C equals the number of constraints only for the two constellations $\{5, 2^2, 1\}_6$ and $\{5, 3, 1^2\}_6$ shown in bold; all larger constellations are overdetermined. (Reproduced with permission from Ref. [78], correcting an erroneous count of the number of constraints pointed out by M. Matolcsi.)

When searching for MU constellations, it is useful to write them in a form containing as few free parameters as possible. Exploiting the dephased form of the associated Hadamard bases, one finds that all candidates for a pair of MU bases $\{(d-1)^2\}_d$ in dimension d , for example, depend on $p_2(d) = (d-2)(d-1)$ real phases. The first Hadamard matrix can be taken as the identity, and dephasing the second matrix leaves $(d-2)$ column vectors with $(d-1)$ free phase factors each (note that one of the columns can be suppressed since $(d-1)$ orthonormal vectors in $\mathbb{C}^d$ fix the last vector). For larger constellations, every additional Hadamard matrix brings another $(d-1)^2$ free phases which means that the candidates $\{(d-1)^\mu\}_d$, $\mu \in \{2 \dots d+1\}$, for MU constellations depend on $p_\mu(d) = (d-1)((\mu-1)(d-1)-1)$ free parameters. Similar arguments lead to the numbers p_C of parameters for the constellations $\mathcal{C} = \{5, x, y, z\}_6$ listed in Table 3.

The numerical searches for MU constellations given in [78] use the same optimisation approach as [91]. They were carried out for subsets of four bases of the form $\{d-1, x, y, z\}_d$, with $d = 5, 6, 7$, and $x, y, z \in [0, d-1]$. In dimension $d = 5$ all of these constellations were identified with sig-

nificant success rates. For dimension $d = 7$, only 46 out of 56 constellations were found directly, although with small success rates; however, *all* constellations were found *indirectly* (the existence of the MU constellation $\{6, 4^2, 2\}_7$, for example, was inferred from identifying a larger one such as $\{6^2, 5, 2\}_7$ containing it).

The success rates (out of 10000 runs for each case) to find constellations $\{5, x, y, z\}_6$ in the space $\mathbb{C}^6$ are reproduced in Table 3. The *largest* MU constellations found were $\{5, 4^2, 1\}_6$ and $\{5^2, 3, 1\}_6$, consisting of 15 and 16 states, respectively. The *smallest* MU constellations which the search failed to find were $\{5, 3^3\}_6$ and $\{5, 4, 3, 2\}_6$ each containing 15 states. The 19-state MU constellation $\{5^3, 1\}_6$ was never found, implying the non-existence of a set of three MU bases together with an additional MU state.

9 Modifying the problem

The difficulty to construct complete sets of MU bases in arbitrary dimensions has led to modifications of the existence problem. The study of closely related structures may provide insights into the original problem, as well as workarounds

in applications such as optimal state reconstruction. In this section we review these approaches. A natural extension consists of replacing the field of complex numbers over which the problem is originally defined, by real numbers, roots of unity, quaternions or finite fields (Secs. 9.1–9.4). Another approach is to modify, in a consistent way, the overlaps defining MU bases and to investigate the resulting structures (Secs. 9.5–9.6). One can generalise the design property of MU bases to include approximate, weighted and conical designs, as described in Secs. 9.7–9.9. More general measurements may also be considered, e.g., POVMs or projectors with rank larger than one (Sec. 9.10–9.12). Finally, infinite-dimensional counterparts of MU bases have been studied, corresponding to quantum systems with continuous variables over the real line, a circle S_1 , or over the p -adic numbers, with associated Hilbert spaces $L^2(\mathbb{R})$, $L^2(S_1)$ and $L^2(\mathbb{Q}_p)$, respectively (Secs. 9.13–9.14).

9.1 Real MU bases

The difficulty of the MU existence problem is related to the large number of parameters needed to parameterise $d(d+1)$ vectors of $\mathbb{C}^d$. Setting the problem in a real Hilbert space $\mathbb{R}^d$ significantly reduces the number of parameters [293, 352]. The modified problem turns the existence question into a search for sets of lines in $\mathbb{R}^d$ which (i) are orthogonal within each set and (ii) otherwise intersect at a specific, fixed angle which depends on the dimension d . These sets of “equiangular” lines in $\mathbb{R}^d$ have been studied in their own right for a long time. Geometric pictures of real MU bases existing in the spaces $\mathbb{R}^3$ and $\mathbb{R}^4$ have been developed in Ref. [54].

An upper limit on the number of MU bases in the space $\mathbb{R}^d$ has been derived by Boykin *et al.* [72]: for any $d \geq 2$, at most $(d/2 + 1)$ real MU bases exist (also see [212]). The proof relies on the link between MU bases and maximally commuting classes of a unitary operator basis (see Equivalence 5.4 of Sec. 5.4). In particular, a set of μ real MU bases $\{\mathcal{B}_0, \dots, \mathcal{B}_{\mu-1}\}$ in $\mathbb{R}^d$ exists if and only if there exists μ classes $\mathcal{C}_0, \dots, \mathcal{C}_{\mu-1}$, of *real symmetric* unitary matrices in $M_d(\mathbb{R})$, each containing d commuting matrices (including the identity), such that all matrices in $\mathcal{C}_0 \cup \dots \cup \mathcal{C}_{\mu-1}$ are pairwise orthogonal. The restriction to *real symmetric* matrices ensures their

eigenstates are real and thus generate MU bases of $\mathbb{R}^d$, not $\mathbb{C}^d$. Comparing the span of this subset of matrices to the space of all real symmetric matrices (which has dimension $d(d+1)/2$), one finds that $\mu \leq d/2 + 1$. Earlier proofs of this result in different contexts can be found in [92, 124].

Stricter bounds can be placed on the number of real MU bases if more is known about the dimension d . If $d \neq 4m$, for $m \in \mathbb{N}$ and $d > 2$, then *no* real Hadamard matrix of order d exists, and therefore no *pair* of real MU bases, in striking contrast to the complex case. Hadamard famously conjectured that if d is a multiple of four then a (real) Hadamard matrix exists [303], leading to the expectation that at least two real MU bases exist for $d = 4m$. However, general constructions of Hadamard matrices have been found only in certain dimensions, e.g. [176, 354], and the smallest matrix for which the conjecture remains unverified is of order 668.

When d is a *non-square* dimension of the form $d = 4m$, $m \in \mathbb{N}$, then at most two real MU bases exist [72]. Clearly, such pairs exist if and only if a real Hadamard matrix of order d exists. Now suppose that d is a square dimension divisible by four. If $d = 4s^2$ for any positive odd integer s , then a simple proof based on lattice lines shows that there exist at most three real MU bases. If $d = 4^k s^2$ with s any positive odd integer, and $k > 1$, then at least $(\ell + 2)$ real MU bases exist provided a real Hadamard of order $2^k s$ exists. Here, ℓ is the maximum number of MO Latin squares of order $2^k s$. This construction, found in [400], is discussed further in Sec. 6.9. Finally, for $d = 4^k$, one can apply connections to algebraic coding theory to construct the maximum number of $(d/2 + 1)$ real MU bases [92, 93]. It remains unknown if maximal numbers of MU bases in $\mathbb{R}^d$ exist when the dimension is not a power of four. For example, when $d = 144$, the construction from Ref. [400] finds only seven bases as opposed to the 73 that could hypothetically exist.

It is possible to establish an equivalence between MU bases in $\mathbb{R}^d$ and specific so-called “4-class cometric association schemes” as explained in Refs. [2, 249]. This observation leads to sets of $(d/2 + 1)$ real MU bases for $d = 4^k$, which are identical to those in [92, 93]. Furthermore, a relation between real MU bases and representations of finite groups of odd order is shown in [161].

This yields a set of $(d/q + 1)$ MU bases in $\mathbb{R}^d$, when $d = q^{2r}$, with q a power of 2 and r a positive integer, by finding a real orthogonal matrix of order q^{2r} , with multiplicative order $(d/q + 1)$, whose powers define the set of real MU bases. When $q = 2$ the upper bound of $(d/2 + 1)$ bases is reached. A proof is also given for the existence of a set of $(2k + 1)$ MU bases in $\mathbb{R}^d$ when $d = 2^{2k-1}$, by taking the real representation of an arbitrary group G of odd order $(2k + 1)$ for $k \geq 3$.

Other studies consider special classes of real Hadamard matrices, e.g. the Bush-type matrices (see Sec. 9.1) yield up to $(4n - 1)$ unbiased real Hadamard matrices when $d = 4n^2$, with even n [190, 223]. For $d > 2$, it is always possible to incorporate free parameters into any collection of real MU bases [162]. For a set of μ MU bases in $\mathbb{R}^d$, one can introduce no fewer than $(\mu - 1)d/2$ free parameters.

We conclude with an upper bound on the number μ of MU bases in a bipartite real vector space, which holds if every vector has a limited Schmidt rank. Corollary 6.5 in Sec. 6.8 provides a bound for bases of a complex Hilbert space $\mathbb{C}^{d_1} \otimes \mathbb{C}^{d_2}$ assuming the Schmidt rank of every vector is at most k , and $k < d_1 \leq d_2$. Under the same assumption on the ranks of the vectors in $\mathbb{R}^{d_1} \otimes \mathbb{R}^{d_2}$, a different bound on the number of MU bases is obtained [96], namely

$$\mu \leq \frac{k}{2} \left(\frac{d_1(d_1 + 1) - 2}{d_1 - k} \right). \quad (9.1)$$

The result follows from a modified version of Thm. 6.10, which limits the purity of a set of MU bases in $\mathbb{R}^d$ rather than $\mathbb{C}^d$. If $k = 1$, all states in each basis are separable, and the bound implies that at most $(d_1 + 2)/2$ real MU product bases exist.

9.2 Butson-type MU bases

As discussed in Sec. 6.1, a special class of $d \times d$ Hadamard matrices known as Butson-Hadamard matrices $BH(d, r)$ have matrix elements which are r -th roots of unity [90]. When $r = 2$, the matrices $BH(d, 2)$ are the real Hadamard matrices of Sec. 9.1; in all other cases, some matrix elements will have non-zero imaginary parts. As all matrix elements are taken from a finite set of complex numbers, searching for MU bases associated with Butson-Hadamard matrices is less

complicated than for general complex Hadamard matrices.

Well-studied examples include the Butson-Hadamard matrices $BH(d, 4)$ containing elements from the set $\{\pm 1, \pm i\}$, first considered in [375, 384]. Constructions appear in orders d where symmetric conference matrices exist, which require dimensions $d = 1 + a^2 + b^2$, with integers a and b . However, it is conjectured that they exist for every even d . If d is an odd integer, at most two unbiased matrices $BH(2d, 4)$ exist, while it is conjectured that pairs exist for all odd integers d when $2d$ is the sum of two squares. A computer search confirms this for $BH(10, 4)$ and $BH(18, 4)$ matrices [58]. An early computer search of all MU Butson-Hadamard matrices $BH(6, 12)$ with twelfth roots of unity was carried out in [49] (see Thm. 7.15 of Sec. 7.6).

Bush-type Butson-Hadamard matrices $BH(d^2, r)$ of square order can be divided into d blocks of order d , such that every block is either a matrix consisting of all ones or a matrix with each row and column summing to zero. It was shown that for every prime power $d \in \mathbb{PP}$, there exists an unextendible set of d MU Bush-type Butson-Hadamard matrices $BH(d^2, r)$ [58].

9.3 Quaternionic MU bases

Conceptually, the generalisation from the complex inner product space $\mathbb{C}^d$ to the quaternionic case $\mathbb{H}^d$ is straightforward. An upper limit on the number of MU bases is given by $(2d + 1)$, as shown by Chterental and Đoković [117] who adapt the proof based on the intersection of hyperplanes in the complex case described in Sec. 3.2 (cf. Refs. [50, 203]). For dimensions $d = 2^{n-2}$, an upper bound of $(2d + 1)d$ lines in $\mathbb{H}^d$ which are either orthogonal or intersect at an angle $\cos^{-1}(1/\sqrt{d})$ had already been found in 1982 [189, 251]. Examples of lines saturating this bound for $\mathbb{H}^2$ and $\mathbb{H}^4$, which correspond to complete sets of five and nine quaternionic MU bases, respectively, can be found in [189].

The five members of the complete set in $\mathbb{H}^2$ consist of the 2×2 identity $\mathbb{I}$ and four structurally simple matrices,

$$\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} 1 & 1 \\ \mathbf{a} & -\mathbf{a} \end{pmatrix}, \quad (9.2)$$

where $\mathbf{a} = \mathbf{i}, \mathbf{j}, \mathbf{k}$ are quaternions satisfying $\mathbf{i}^2 = \mathbf{j}^2 = \mathbf{k}^2 = \mathbf{ijk} = -1$; the common factor of $1/\sqrt{2}$ has been dropped. This complete set is unique up to equivalence [117].

In the space $\mathbb{H}^3$, a complete set consists of seven MU bases. All *triples* of MU bases in $\mathbb{H}^3$ have been identified in [117]; they necessarily contain (an equivalent of) the standard complex-valued Fourier matrix. The third basis can be chosen either from one three-parameter family or from one of five families depending on two parameters each. Furthermore, a *quadruple* of quaternionic MU bases depending on three real parameters has been identified. It is unextendible (see Sec. 6.10) and contains a one-parameter family which, in turn, has the complete set of four MU bases in $\mathbb{C}^3$ as a subset. No sets with more than four elements have been constructed, meaning that the (expected) complete set of seven MU bases for $d = 3$ remains elusive.

The existence of complete sets in general quaternionic spaces $\mathbb{H}^d$ with arbitrary dimension $d \in \mathbb{N}$, is, to our knowledge, an open question. However, in 1995, Kantor presented quaternionic line-sets in spaces of dimension $d = 2^{n-2}$, with n even, whose angles are either 90° or $\cos^{-1}(2^{-(n-2)/2})$ [214]. These sets translate into complete sets of $(2d + 1)$ MU bases in $\mathbb{H}^d$. This approach, in analogy with constructions of complete sets described in Appendix A.8 for $\mathbb{C}^d$, utilises symplectic spreads.

More recently, constructions of quaternionic Hadamard matrices of small orders—each such matrix giving rise to a pair of quaternionic MU bases—as well as infinite families of larger orders, have been found in [187] and [37], respectively. Quaternionic Hadamard matrices prove useful in connection to generalised unbiasedness (see Sec. 9.12).

Quaternionic extensions of tight frames (cf. Sec. 3.9), equiangular lines, and t -designs, have also been studied [382, 383]. A maximal set of equiangular lines in $\mathbb{C}^d$ consists of d^2 vectors and defines a SIC, while in $\mathbb{H}^d$ there are at most $(2d^2 - d)$ equiangular lines. Thus, for $d = 2$, six such lines may exist for $\mathbb{H}^2$ that, in fact, have been described explicitly [224]. The allowed maximum number of equiangular lines in $\mathbb{H}^d$ is conjectured to exist for every finite d [382], in analogy with SICs in $\mathbb{C}^d$.

It is worth pointing out that, obviously, each set of MU bases in $\mathbb{C}^d$ also can be thought of as a set in the space $\mathbb{H}^d$. Consequently, the known complete sets of $(d + 1)$ MU bases in prime-power dimensions define sets in $\mathbb{H}^d$ which are, however, still d bases away from a complete set.

9.4 MU bases over finite fields

The definition of mutually unbiased bases extends naturally to vector spaces over finite fields, as shown by McConnell *et al.* [280]. Let F^d denote a d -dimensional vector space over a finite field F with a characteristic not dividing $2d$. For $u = (u_j), v = (v_j) \in F^d$, a Hermitian form is defined as $\langle u|v \rangle = \sum_{j=1}^d u_j^\sigma v_j$, where σ denotes the automorphic involution of F which leaves invariant a subfield K contained in F . Pairs of (normalised) vectors $u, v \in F^d$ are mutually unbiased if the identity $\langle u|v \rangle \langle u|v \rangle^\sigma = 1/d$ holds. As in the case of real or complex number fields, orthonormal bases are mutually unbiased if every pair of vectors taken from different bases satisfy the identity just given. The infinite-dimensional equivalent of this generalisation corresponds to p -adic MU bases [425] considered in Sec. 9.14.

It is possible to bound the cardinality of the largest set of MU bases in F^d . For any quadratic extension of F/K and $d > 2$ coprime to the characteristic p of K , the maximum number μ of MU bases in F^d satisfies $1 \leq \mu \leq d + 1$. Interestingly, three MU bases in F^d do not always exist, in contrast to the case of $\mathbb{C}^d$. However, for prime powers $d \in \mathbb{PP}$, complete sets of $(d + 1)$ MU bases in F^d exist for many fields F , as described in [280].

The properties of MU bases over finite fields in a vector space of dimension $d = 6$ can be considered as partial evidence both *for* and *against* Conjecture 1.1. For prime powers $q = p^r \in [5, 41]$, there exist at most three MU bases in F^6 when $F = \mathbb{F}_{q^2}$. However, for some values $q \equiv 5 \pmod{12}$ there exist three MU bases in F^6 together with four orthonormal vectors that are mutually unbiased to the triple [280]. In contrast, all known MU triples in $\mathbb{C}^6$ appear to be strongly unextendible, i.e. no vector unbiased to three MU bases has been found (cf. Sec. 7). This situation may represent a "shadow" [280] of an original (unknown) set of MU bases in $\mathbb{C}^6$, mirroring a phenomenon that has been observed for SIC-POVMs.

Extensions to finite fields have also been considered for other discrete structures in Hilbert space. For example, Greaves *et al.* [169] study equiangular lines as well as frames (see Sec. 3.9 and Sec. 9.11) over finite fields.

9.5 Weak MU bases

A attempt to allow for overlaps other than the standard ones between vectors in Def. 1.1 has been proposed for composite dimensions $d \notin \mathbb{P}$ in Ref. [339]. Suppose $d = d_1 \dots d_r$ is a particular factorisation of the Hilbert space dimension d . Then, a pair of orthonormal bases $\mathcal{B}_b = \{|v_b\rangle\}$ and $\mathcal{B}_{b'} = \{|v'_{b'}\rangle\}$ are weak MU bases if either $|\langle v_b | v'_{b'} \rangle|^2 = \frac{1}{d}$ for all v and v' , or $|\langle v_b | v'_{b'} \rangle|^2 \in \{\frac{1}{d_j}, 0\}$ for a given d_j ($\neq 1, d$) and all v and v' .

For an explicit example of the modification, consider the case when $d = p_1 p_2$ with both p_1 and p_2 prime. Then a pair of bases $\mathcal{B}_b = \{|v_b\rangle\}$ and $\mathcal{B}_{b'} = \{|v'_{b'}\rangle\}$, with $v, v' = 1, \dots, d$, of the space $\mathbb{C}^{p_1} \otimes \mathbb{C}^{p_2}$ are *weakly* MU if their overlap is either (i) standard: $|\langle v_b | v'_{b'} \rangle|^2 = 1/d \quad \forall v, v'$, or one of the conditions

$$(ii) \quad |\langle v_b | v'_{b'} \rangle|^2 = \begin{cases} 1/p_1 & v \equiv v' \pmod{p_2}, \\ 0 & \text{otherwise;} \end{cases} \quad (9.3)$$

$$(iii) \quad |\langle v_b | v'_{b'} \rangle|^2 = \begin{cases} 1/p_2 & v \equiv v' \pmod{p_1}, \\ 0 & \text{otherwise} \end{cases} \quad (9.4)$$

holds. A set of bases $\mathcal{B}_0, \dots, \mathcal{B}_{\mu-1}$, are weak MU bases if every pair satisfies one of the constraints (i)–(iii). For example, suppose $\mathcal{B}_0^{(2)}, \mathcal{B}_1^{(2)}, \mathcal{B}_2^{(2)}$ and $\mathcal{B}_0^{(3)}, \mathcal{B}_1^{(3)}, \mathcal{B}_2^{(3)}, \mathcal{B}_3^{(3)}$ are complete sets of MU bases in $\mathbb{C}^2$ and $\mathbb{C}^3$, respectively. We can construct 12 weak MU product bases $\mathcal{B}_{j_1}^{(2)} \otimes \mathcal{B}_{j_2}^{(3)}$ by using all combinations of the labels $j_1 = 0, 1, 2$, and $j_2 = 0, 1, 2, 3$.

Thm. IV.2 of [339] states that any set of weak MU bases of dimension $d = d_1 d_2$ take the form $\mathcal{B}_{j_1}^{(d_1)} \otimes \mathcal{B}_{j_2}^{(d_2)}$, where $\mathcal{B}_{j_1}^{(d_1)}$ and $\mathcal{B}_{j_2}^{(d_2)}$ are MU bases in $\mathbb{C}^{d_1}$ and $\mathbb{C}^{d_2}$, respectively, and that the maximal number of weak MU bases is $(d_1 + 1)(d_2 + 1)$. The proof makes the assumption that all product bases in composite dimensions can be written as a direct product. However, *indirect* product bases (cf. Sec. 7.4) can also be used to construct weak MU bases: for $d = 6$ the pair $\mathcal{B}_0^{(2)} \otimes \mathcal{B}_0^{(3)}$ and $\{|0\rangle \otimes \mathcal{B}_1^{(3)}, |1\rangle \otimes \mathcal{B}_2^{(3)}\}$ are weak MU bases but not covered by Thm. IV.2; here $\mathcal{B}_0^{(2)}$ and $\mathcal{B}_0^{(3)}$ are the

standard bases of $\mathbb{C}^2$ and $\mathbb{C}^3$, respectively. Thus, the general structure of weak MU bases and their maximal number is still unknown.

9.6 Approximately MU bases

Another approach to introduce bases with overlaps similar to MU bases are the so-called *approximately* mutually unbiased bases, defined by the asymptotic behaviour of their inner products. The idea, introduced by Klappenecker *et al.* [228], is to construct a system of $(d+1)$ orthonormal bases of $\mathbb{C}^d$ which satisfies the inequality

$$|\langle v_b | v'_{b'} \rangle|^2 \leq \frac{1 + o(1)}{d}, \quad (9.5)$$

for all v, v' and $b \neq b'$. The o -notation $f(d) = o(g(d))$ implies that for *any* positive constant c , there exists a constant $d_0 > 0$ such that $0 < f(d) < cg(d)$ for all $d \geq d_0$, i.e., the ratio $f(d)/g(d)$ approaches zero in the limit of increasing dimension, $d \rightarrow \infty$.

A construction of sets of bases which exhibit asymptotic bounds of this type is provided in [228]. To begin, for arbitrary dimension d , and any positive integer n , they construct a set of $(d^n + 1)$ orthonormal bases from exponential sums, where the constant overlap property of Def. 1.1 is modified such that the inner product of any two vectors from different bases becomes $O(d^{-1/4})$. When $n = 1$, the upper bound can be improved to $O(d^{-1/3})$. Here, the O -notation $f(d) = O(g(d))$ implies that there exist positive constants c and d_0 such that $0 < f(d) \leq cg(d)$ for all $d \geq d_0$, hence there exists $c > 0$ such that the inner product $|\langle v_b | v'_{b'} \rangle| \leq cd^{-1/3}$ for all $d \geq d_0$. Note that the two asymptotic bounds can differ since the O -notation may or may not lead to asymptotically tight bounds while the o -notation is compatible with an upper bound that is not tight.

Explicitly, the $(d+1)$ asymptotically MU bases consist of the standard basis $\mathcal{B}_0$ together with the bases $\mathcal{B}_b = \{|v_b\rangle\}_{v=0}^{d-1}$, $b = 1, \dots, d$, with orthonormal vectors

$$|v_b\rangle = \frac{1}{\sqrt{d}} \sum_{k=0}^{d-1} e^{2\pi i b k^2 / p} e^{2\pi i v k / d} |k\rangle. \quad (9.6)$$

In a related paper it is shown that the bound $O(d^{-1/3})$ for the inner products may be strengthened to $O(d^{-1/2}(\log d)^{1/2})$ [342].

When p is the smallest prime such that $p \equiv 1 \pmod d$ for a given dimension d , the construction described in Ref. [228] can be improved by using multiplicative and mixed character sums, to provide a set of $(d^n + 1)$ orthonormal bases satisfying

$$|\langle v_b | v_{b'} \rangle|^2 \leq \frac{np^{1/2}}{d}. \quad (9.7)$$

If $p = d + 1$, this construction gives a set of $(d + 1)$ approximately MU bases satisfying Eq. (9.5). In fact, the bound given in Eq. (9.7) improves to $O(d^{-1/2} \log d)$ if one relies on a widely believed conjecture on the distribution of primes in arithmetic progressions.

A different construction with an overlap bound of $O(d^{-1/2})$ was given in [342] for almost all d , based on elliptic curves. An extension to all dimensions d exists if one assumes Cramér's conjecture which provides an estimate for the gap size between consecutive prime numbers. Two further constructions based on mixed character sums of functions over finite fields yield sets of $(d + 1)$ and $(d + 2)$ approximately MU bases when $d = p - 1$, for p a prime-power [385].

A construction of up to $\sqrt{d} + 1$ approximately MU bases for $d = q^2$, where q is a positive integer, is presented in [242]. If $q \equiv 0 \pmod 4$, and a $q \times q$ real Hadamard matrix exists, the construction gives rise to approximately real MU bases (cf. Sec. 9.1).

Almost perfect MU bases [243] represent another modification of *approximately* MU bases. Given a set of vectors, a restriction is placed on the magnitudes of all inner products: they are allowed to take only two values. The resulting vectors contain a large number of components equal to zero, and every non-zero component is of equal magnitude.

9.7 Approximate 2-designs

Let us now turn to a modification of mutual unbiasedness by Ambainis and Emerson [10] which involves revising the design property of complete sets explained in Sec. 5.11. *Approximate* complex-projective t -designs are defined in the following way [10]:

Definition 9.1. Let $\mathcal{D} = \{x : x \in \mathbb{C}P^{d-1}\}$ be a finite subset of $\mathbb{C}P^{d-1}$ and a 1-design. Then $\mathcal{D}$ is

an ϵ -approximate t -design if for all $f \in \text{Hom}(t, t)$,

$$(1 - \epsilon) \int_{\mathbb{C}P^{d-1}} f(x) d\nu(x) \leq \frac{1}{|\mathcal{D}|} \sum_{x \in \mathcal{D}} f(x) \quad (9.8)$$

$$\leq (1 + \epsilon) \int_{\mathbb{C}P^{d-1}} f(x) d\nu(x).$$

where the integral is evaluated over the unitarily invariant Haar measure ν on the unit sphere in $\mathbb{C}^d$.

The above inequalities clearly relax the identity (5.16) valid for standard t -designs. It is known that for $d \geq 2t$, there exists an $O(d^{-1/3})$ -approximate t -design such that $|\mathcal{D}| = O(d^{3t})$ [10] (see Sec. 9.6 for the definition of the O -notation). Hence, there exists an $O(d^{-1/3})$ -approximate 2-design containing $O(d^6)$ elements for $d \geq 4$.

Since we are interested in finding bases, it makes sense for the ϵ -approximate 2-design $\mathcal{D} \subset \mathbb{C}P^{d-1}$ to be the union of a set of orthonormal bases $\mathcal{B}_b = \{|v_b\rangle\}_{v=0}^{d-1} \subset \mathbb{C}^d$, with $b = 0, \dots, \mu - 1$. Approximate 2-designs of this type were considered in relation to cyclic 2-designs [22]. These designs, composed of sets of bases, generalise cyclic MU bases—i.e. MU bases generated from the powers of a single unitary (cf. Appendix A.8)—which appear only to exist in even prime-power dimensions.

To our knowledge, the construction of minimal sets of bases which form an approximate 2-design, for arbitrary dimension d , remains an open problem.

9.8 Weighted 2-designs

Complex projective t -designs (defined in Sec. 5.11) can be generalised by adding a normalised positive-valued weight function to the finite set $\mathcal{D} \subset \mathbb{C}P^{d-1}$.

Definition 9.2. Let $\mathcal{D} = \{x : x \in \mathbb{C}P^{d-1}\}$ be a finite subset of $\mathbb{C}P^{d-1}$, and $w : \mathcal{D} \rightarrow [0, 1]$ a normalised weight function. Then $(\mathcal{D}, w)$ is a weighted complex projective t -design if for all $f \in \text{Hom}(t, t)$,

$$\sum_{x \in \mathcal{D}} w(x) f(x) = \int_{\mathbb{C}P^{d-1}} f(x) d\nu(x), \quad (9.9)$$

where the integral is evaluated over the unitarily invariant Haar measure ν on the unit sphere in $\mathbb{C}^d$.

This relation generalises Eq. (5.16). Equivalently, and in analogy to Eqs. (5.17), a weighted t -design $(\mathcal{D}, w)$ is a subset of $\mathbb{C}P^{d-1}$ which satisfies

$$\begin{aligned} \sum_{x \in \mathcal{D}} w(x) P(x)^{\otimes t} &= \int_{\mathbb{C}P^{d-1}} P(x)^{\otimes t} d\nu(x) \\ &= \binom{d+t-1}{t}^{-1} \Pi_{\text{sym}}^{(t)}, \end{aligned} \quad (9.10)$$

where $P(x) = |x\rangle\langle x|$ is the projection operator associated with $x \in \mathbb{C}P^{d-1}$, and $\Pi_{\text{sym}}^{(t)}$ is the projector onto the symmetric subspace of $(\mathbb{C}^d)^{\otimes t}$. As seen in Sec. 5.11, (unweighted) t -designs exist for all choices of t and d .

Since a complete set of MU bases forms a complex projective 2-design consisting of $(d+1)$ orthogonal bases (each contributing equally), one way to generalise sets of MU bases is to consider a *weighted* 2-design formed from the union of a set of orthonormal bases in $\mathbb{C}^d$. Suppose we have a set of μ orthonormal bases $\mathcal{B}_0, \dots, \mathcal{B}_{\mu-1} \subset \mathbb{C}P^{d-1}$, such that $\mathcal{B}_b = \{|v_b\rangle\}_{v=0}^{d-1}$, and an associated weight w_b assigned to each basis. Then the weight function together with the set $\mathcal{D} = \cup_b \mathcal{B}_b$ forms a 2-design if

$$\sum_{b=0}^{\mu-1} w_b \sum_{v=0}^{d-1} P_b(v)^{\otimes 2} = \binom{d+1}{2}^{-1} \Pi_{\text{sym}}^{(2)}, \quad (9.11)$$

where $P_b(v) = |v_b\rangle\langle v_b|$. This holds only if $\mu \geq d+1$, with equality when the bases are mutually unbiased [322].

Provided μ is sufficiently large, weighted 2-designs from bases exist in all dimensions d [322, 337]. The construction is based on highly non-linear functions on Abelian groups. For prime-power dimensions $d = p^n$, there exist maximally nonlinear functions which generate a 2-design containing the minimal $\mu = d+1$ orthonormal bases [322]. When $d = p^n - 1$, this technique is used to generate a 2-design with $\mu = d+2$. Let $\mathcal{B}_0$ be the standard basis of $\mathbb{C}^d$ with corresponding weight

$$w_0 = \frac{1}{d(d+1)}. \quad (9.12)$$

For the remaining $(\mu-1)$ bases, the v -th vector of basis $\mathcal{B}_b$, $b = 1 \dots d+1$, is defined as

$$|v_b\rangle = \frac{1}{\sqrt{d}} \sum_{k=0}^{d-1} e^{2\pi i v k / d} e^{2\pi i \text{Tr}[b y^k] / p} |k\rangle, \quad (9.13)$$

where the trace function is $\text{Tr}[x] = x + x^p + \dots + x^{p^{n-1}}$, and y is a primitive element of $\mathbb{F}_{d+1}$. The weight assigned to the basis $\mathcal{B}_b$ is given by

$$w_b = \frac{1}{(\mu-1)(d+1)}, \quad b = 1 \dots d+1, \quad (9.14)$$

and the overlaps between elements of different bases read

$$|\langle v_b | v'_{b'} \rangle|^2 = \begin{cases} \frac{1}{d^2} & \text{if } b \neq b', v \neq v', \\ \frac{d+1}{d^2} & \text{if } b \neq b', v = v'. \end{cases} \quad (9.15)$$

Weighted 2-designs of this type provide a good generalisation for MU bases in quantum tomography as they yield an optimal approach for quantum state reconstruction (see Sec. 4.1).

9.9 MU measurements and conical 2-designs

Another natural generalisation of MU bases relaxes the rank-one restriction on the projection operators $P_b(v) = |v_b\rangle\langle v_b|$ from the bases $\mathcal{B}_b = \{|v_b\rangle\}$. Suppose that for each b , $M_b = \{M_b(v) : v = 0 \dots d-1\}$ is a d -outcome POVM on the space $\mathbb{C}^d$ such that $\text{Tr}[M_b(v)] = 1$, for all v . A suitable modification of the fundamental conditions (1.3) leads to one-parameter-families of sets of *MU measurements*.

Definition 9.3. A collection of μ POVMs M_b , with $b = 0, \dots, \mu-1$, forms a set of μ *MU measurements* if $\text{Tr}[M_b(v)M_{b'}(v')] = 1/d$ for $b \neq b'$, and

$$\text{Tr}[M_b(v)M_{b'}(v')] = \kappa \delta_{v,v'} + (1 - \delta_{v,v'}) \frac{1 - \kappa}{d-1}, \quad (9.16)$$

for $b = b'$, with $v, v' = 0 \dots d-1$ and $1/d < \kappa \leq 1$.

When $\kappa = 1$ the condition is equivalent to the definition of MU bases since the operators $M_b(v)$ become rank-one projectors. However, for $\kappa < 1$ we obtain a new set of measurements such that the inner product between any two elements from a single POVM depends on the parameter κ , while the inner product between any elements from a pair of POVMs have the overlap $1/d$. The value κ determines how close the POVM elements are to rank-one projectors.

A set of $(d+1)$ MU measurements $M_b = \{M_b(v) : v = 0 \dots d-1\}$ has been constructed in Ref. [210]. Let $F_{v,b}$ be the $d(d+1)$ elements of the

generalised Gell-Mann operator basis of bounded operators on the Hilbert space $\mathbb{C}^d$, and define

$$F_b(v) = \begin{cases} (1 + \sqrt{d})F_b & \text{for } v = d, \\ F_b - (d + \sqrt{d})F_{v,b} & \text{otherwise,} \end{cases} \quad (9.17)$$

where $F_b = \sum_{v=1}^{d-1} F_{v,b}$. The operators $M_b(v) = \mathbb{I}/d + tF_b(v)$, with t chosen such that $M_b(v) \geq 0$, define a set of MU measurements for arbitrary d when $\kappa = 1/d + 2/d^2$. Note that while MU measurements exist for any d , if one initially fixes κ , their existence is not guaranteed.

Since MU measurements share many features with MU bases, they are useful for applications such as entanglement detection [106, 252, 317, 325], especially in composite dimensions $d \notin \mathbb{PP}$ where complete sets are not known.

Mutually unbiased measurements are examples of conical 2-designs [168] which generalise complex projective 2-designs by dropping the restriction on the rank of the projection operators. As we have seen in Sec. 5.11, a complex projective 2-design $\mathcal{D}$ is a finite set of rank-one projection operators $P(x) = |x\rangle\langle x|$ such that $\sum_{x \in \mathcal{D}} P(x) \otimes P(x)$ is proportional to the symmetric projection Π_{sym} onto $\mathbb{C}^d \otimes \mathbb{C}^d$. Allowing for asymmetric projections leads to the definition of conical 2-designs.

Definition 9.4. A *conical 2-design* is a finite set $\mathcal{D} = \{M(x) : x = 1, \dots, n\}$ of positive semi-definite operators such that

$$\sum_{x=1}^n M(x) \otimes M(x) = k_s \Pi_{\text{sym}} + k_a \Pi_{\text{asym}}, \quad (9.18)$$

where $k_s > k_a \geq 0$, and $\Pi_{\text{sym}}, \Pi_{\text{asym}}$ are the symmetric and antisymmetric projectors onto $\mathbb{C}^d \otimes \mathbb{C}^d$.

Both conical and complex projective 2-designs are sets of projection operators such that their linear combinations $\sum_x M(x) \otimes M(x)$ commute with $U \otimes U$ for all unitary operators U . The weighted complex projective 2-designs discussed in Sec. 9.8 form a subset of conical 2-designs if the parameter k_a takes the value zero. In fact, $k_a = 0$ holds if and only if all projectors are rank-one. In addition to mutually unbiased measurements, arbitrary-rank symmetric informationally complete measurements also form conical 2-designs [16]. Another class of generalised designs, called *mixed 2-designs* were introduced

in Ref. [74] and they also contain MU measurements as a subclass. Mixed designs of finite cardinality form a subset of the homogeneous conical 2-designs [168].

9.10 MU POVMs

Beneduci *et al.* [47] generalised the definition of MU bases to POVMs. This notion of unbiasedness is more general than the definition of MU measurements from Sec. 9.9.

Definition 9.5. A pair of d -outcome POVMs $M = \{M(i)\}_{i=1}^d$ and $N = \{N(j)\}_{j=1}^d$ acting on a d dimensional Hilbert space $\mathcal{H}$ are called *mutually unbiased* if

$$\text{Tr}[M(i)N(j)] = 1/d, \quad i, j = 1, \dots, d. \quad (9.19)$$

Mutually unbiased POVMs shed some light on the connection between SICs (cf. Sec. 3.9) and MU bases. For instance, MU POVMs arise as marginals of a SIC (cf. Sec. 3.4), and any SIC is, in fact, a joint measurement of at least three and at most $(d+1)$ mutually unbiased POVMs [47]. Given a set of $(d-1)$ pairwise mutually orthogonal Latin squares of order d (cf. Appendix C), a SIC yields $(d+1)$ mutually unbiased POVMs as marginals. If the resulting POVMs are *commutative*, e.g. the elements of $M(i)$ pairwise commute, it is possible to construct a system of MU bases. In particular, mutually unbiased POVMs are smearings of MU bases.

9.11 MU frames

Pérez *et al.* [314] generalised the concept of unbiasedness to finite frames (cf. Sec. 3.9).

Definition 9.6. A pair of frames $\{|\phi_i\rangle\}_{i=1}^{m_1}$ and $\{|\psi_j\rangle\}_{j=1}^{m_2}$ in a d dimensional Hilbert space $\mathcal{H}$ are called *mutually unbiased frames* if there exists $c > 0$ such that

$$|\langle \phi_i | \psi_j \rangle|^2 = c, \quad (9.20)$$

for $i = 1, \dots, m_1$ and $j = 1, \dots, m_2$.

Sets of pairwise mutually unbiased frames include MU bases and SICs, as well as mutually unbiased rank-one POVMs. If at least one of the frames is tight, i.e. the projections onto the frame elements sum to a multiple of the identity, the overlap takes the value $c = 1/d$. Hence, mutually unbiased tight frames satisfy Eq. (9.19) and correspond to the MU-POVMs of Sec. 9.10.

The notion of MU frames covers other extensions of unbiasedness, including MU equiangular tight frames [145] and MU regular simplices [146]. An equiangular tight frame in the space $\mathbb{C}^d$ is a collection of $m \geq d$ vectors which have constant overlap (e.g. a SIC), and a regular simplex is an equiangular tight frame with $m = d + 1$. For equiangular tight frames with m vectors in $\mathbb{C}^d$, the number μ of pairwise mutually unbiased equiangular tight frames satisfies

$$\mu \leq \left\lfloor \frac{d^2 - 1}{m - 1} \right\rfloor. \quad (9.21)$$

This reproduces previously derived bounds for MU bases and MU regular simplices when $m = d$ and $m = d + 1$, respectively. MU equiangular tight frames have also been applied to construct equiangular tight frames in composite dimensions [145].

9.12 Generalised unbiasedness

In the context of Bell inequalities (see Sec. 3.11), a notion of unbiasedness was introduced which imposes no constraints on the dimension of the Hilbert space and fixes only the number of measurement outcomes [366]. Although this definition differs from the one given in Sec. 9.9, both share the same name.

Definition 9.7. Two d -outcome POVMs $M = \{M(i)\}_{i=1}^d$ and $N = \{N(j)\}_{j=1}^d$, acting on a Hilbert space $\mathcal{H}$ (not necessarily of dimension d), are called *mutually unbiased measurements* (MUMs) if

$$\begin{aligned} M(i) &= d M(i) N(j) M(i), \\ N(j) &= d N(j) M(i) N(j), \end{aligned} \quad (9.22)$$

for all $i, j = 1, \dots, d$.

Here, the dimension of the Hilbert space $\mathcal{H}$ is undefined, but the notion of complementarity remains a key feature. The formulation is linked to a class of tailor-made Bell inequalities that are maximally violated by MU bases. Introducing MUMs ensures that the inequalities are *only* maximally violated by this class of measurements and, hence, provides a means of self-testing. A similar modification—removing the fixed dimension of the Hilbert space and only requiring d^2 outcomes—has been made for SIC-POVMs [366].

The structure and properties of MUMs as well as their construction have been studied extensively in [140]. It is clear that both MU bases and direct sums of MU bases provide examples of MUMs. Other distinct examples have been constructed, including a method based on quaternionic Hadamard matrices. A fundamental difference between MU bases and MUMs is the existence of an unbounded number of pairwise d -outcome measurements satisfying Eq. (9.22).

9.13 MU bases for continuous variables

Mutually unbiased bases in an infinite-dimensional Hilbert space emerge naturally for position and momentum observables of quantum particles (cf. Sec. 1.1) which are known as (a pair of) “continuous variables” [75]. Only a few results have been obtained for composite systems; they will be described after discussing the case of a single continuous variable.

Consider two different bases $\mathcal{B}_r = \{|r\rangle, r \in I\}$ and $\mathcal{B}_s = \{|s\rangle, s \in I\}$ of the Hilbert space $\mathcal{H} = L^2(I)$, with some interval $I \subseteq \mathbb{R}$. The bases consist of (generalised) states which satisfy orthonormality conditions expressed in terms of Dirac delta functions, i.e. $\langle r|r'\rangle \propto \delta(r - r')$, $r, r' \in I$, and $\langle s|s'\rangle \propto \delta(s - s')$, $s, s' \in I$, must hold. The labels of the states vary over a *continuous* range, and the interval $I \subseteq \mathbb{R}$ may be infinitely large. The bases are mutually unbiased if the *transition probability densities* for all pairs of vectors $|r\rangle \in \mathcal{B}_r$ and $|s\rangle \in \mathcal{B}_s$ equal some constant, i.e. $|\langle r|s\rangle|^2 = \kappa > 0$. The best-known examples of such sets of states are the generalised eigenstates of position or momentum for the space, with $I = \mathbb{R}$. According to Eq. (1.1), the constant overlaps guarantee that the probabilities $\text{prob}(r, dr)$ and $\text{prob}(s, ds)$ to find outcomes near r and s , initially given $|s\rangle$ and $|r\rangle$, respectively, are all equal.

MU bases can be defined either directly in the setting of an infinite-dimensional Hilbert space or by constructing them through a limiting procedure of a d -dimensional Hilbert space and taking the limit of $d \rightarrow \infty$. The second approach has been carried out in considerable detail in [133].

The state space $L^2(\mathbb{R})$ of a quantum particle hosts, in fact, not only pairs of MU bases associated with the position operator $\hat{q}$ and the momentum operator $\hat{p}$. All rotated position observables $\hat{q}_\theta = \hat{q} \cos \theta + \hat{p} \sin \theta$, $\theta \in [0, \pi)$, possess

complete sets of (generalised) eigenstates. The overlap of two states $|q_\theta\rangle$ with $|q_{\theta'}\rangle$ associated with the bases $\mathcal{B}_\theta$ and $\mathcal{B}_{\theta'}$, respectively, can be calculated from their Wigner functions [390],

$$|\langle q_\theta | q_{\theta'} \rangle|^2 = \frac{1}{2\pi\hbar |\sin(\theta - \theta')|}. \quad (9.23)$$

Since the overlap only depends on the angles θ and θ' (i.e. the chosen pair of bases) but not on the values q_θ and $q_{\theta'}$, the bases $\mathcal{B}_\theta$ and $\mathcal{B}_{\theta'}$ are mutually unbiased. This property of the rotated position bases has been noticed previously, for example in [70], where the mean-king problem (cf. Sec. 4.5) is formulated and solved in the continuous-variable setting. The fact that the overlap can vary as a function of the difference $(\theta - \theta')$, i.e. the pair of bases considered, represents a new feature of the continuous-variable case. In finite-dimensional spaces, the overlap of MU bases cannot vary from one pair to the next since, for given dimension d , a specific fixed value is required for consistency.

As an immediate consequence of Eq. (9.23) we are now presented with two possibilities when looking for *sets* of MU bases; both choices have their merits. If we allow for *basis-dependent* overlaps, then a *continuous* family of MU bases $\mathcal{B}_\theta$, $\theta \in [0, \pi)$ in the space $L^2(\mathbb{R})$ [390] exists. This situation is natural in the sense that the number of MU bases in prime-power dimensions increases without bound. In addition, the MU bases of Heisenberg-Weyl type in finite-dimensional systems, for ever larger dimensions d , have been shown to approach the MU bases $\mathcal{B}_\theta$, $\theta \in [0, \pi)$ for a particle moving on a line [133]. Taking the limit is, however, a rather subtle affair since the density of prime-powers among all integers approaches zero for $d \rightarrow \infty$ according to Eq. (2.4).

Alternatively, one may decide to only consider sets of MU bases with *basis-independent* pairwise overlaps, just as in the finite-dimensional case where this property is the only option. In other words, we require all overlaps to take a single value only. This stronger condition leaves us with a maximum of *three* MU bases among the set $\mathcal{B}_\theta$, $\theta \in [0, \pi)$ (cf. below). In both cases, the link between sets of MU bases and non-redundant quantum tomography seems to be broken: three MU bases are not tomographically complete for arbitrary quantum states while measurements associated with a continuous family of MU bases will be overcomplete, i.e. they contain redundant

information. A suitably chosen countable subset, however, might represent the most appropriate equivalent of a complete set of MU bases in a finite-dimensional space.

A *symmetric* triple of MU bases [390] is given by the set $\{\mathcal{B}_0, \mathcal{B}_{2\pi/3}, \mathcal{B}_{4\pi/3}\}$ where $\mathcal{B}_0$ is the basis of position eigenstates $|q\rangle$, $q \in \mathbb{R}$, and two other bases associated with the observables $\hat{q}_\pm = \hat{q} \cos(2\pi/3) \pm \hat{p} \sin(2\pi/3)$, obtained by three-fold rotations of the position operator. Denoting their eigenstates by $|q_\pm\rangle$, $q_\pm \in \mathbb{R}$, the second basis is given by $\mathcal{B}_{2\pi/3} \equiv \mathcal{B}_+ = \{|q_+\rangle, q_+ \in \mathbb{R}\}$, and we define $\mathcal{B}_{4\pi/3} \equiv \mathcal{B}_-$ in a similar way. The observables $\hat{p}$ and $\hat{q}_\pm$ are (non-unitarily) equivalent to the *asymmetric* set of operators $\hat{q}$, $\hat{p}$ and $\hat{r} = -\hat{q} - \hat{p}$ which have the advantage of being “equi-commutant” [221], in the sense that

$$[\hat{p}, \hat{q}] = [\hat{q}, \hat{r}] = [\hat{r}, \hat{p}] = \frac{\hbar}{i}. \quad (9.24)$$

The *Schrödinger triple* $(\hat{p}, \hat{q}, \hat{r})$ is a *maximal* set of equi-commutant observables and is *unique* (up to unitary transformations). First, assume that another observable $\hat{r}' \neq \hat{r}$ exists which equi-commutes with both $\hat{p}$ and $\hat{q}$, i.e. we have

$$[\hat{q}, \hat{r}'] = [\hat{r}', \hat{p}] = \frac{\hbar}{i}, \quad (9.25)$$

in analogy to Eq. (9.24). It follows immediately that the operator $(\hat{r}' - \hat{r})$ commutes with both generators of the Heisenberg algebra but the only Hermitian operators with this property are multiples of the identity so that

$$\hat{r}' = \hat{r} + c\hat{I}, \quad c \in \mathbb{R}. \quad (9.26)$$

Thus, discounting the irrelevant constant shift, there is no observable other than $\hat{r}$ which equi-commutes to $\hbar/i$ with both position and momentum.

The *uniqueness* of the Schrödinger triple $(\hat{p}, \hat{q}, \hat{r})$ follows from the fact that all irreducible representations of equi-commutant triples are unitarily equivalent. This result is a consequence of the theorem by *Stone* and *von Neumann* stating that (under some mild conditions) all irreducible representations of the canonical commutation relation $[\hat{p}, \hat{q}] = \hbar/i$ are unitarily equivalent [426]. Now assume that we have three observables $(\hat{P}, \hat{Q}, \hat{R})$ satisfying the relations (9.24) and that an irreducible representation of these relations on the space $L^2(\mathbb{R})$ is

given. Consequently, we have an irreducible representation of two observables with a canonical commutator, $[\hat{P}, \hat{Q}] = \hbar/i$. However, due to the Stone-von Neumann theorem, there exists a unitary operator $\hat{U}$ which maps this representation to the one we have used to initially represent the particle's position and momentum, i.e. we conclude

$$\hat{P} = \hat{U}\hat{p}\hat{U}^\dagger, \text{ and } \hat{Q} = \hat{U}\hat{q}\hat{U}^\dagger. \quad (9.27)$$

This relation leads to

$$[\hat{p}, \hat{q}] = [\hat{q}, \hat{R}'] = [\hat{R}', \hat{p}] = \frac{\hbar}{i}, \quad (9.28)$$

where $\hat{R}' \equiv \hat{U}^\dagger \hat{R} \hat{U}$. However, as shown before, the only observable equi-commutant to $\hbar/i$ with position $\hat{q}$ and momentum $\hat{p}$ is given by $\hat{R}' \equiv \hat{r}$, leading to

$$\hat{R} = \hat{U}\hat{r}\hat{U}^\dagger. \quad (9.29)$$

Combining this result with Eqs. (9.27) establishes the unitary equivalence of the triples $(\hat{P}, \hat{Q}, \hat{R})$ and $(\hat{p}, \hat{q}, \hat{r})$, i.e. the essential uniqueness of triples equi-commutant to $\hbar/i$. Therefore, no more than three MU bases can indeed be associated with a set of three equi-commutant observables, and these triples are all unitarily equivalent.

The argument just given is not strong enough to limit the number of MU bases for continuous variables with basis-independent overlaps to three; other constructions may exist, unrelated to equi-commutant operators. Interestingly, the situation changes if one replaces the real numbers $\mathbb{R}$ by the p -adic numbers $\mathbb{Q}_p$ since the space $L(\mathbb{Q}_p)$ is known to support $(p+1)$ MU bases (see Sec. 9.14).

MU bases for other continuous degrees of freedom have been introduced as well. For both motion on a half-line and a finite line segment, continuously many pairs of MU bases exist [133], each containing subsets of three bases with basis-independent overlaps.

The quantum mechanical rotor, i.e. motion on a circle, poses an unexpected challenge. The basis associated with a shift of the discretised angular momentum states (which obey a Kronecker-delta type normalisation) and the basis associated with the continuous rotations of the azimuthal position (with a Dirac-delta type normalisation) are mutually unbiased. However, this pair of bases is *strongly* unextendible (cf. Sec. 6.10): not a single

state MU to both of them can be constructed, seemingly due to the different normalisation conditions [133]. In stark contrast, no pair of MU bases in finite dimensions is strongly unextendible: one can always find at least one vector MU to any two bases (Cor. 6.3). Guided by the fact that Hilbert spaces with countably infinite dimensions are isomorphic, two different continuous sets of triples of MU bases have, however, been identified for the quantum rotor [265].

In composite systems with $N > 1$ continuous variables, it is straightforward to construct infinitely large families of MU bases with basis-dependent overlaps, simply by tensoring copies of the bases $\mathcal{B}_\theta$, $\theta \in [0, \pi)$. The overlaps of the product states $|q_{\theta_1} \dots q_{\theta_N}\rangle$ follow from Eq. (9.23),

$$|\langle q_{\theta_1} \dots q_{\theta_N} | q_{\theta'_1} \dots q_{\theta'_N} \rangle|^2 = \kappa \prod_{n=1}^N \frac{1}{|\sin(\theta_n - \theta'_n)|}, \quad (9.30)$$

where $\kappa = (2\pi\hbar)^{-N}$. This construction is expected to also work for the other types of continuous degrees of freedom discussed in [133]. Further MU bases may be found if the restriction to product states is dropped.

Asking for *basis-independent* overlaps drastically reduces the number of MU bases. For two continuous variables, five MU product bases with unit overlap have been constructed explicitly [390]. They are characterised by pairs of vectors with two components all of which are elements of a Galois field obtained by a quadratic extension of the integer numbers. Having three and five MU bases in both the two- and the infinite-dimensional Hilbert space, respectively, suggests an analogy which has not been formalised but speculated about [64]. However, the analogy is unlikely to be straightforward since a complete set of MU bases for two qubits with state space $\mathbb{C}^2 \otimes \mathbb{C}^2$ contains both product states and entangled states, while the five bases of the space $L^2(\mathbb{R}) \otimes L^2(\mathbb{R})$ contain product states only. In addition, a one-parameter family of inequivalent sets of five MU bases exists, and one can construct yet other pentuples [42] taking inspiration from the continuous-variable analogue of indirect product bases described in Sec. 7.4.

For $N \geq 2$, conditions for the existence of specific types of MU bases, not necessarily of product form, have been expressed in terms of metaplectic operators [390]. So far, no solutions have been found.

The position and momentum variables of a quantum particle can be “coarse-grained” in a periodic fashion to introduce a situation which sits between the finite- and the infinite-dimensional case [364]. The new observables are constructed by means of a set of infinite periodic square waves which, when taken together, cover all of $\mathbb{R}$. Effectively, one lumps together all those projectors onto (generalised) position eigenstates which have labels in regions where the square waves are non-zero. The construction ensures that quantum states contained entirely in one of the position bins, say, is evenly spread out across all momentum bins [343].

The construction can be generalised by using arbitrary straight lines in phase space as a starting point [308]. It has been shown that this approach cannot lead to more than three MU bases with basis-independent overlaps. Both of the papers just mentioned report quantum optical experiments which implement the required measurements and confirm that they are unbiased. Composite systems with two or more (pairs of) continuous variables have not been considered.

A conceptual link between Feynman’s path integral and mutually unbiased bases for continuous variables has been described in Refs. [353, 374]. Furthermore, it is pointed out that the basis of position eigenstates at time t and its image under the free-particle dynamics at time t' are mutually unbiased since we have

$$\langle x', t' | x, t \rangle = \left(\frac{m}{2\pi i(t' - t)} \right)^{\frac{1}{2}} \exp \left[\frac{im(x' - x)^2}{\hbar t} \right]. \quad (9.31)$$

This relation effectively defines a continuous family of MU bases for a continuous variable with basis-dependent overlaps, parameterised by the variable t . In contrast to the three rotated position bases satisfying Eq. (9.23), only two bases with identical overlap exist.

9.14 p -adic MU bases

van Dam and Russell [425] studied the properties of MU bases in the infinite-dimensional Hilbert space $L^2(\mathbb{Q}_p)$, where $\mathbb{Q}_p$ is the field of p -adic numbers. The p -adic numbers, which pervade the field of number theory, as well as other areas of mathematics [159], have led to p -adic variants of much of theoretical physics, including quantum mechanics and quantum field theory [378].

In a non-relativistic setting, states take the form $|\psi\rangle = \int_{x \in \mathbb{Q}_p} \psi(x) |x\rangle d\nu(x) \in L^2(\mathbb{Q}_p)$, with ν being the Haar measure on $\mathbb{Q}_p$ [425]. At least $(p + 1)$ MU bases in $L^2(\mathbb{Q}_p)$ can be found for $p > 2$. The construction is a generalisation of Wootters’ approach to obtaining $(d + 1)$ MU bases in $\mathbb{C}^d$ for prime-powers d , as described in Appendix A.1. The original method relies on properties of quadratic Gauss sums over finite fields, while the p -adic construction relies on similar results for quadratic Gauss integrals over $\mathbb{Q}_p$. More explicitly, suppose that p orthonormal bases $\mathcal{B}_b = \{|v_b\rangle\}$ of $L^2(\mathbb{Q}_p)$ are given, with $b \in \{0, \dots, p-1\}$ and $v \in \mathbb{Q}_p$. Each basis is a collection of states

$$|v_b\rangle = \int_{x \in \mathbb{Q}_p} e^{bx^2 + vx} |x\rangle d\nu(x), \quad (9.32)$$

with the function $e : \mathbb{Q}_p \rightarrow \mathbb{C}$ defined in the p -adic sense as $e(x) = \exp(2\pi i\{x\})$ where $\{x\}$ is the fractional part of $x \in \mathbb{Q}_p$. In addition, there is a basis $\mathcal{B}_\infty = \{|v_\infty\rangle\}$ defined by the Fourier transform of the states in $\mathcal{B}_0$. Taken together, one obtains a collection of $(p + 1)$ MU bases in $L^2(\mathbb{Q}_p)$.

A similar construction for the Hilbert space $L^2(\mathbb{R})$ over the field of *real* numbers rather than $\mathbb{Q}_p$ produces only three MU bases with basis-independent overlaps (cf. Sec. 9.13). The greater abundance of MU bases in $L^2(\mathbb{Q}_p)$ is due to a “coarser” p -adic norm than the one for real numbers, as explained in Ref. [425]. There are more possibilities to create numerically identical “overlaps” in the p -adic equivalent of Eq. (9.23). It is likely that products of the MU bases of $L^2(\mathbb{Q}_p)$ will lead to MU bases in product spaces such as $L^2(\mathbb{Q}_p) \otimes L^2(\mathbb{Q}_p)$ but we are not aware of any published results. Relations between coherent states over a field of p -adic numbers, canonical commutation relations and MU bases have been explored in Ref. [414].

10 Summary and outlook

This section summarises what we know about MU bases in composite dimensions $d \notin \mathbb{P}\mathbb{P}$ by making explicit the *properties* which a complete set in dimension $d = 6$ would need to possess. We will also collect *strategies* to solve the existence problem which have not yet been fully exhausted. Then, we formulate a number of open problems related to the existence of complete sets. The

problems are interesting in themselves but do not necessarily contribute directly to the existence problem in non-prime-power dimensions $d \notin \mathbb{PP}$. We conclude with a few remarks and an outlook.

10.1 Constraints on complete sets in $\mathbb{C}^6$

Sections 5 and 6 describe structural features of complete sets of MU bases $\mathcal{M}_d = \{\mathcal{B}_0, \dots, \mathcal{B}_d\}$ for arbitrary dimensions $d \geq 2$. We spell out some of these properties for the case of $d = 6$ and combine them with results which apply only to bases in composite dimension (cf. Sec. 6) or dimension six (cf. Sec. 7). Hence, if a complete set of seven MU bases $\mathcal{M}_6 = \{\mathcal{B}_0, \dots, \mathcal{B}_6\}$ were to exist, it would necessarily have the properties listed in the corollary.

Corollary 10.1. *A complete set of seven MU bases $\mathcal{M}_6 = \{\mathcal{B}_0, \dots, \mathcal{B}_6\}$ in the space $\mathbb{C}^6$ has the following properties:*

1. The seven bases $\mathcal{B}_0, \dots, \mathcal{B}_6$ can be written in terms of *six mutually unbiased Hadamard matrices* $\mathcal{M}_6 = \{\mathbb{I}_6\} \cup \{H_1, \dots, H_6\}$, i.e. the union of the identity and six complex Hadamard matrices H_i of order six such that the product $H_i^\dagger H_j$ of any two of them is another Hadamard matrix (see Equivalence 5.2).
2. The matrix H_1 can be written in *dephased* form with its first row and column entries given by $H_{1j} = H_{i1} = 1/\sqrt{6}$ for $i, j = 1, \dots, 6$ (see Sec. 3.13).
3. Given *five* mutually unbiased Hadamard matrices one can construct a sixth one to obtain the complete set $\mathcal{M}_6$ (Thm. 6.2).
4. The set $\mathcal{M}_6$ defines a *unitary operator basis* of the space $\mathbb{C}^6$ which partitions into $d + 1$ maximally commuting classes (Equivalence 5.4).
5. The bases in $\mathcal{M}_6$ provide a set of seven *pair-wise orthogonal Cartan subalgebras* such that the simple Lie algebra $sl_6(\mathbb{C})$ admits an orthogonal decomposition (Equivalence 5.5).
6. The vectors in $\mathcal{M}_6$ saturate the *Welch bounds* (5.20) and (5.21) (Equivalence 5.12).
7. The vectors in $\mathcal{M}_6$ form a *complex projective 2-design* and hence satisfy Eq. (5.18).

8. The average *entanglement content* over the states in $\mathcal{M}_6$ is fixed by Thm. 6.9.
9. The set $\mathcal{M}_6$ contains at most one product basis (Thm. 7.10).
10. No Hadamard matrix in $\mathcal{M}_6$ contains three or more columns which are product states (Thm. 7.11).
11. The set $\mathcal{M}_6$ contains no Butson-type Hadamard matrices $BH(6, 12)$ (Thm. 7.15).
12. The six Hadamard matrices in $\mathcal{M}_6$ form a projective toric 2-design of $P(T^6)$ that is not a group (Thm. 7.13).
13. No more than three bases in $\mathcal{M}_6$ are monomial (Thm. 6.7).
14. Each Hadamard matrix in $\mathcal{M}_6$ has Schmidt rank $r > 2$ (Thm. 7.12).
15. No Hadamard matrix in $\mathcal{M}_6$ contains a 3×3 submatrix proportional to a unitary (Lem. 7.1).
16. Each Hadamard matrix in $\mathcal{M}_6$ is equivalent to a Hadamard in which all or none of the nine 2×2 blocks are *unitary* (Thm. 7.2).
17. The set $\mathcal{M}_6$ does not include the isolated matrix S_6 (Thm. 7.14) or the Fourier family $F_6^{(6)}$ (Thm. 7.7).

The first seven statements are generic in the sense that complete sets of MU bases in any dimension have analogous properties. *Mutatis mutandis*, property 8 holds for other composite dimensions, as well as a weaker version of property 9 (Thm. 6.8). The remaining eight properties have been derived for the case of $d = 6$; their generalizations to other dimensions may exist but are not known. Furthermore, in dimensions where real Hadamard matrices exist, we also know that a complete set will contain at most one of those (Thm. 6.16).

At this point, musings by Sylvester spring to mind when, in 1887, he pondered the existence of odd perfect numbers:

... a prolonged meditation on the subject has satisfied me that the existence of any one such [odd perfect number] – its escape, so to say from the complex

web of conditions which hem it in on all sides – would be little short of a miracle [355, pp. 152-3].

The problem is still open today. The existence problem for complete sets of MU bases puts us in a similar situation, although perhaps not (yet) as dire as Sylvester’s case. A viable strategy to prove their non-existence is to further “hem them in on all sides” so that their construction becomes impossible. The following section summarises some alternative proof strategies.

10.2 Solution strategies

Arbitrary composite dimension

We now summarise several strategies which could be used to prove non-existence of complete sets in any composite dimension, i.e. when $d \notin \mathbb{PP}$.

Strategy 10.1. *Equivalent formulations*

If true, each of the fourteen conjectures listed in Sec. 5 ensures the non-existence of complete MU bases in any composite dimension. For instance, one could attempt to show that no suitable partitioning of a unitary operator basis (as defined in Sec. 5.4) exists, or that $sl_d(\mathbb{C})$ has no orthogonal decomposition (cf. Sec. 5.5). Alternatively, a solution would follow if the Welch bounds were found not to be tight, or if the optimal success probability of a p-QRAC is unachievable (see Secs. 5.12 and 5.9, respectively). One popular (numerical) strategy is to search for the global minimum (or minima) of the function defined in Eq. (5.2) of Sec. 5.1, with the main findings of this approach summarized in Secs. 8.2 and 8.3. Similar methods can be applied to other functions optimised by MU bases, e.g., the measure of non-commutativity introduced by Bandyopadhyay and Mandayam [32] (cf. Sec. 3.3). While some of these techniques rely on numerics, others can be formulated in terms of semidefinite programming, allowing for the possibility of a rigorous non-existence proof.

Strategy 10.2. *Semidefinite programming*

Expressing the search for MU bases as a semidefinite program is a promising computational approach to rigorously prove Conjecture 1.1. There are different methods to do so, depending

on the type of optimisation, and whether commutative or non-commutative polynomial optimisations are considered.

One technique involves solving a system of coupled polynomials $p_i(\alpha)$ which represent the constraints for the MU basis vectors [80, 373] (see Sec. 5.3). The real *commutative* variables $\alpha \equiv (\alpha_1, \dots, \alpha_n)$, with $\alpha_i \in [0, 2\pi)$, parameterise the candidate MU vectors. The idea is to minimise one polynomial, $(p_k(\alpha))^2$, subject to the condition $p_i(\alpha) = 0$ for all $i \neq k$. Since the polynomials are non-convex, Lasserre’s hierarchy of semidefinite programs can be applied [247], and for each level of relaxation the existence of MU bases is ruled out or the result is inconclusive. If a positive global bound is obtained by this minimisation, the coupled polynomial equations have no solution and, therefore, no set of MU bases exists. This method successfully confirms the non-existence of an MU triple containing the pair $\{\mathbb{I}, S_6\}$, where S_6 is the isolated Hadamard matrix, but has been unsuccessful for the constellation $\{5^3, 1\}$ (see Sec. 8.3 for the definition of constellations), due to the increase in computational complexity [80].

One can also formulate the existence question in terms of a certain C^* -algebra (Sec. 5.7) to provide a *non-commutative* polynomial optimisation strategy, leading to semidefinite programming relaxations [170]. Proving infeasibility of these relaxations provides a strategy to rule out the existence of $(d+1)$ MU bases in dimension d . In [170], by exploiting symmetries of the problem, this technique was used to show that $d+2$ MU bases do not exist if $d \leq 8$.

Another approach, which also involves a non-commutative polynomial optimisation, uses the equivalence between QRACs and MU bases, as described in Sec. 5.9. The idea is to apply a specific semidefinite-programming hierarchy [298] to find an upper bound for the optimal success probability of the $(4, 2)^6 \rightarrow 1$ p-QRAC. If the bound falls below the optimal value defined in Eq. (5.13) one can conclude that four MU bases do not exist. As with the commutative case, the method has been unsuccessful due to insufficient computational resources. For example, the k -th level of the hierarchy for the $(4, 2)^6 \rightarrow 1$ p-QRAC requires roughly 2^{32k} bits of memory, although a quadratic reduction is feasible by exploiting certain symmetries of the QRAC [7].

Strategy 10.3. *Discretisation of the parameter space*

Thm. 7.7 of Sec. 7.3 states that any triple of MU bases containing the two-parameter Fourier family is unextendible. The proof, which relies on a discretisation of the parameter space and a computational search over a finite set of vectors, can also be applied as a strategy to disprove the existence of any four MU bases in $d = 6$, as well as generalising to larger dimensions. Suppose that four MU bases $\{\mathbb{I}, H_1, H_2, H_3\}$ exist which can be parameterised in terms of m phases, $\alpha \equiv (\alpha_1, \dots, \alpha_m)$, where $\alpha_j \in [0, 2\pi)$. The discretisation approximates the original MU bases by the set $\{\mathbb{I}, \tilde{H}_1, \tilde{H}_2, \tilde{H}_3\}$ where the phases are restricted to N -th roots of unity. For instance, if the phase $\alpha_j \in [0, 2\pi)$ initially lies in the interval $[(2k-1)\pi/N, (2k+1)\pi/N)$, then we approximate α_j by $\tilde{\alpha}_j = 2\pi k/N$. If we choose a sufficiently large positive integer N , rigorous bounds of the errors given by the inner products of the approximated states can be established. If the errors lie outside these bounds, the original bases cannot be mutually unbiased. The efficiency of this approach can be improved by considering suitable MU constellations which will depend on fewer parameters (see Sec. 8.3).

Strategy 10.4. *Positive definite functions*

An approach exploiting positive definite functions (Sec. 6.11) on the group $G = U(d)$ of unitary matrices may provide a means to upper-bound the cardinality of the maximal set of MU bases for a given dimension. Introduced in [235, 276], the cardinality of the maximal set of MU bases is bounded from above by $h(e)/\int h d\nu$ where $h : G \rightarrow \mathbb{R}$ is a positive definite function with the properties (i) $h(H) \leq 0$ for all $d \times d$ Hadamard matrices H ; (ii) $h(e) = 0$; and (iii) $\int h d\nu > 0$, where ν is the normalised Haar measure.

The function given in Eq. (6.21) yields a tight upper bound when the dimension is a prime power. The aim is to construct a positive definite function which would lower this bound for composite dimensions $d \notin \mathbb{PP}$.

Strategy 10.5. *Linear constraints*

Treating the columns of a set of mutually unbiased Hadamard matrices as elements of the

group $\mathbb{T}^d$, the usual polynomial conditions of orthogonality and unbiasedness for a set of MU bases can be transformed into linear constraints. The constraints, which are derived via Fourier analytic methods, apply to the functions $E(\gamma)$ and $F(\gamma)$ (see Eqs. (6.27)–(6.30) of Sec. 6.12) and are linear by treating each function $E(\gamma)$ and $F(\gamma)$ as a variable for each value of $\gamma \in \mathbb{Z}^d$.

There are two ways to apply these constraints to prove that complete sets do not exist. First, one can attempt to find some structural results on the entries of the Hadamard matrices. A contradiction would follow if the additional structure imposes a restriction on the complete set that cannot hold. For instance, if $F(\rho) = d^4$ holds for all permutations of $\rho = (d, -d, 0, \dots, 0) \in \mathbb{Z}^d$, then the matrix entries of a set of MU bases are all d -th roots of unity. While this constraint has been used to classify all MU bases for $d \leq 5$, it is not expected to hold when $d = 6$ [272].

Secondly, one can attempt to prove directly the non-existence of a complete set by applying a linear programming code to show that the constraints in Eqs. (6.27)–(6.30) do not hold. For instance, if maximising the variable $E(\gamma)$ for a given $\gamma \in \mathbb{Z}^d$ yields $E(\gamma) \geq d^3$, then a contradiction and ultimately a proof would follow. It is surmised that a proof of Conjecture 6.4 will be an important ingredient in this approach since it establishes an additional linear constraint which is expected to hold for almost all 6×6 Hadamard matrices. While the conjecture is true for the three-parameter Karlsson family $K_6^{(3)}$, a linear program is unable to capitalise on the additional constraint and fails to rule out the existence of a complete set containing only Hadamard matrices from $K_6^{(3)}$ [278].

Dimension six

The ultimate goal, to prove that a complete set of MU bases in $\mathbb{C}^d$ exists if and only if the dimension is a prime-power, would simultaneously prove the conjectures of Sec. 5. A slightly more feasible challenge is to focus on dimension six rather than arbitrary composite dimensions $d \notin \mathbb{PP}$.

Problem 10.1. Show that no complete set of seven MU bases exists when $d = 6$.

Simplifying further, one could aim for a proof of Zauner's conjecture given in Sec. 2.3.

Problem 10.2. Show that no set of four MU bases exists when $d = 6$.

This approach is, of course, sufficient to solve the existence problem for complete sets in $\mathbb{C}^6$. Instead, it might be easier to solve a pared-down version of this question by showing that any three MU bases are strongly unextendible when $d = 6$.

Problem 10.3. Show that no single vector is mutually unbiased to any triple of three MU bases when $d = 6$.

An exhaustive classification of all MU triples would probably be necessary for this method. To make progress, an exhaustive classification of all pairs of MU bases in $d = 6$ (Sec. 7.1) should be given.

Problem 10.4. Classify all complex Hadamard matrices of order six.

This problem was addressed in Sec. 7.1 where all known Hadamard matrices of order six were reported: an isolated matrix S_6 , a three-parameter family $K_6^{(3)}$ and a four-parameter family $G_6^{(4)}$. It is expected that any Hadamard matrix is equivalent to a member of these families, but a proof that this list is exhaustive remains elusive (Conjecture 7.1). The structure of the four-parameter family and its relation to $K_6^{(3)}$ is not well understood; for instance, does the general construction presented in [357] include $K_6^{(3)}$ as a subfamily? Even simpler problems remain open, such as the question of whether F_6 is a member of a four-parameter family (although substantial evidence points towards this being true; cf. Appendix B).

Given an exhaustive list, all candidates for the six MU Hadamard matrices would be known. Still, a non-trivial task remains, namely to identify all triples of MU bases in dimension six or, equivalently, to identify all pairs of Hadamard matrices H_1 and H_2 such that $H_1^\dagger H_2$ is another Hadamard matrix (see Sec. 7.2).

Problem 10.5. Find all pairs of 6×6 complex Hadamard matrices H_1 and H_2 such that their product $H_1^\dagger H_2$ is another Hadamard matrix.

Conjecture 8.1 suggests a solution to this problem, with the Fourier family $F_6^{(2)}$, its transpose, and Szöllősi's family $X_6^{(2)}$ proposed as the only viable candidates.

If these problems are still too difficult, one could perhaps try to complete Table 2 by providing a rigorous proof confirming the numerical evidence that certain families are unextendible.

Problem 10.6. Show that a given pair of MU bases in $\mathbb{C}^6$ does not extend to a triple (or quadruple) of MU bases.

Examples would include a proof that, for certain parameter values, $\{\mathbb{I}, M_6^{(1)}\}$, $\{\mathbb{I}, K_6^{(2)}\}$ or $\{\mathbb{I}, K_6^{(3)}\}$ do not extend to a triple, in analogy with the isolated case $\{\mathbb{I}, S_6\}$. A general analytic proof similar to Thm. 7.7 would represent a major step forward.

10.3 Related open problems

For general composite dimensions, and for the case of continuous variables, there are several open problems related indirectly to the existence of MU bases. Some are mathematical in nature, others concern the physics behind MU bases.

For even dimensions such as $d = 2 \times p$ with p an odd prime, Thm. 6.1 yields only three MU bases, even when the dimension d is arbitrarily large. Do more effective construction methods exist in this situation, even if they do not lead to complete sets?

Problem 10.7. Can one improve the lower bound provided in Thm. 6.1, to find larger sets of MU bases in composite dimensions?

Theorem 6.8 states that the lower bound cannot be improved if one considers product bases only. However, a method based on Latin squares and maximally entangled bases successfully improves the bound in certain square dimensions, as discussed in Sec. 6.9 and Thm. 6.11.

One can also attempt to extend the minimal set of MU bases used to derive the lower bound in Thm. 6.1.

Problem 10.8. Is the set of MU product bases from Thm. 6.1 unextendible?

The solution is known for dimension six: any set of three MU product bases is *strongly unextendible* (Sec. 7.4). We may also ask a similar question for the Latin square construction in square dimensions.

Problem 10.9. Is the set of $(\mu + 2)$ MU bases from Thm. 6.11 unextendible?

One construction method of MU bases proceeds by partitioning a subset of the elements of a nice error basis into maximally commuting classes (cf. Sec. 6.5). According to Thm. 6.6, a set of $\min_i(p_i^{n_i} + 1)$ weakly unextendible “nice” MU bases results for $d = p_1^{n_1} \dots p_r^{n_r} \notin \mathbb{PP}$.

Problem 10.10. For $d = p_1^{n_1} \dots p_r^{n_r} \notin \mathbb{PP}$, is a set of $\min_i(p_i^{n_i} + 1)$ nice MU bases *strongly* unextendible?

This relates to another open problem, namely Conjecture 6.2, which predicts that the eigenbases of a smaller set of Heisenberg-Weyl operators (defined globally rather than as a tensor product of each system) are unextendible. The conjecture has been confirmed for $d \leq 15$ (Sec. 6.10). Recall, from Sec. 6.10, that if a set of weakly unextendible nice MU bases is sufficiently large, it cannot form a complete set.

MU bases also give rise to an interpretational question which asks about the consequences of inequivalent pairs of complementary observables for the description or the properties of a physical system (see Sec. 3.13).

Problem 10.11. What does it mean for a physical system if inequivalent complementary pairs of observables exist?

Since a continuous family of inequivalent Hadamard matrices exists already for $d = 4$, this question can be addressed in full for a quantum system composed of two qubits. So far, inequivalent *pairs* are not known to exhibit operational differences. For example, methods of self-testing (cf. Sec. 3.11) are unable to distinguish between complementary pairs. However, for *sets of μ MU bases* in $\mathbb{C}^d$, with $2 < \mu < d$, there are some known consequences. Different sets affect the success of a p-QRAC protocol (Sec. 4.6) and the ability to detect (bound) entangled states (Sec. 4.2). Furthermore, certain sets exhibit more measurement incompatibility than others (Sec. 3.4). Curiously, these discrepancies no longer hold for complete sets, which suggests another question.

Problem 10.12. What are the consequences for a physical system if inequivalent complete sets of MU bases exist?

So far, the existence of inequivalent complete sets (see Appendix A.8) is known for *prime-power* dimensions $d = p^n$ with $p \in \mathbb{P}$ and $n > 1$. No

examples have been found when the dimension is a *prime* number, $d \in \mathbb{P}$.

Problem 10.13. Do inequivalent complete sets of MU bases exist in prime dimensions?

MU bases for continuous variables bring their own existence problems. For example, the maximal number of MU bases with identical overlaps (see Sec. 9.13) is not known even in the simplest case of a single continuous-variable pair.

Problem 10.14. For a quantum particle with one degree of freedom, do more than three MU bases with basis-independent overlaps exist?

A somewhat less general question concerns the extendability of the “standard triple” of MU bases by a single state.

Problem 10.15. For a quantum particle with one degree of freedom, is the Heisenberg-Weyl type triple of MU bases with basis-independent overlaps strongly unextendible?

A positive answer would establish a desirable similarity between the three MU bases of Heisenberg-Weyl type for a discrete and for a continuous degree of freedom, respectively.

10.4 Conclusions

The concept of mutual unbiasedness in linear spaces with an inner product turns out to be *structurally rigid*: the definition of MU bases makes sense for real, complex, quaternionic and even *p*-adic numbers (cf. Sec. 9). In the standard setting of the space $\mathbb{C}^d$, a parameter count reveals that the existence of complete MU sets in prime-power dimensions is, in fact, a remarkable surprise: the number of constraints exceeds the number of free parameters for $d > 2$, both in composite *and* prime-power dimensions (see Sec. 2.3). To understand the (im-) possibility to solve the coupled polynomial equations defining the existence problem (cf. Equivalence 5.3) is probably at the heart of the matter. The number-theoretical identities which entail solutions in prime-power dimension are absent in composite dimensions. At the same time, the existence problem of complete sets of MU bases in a given composite dimension $d \notin \mathbb{PP}$ is *decidable* since an algorithm detecting MU bases (or their absence) is known (cf. the end of Sec. 2.3).

Being set in a complex inner product space, quantum theory is a natural home for mutually unbiased bases. However, it is important to acknowledge that they also arise when studying complex-valued *classical* signals or within Fourier theory (cf. Sec. 1.1). Nevertheless, the existence problem is particularly important in quantum theory and quantum information since complete sets of MU bases often represent “extreme” cases: they maximise or minimise uncertainty relations or entropies, they exhibit maximal non-classicality in the form of measurement incompatibility and coherence, and they optimise information processing protocols making them suitable for benchmarking (cf. Sec. 3).

The existence problem of complete sets clearly represents yet another instance where quantum theory meets number theory (see e.g. [57, 268, 341]). For discrete structures such as SICs (cf. Sec. 3.9), the link is even more explicit and possibly “mathematically deeper” (cf. [17, 18]). The problem is also linked with the tensor-product structure used to describe composite quantum systems. There are, in fact, alternatives to the commonly used tensor product [232] such as the “maximal” or “minimal” tensor product, which differ from the standard one used in quantum theory that sits between the extreme cases.

Mapping the search for complete sets of MU bases onto equivalent problems (cf. Sec. 5) has led to *new perspectives* and confirms the *genuine difficulty* of the open question. For example, rephrasing the existence problem in terms of orthogonal decompositions of $sl_d(\mathbb{C})$ has revealed the existence of a single family of mutually unbiased bases which—although it has not yet been fully characterised analytically—is conjectured to contain all previously known examples, except for isolated ones. The equivalence of a complete set of MU bases with a complex projective 2-design implies that their entanglement content is restricted in any composite dimension. Furthermore, research into MU bases has (re-) established interest in *complex* Hadamard matrices which have become a mathematical topic of its own.

This review collects a considerable number of properties of mutually unbiased bases in composite dimensions. Nevertheless, no overarching or underlying structure emerges, not even in dimension six (cf. Sec. 10.1), the composite dimension for which most is known. A definite *lack of recog-*

nisable patterns reflects our lack of understanding. Attempts to simplify or modify the main existence problem—by focussing on a particular dimension or by restricting the candidate states of MU bases to product form, for example—have led to a plethora of apparently unrelated observations, without shedding much light on the original existence problem.⁸ We continue to divide but do not conquer. From a mathematical point of view, our current fragmented knowledge about mutually unbiased bases makes one think of the problem of radicals before Galois’ solution by introducing entirely new mathematical concepts [156].

On the basis of the results gathered in these pages, we expect the generalisation of *Zauner’s Conjecture* to be true: complete sets of mutually unbiased bases do not exist in dimension six or any other composite dimensions. While the search for a mathematical proof of Zauner’s conjecture continues, we suggest pondering the relevance of MU bases for the description of nature: would existence or non-existence of complete sets have far-reaching consequences in quantum theory, or in some other context? Are complete sets of MU bases “luxury items” which are nice to have in prime-power dimensions but not really essential otherwise?

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⁸“There are thing[s] we know that we know. There are known unknowns. That is to say there are things that we now know we don’t know. But there are also unknown unknowns. There are things we don’t know we don’t know” [323].

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A Constructions of complete sets

Early constructions of complete sets of MU bases covering prime dimensions $d = p \in \mathbb{P}$ were provided in the early eighties by Alltop and Ivanović [9, 203], at a time when MU bases had not been formally defined. Alltop's implicit construction for prime dimensions $p \geq 5$ was given in terms of complex periodic sequences (see Sec. 2). A year later Ivanović discovered these bases in the context of optimal quantum state tomography, as described in Sec. 4.1. They can be written in the form $\mathcal{B}_b = \{|v_b\rangle\}$, $b, v \in \mathbb{Z}_p$, with basis vectors,

$$|v_b\rangle = \frac{1}{\sqrt{p}} \sum_{k=0}^{p-1} e^{(2\pi i/p)(bk^2+vk)} |k\rangle. \quad (\text{A.1})$$

Here the label b denotes different bases, v the vectors within each basis, and $|k\rangle$ the elements of the computational basis. Together with the standard basis they form a set of $(p+1)$ MU bases. Throughout this appendix, $\mathcal{B}_0$ will not necessarily denote the standard basis.

Ivanović's construction was extended by Wootters and Fields [401] to include (both odd and even) powers of primes, $d = p^n \in \mathbb{PP}$, using field extensions $\mathbb{F}_{p^n}$. For odd prime-powers we will follow the method of Wootters and Fields, but for even prime-powers we will review a simpler construction by Klappenecker and Rötteler [229] based on Galois rings.

We will summarise several other construction methods, roughly in chronological order, and describe why they fail in non-prime-power dimensions $d \notin \mathbb{PP}$. Our aim is to give a flavour of the diverse (but not exhaustive) methods used to construct MU bases.

A.1 Odd prime-powers

Since the construction of Wootters and Fields [401] relies on finite fields $\mathbb{F}_{p^n}$, we will briefly describe some of their basic properties. To construct the field $\mathbb{F}_{p^n}$ from the field $\mathbb{F}_p$ one starts by adding an element α which is a root of an *irreducible* polynomial $f(x)$ of degree n , with coefficients from the field $\mathbb{F}_p$. A polynomial of order n is irreducible if it cannot be expressed as the product of two polynomials over $\mathbb{F}_p$ of smaller degree. The remaining elements of $\mathbb{F}_{p^n}$ are then given by the set of all polynomials of the form $g(\alpha) = g_0 + g_1\alpha + \dots + g_n\alpha^n$ were $g_i \in \mathbb{F}_p$. In

this representation we say that $\{\alpha, \alpha^2, \dots, \alpha^n\}$ is a *basis* of $\mathbb{F}_{p^n}$.

Addition and multiplication within the field are defined by the usual addition and multiplication of polynomials *modulo* the irreducible polynomial. In the construction of the extension $\mathbb{F}_{p^n}$ one is free to choose any irreducible polynomial of order n and any root α of the polynomial as they result in the same field up to isomorphism. If, however, one chooses the irreducible polynomial to be a *primitive* polynomial $p(x)$, then all non-zero elements of the field can be generated through powers of γ , i.e. $\mathbb{F}_{p^n} \setminus \{0\} = \{\gamma^0, \gamma, \dots, \gamma^{p^n-2}\}$, where $p(\gamma) = 0$. A polynomial $p(x)$ of degree n is called primitive if the smallest positive integer m for which $p(x)$ divides $(x^m - 1)$ is $m = p^n - 1$.

For powers of odd primes the construction leads to a set of $d = p^n$ bases $\mathcal{B}_b = \{|v_b\rangle\}$, $b, v \in \mathbb{F}_{p^n}$, consisting of the the vectors

$$|v_b\rangle = \frac{1}{\sqrt{p^n}} \sum_{k \in \mathbb{F}_{p^n}} e^{(2\pi i/p)\text{Tr}[bk^2+vk]} |k\rangle. \quad (\text{A.2})$$

The trace of $\alpha \in \mathbb{F}_{p^n}$ is defined as $\text{Tr } \alpha = \alpha + \alpha^p + \dots + \alpha^{p^{n-1}}$, and $|k\rangle$ again denotes elements of the standard basis. The bases are pairwise mutually unbiased due to the quadratic Gaussian sum over finite fields taking values independent of both b and v , i.e.

$$\left| \sum_{k \in \mathbb{F}_{p^n}} e^{(2\pi i/p)\text{Tr}[bk^2+vk]} \right| = \sqrt{p^n}, \quad (\text{A.3})$$

if p is an odd prime and $b \neq 0$. Thus, together with the standard basis, the vectors in Eq. (A.2) form a complete set of $(p^n + 1)$ MU bases.

This approach fails for $p = 2$ since Eq. (A.3) does not hold. The bases defined through Eq. (A.2) can also be written in a form without explicitly referring to the field elements, as shown in Ref. [401]. This specific representation can then be used to write out explicitly the complete set of MU bases for even dimensions $d = 2^n$. Galois rings provide an alternative way to construct complete sets in even prime-powers.

A.2 Even prime-powers

For spaces $\mathbb{C}^d$ with even prime-power dimensions $d = 2^n$, a construction of complete sets of MU

bases using Galois rings was found by Klappenecker and Rötteler [229]. In particular, they employ properties of exponential sums over $GR(4, n)$ (the Galois ring of degree n over $\mathbb{Z}/4\mathbb{Z}$) to obtain sets consisting of $(2^n + 1)$ MU bases.

The Galois ring $GR(4, n)$ is the unique Galois extension of $\mathbb{Z}/4\mathbb{Z}$ (the residue class ring of integers modulo 4) of degree n . The 4^n elements of $GR(4, n)$ can be written in the form $r = b + 2v$ where b and v are elements of the Teichmüller set $\mathcal{T}_n$ of order $(2^n - 1)$. For $b \in \mathcal{T}_n$, elements of $\mathcal{B}_b$ are given by

$$|v_b\rangle = \sum_{k \in \mathcal{T}_n} \frac{1}{\sqrt{2^n}} e^{(2\pi i/4)\text{Tr}[(b+2v)k]} |k\rangle. \quad (\text{A.4})$$

Together with the standard basis they provide the desired set of $(2^n + 1)$ MU bases of $\mathbb{C}^{2^n}$. The trace map $\text{Tr} : GR(4, n) \rightarrow \mathbb{Z}/4\mathbb{Z}$ is defined as $\text{Tr } x = \sum_{j=0}^{n-1} \sigma^j(x)$ where σ is the automorphism $\sigma(b + 2v) = b^2 + 2v^2$. The proof follows straightforwardly by replacing Eq. (A.3) with the identity

$$\left| \sum_{x \in \mathcal{T}_n} e^{(2\pi i/4)\text{Tr}[rx]} \right| = \begin{cases} 0 & r \in 2\mathcal{T}_n, r \neq 0; \\ 2^n & r = 0; \\ \sqrt{2^n} & \text{otherwise.} \end{cases} \quad (\text{A.5})$$

The relations (A.3) and (A.5) have no equivalents in composite cases $d \notin \mathbb{PP}$. Moreover, it has been shown that a generalisation of Eqs. (A.2) and (A.4) to any finite ring leads to no more than $(p_1^{n_1} + 1)$ MU bases in $\mathbb{C}^d$, where $p_1^{n_1}$ is the smallest prime-power factor of a given composite number d [20].

A.3 Generalised Alltop construction

Alltop's construction of complete sets in terms of complex periodic sequences for prime dimensions $p \geq 5$ (mentioned in Appendix A.1) has been generalised by Klappenecker and Rötteler in [229] to prime-power dimensions $d = p^n$ with $p \geq 5$. For a finite field $\mathbb{F}_{p^n}$ of characteristic $p \geq 5$, the bases $\mathcal{B}_b = \{|v_b\rangle : v \in \mathbb{F}_{p^n}\}$ are expressed as

$$|v_b\rangle = \frac{1}{\sqrt{p^n}} \sum_{k \in \mathbb{F}_{p^n}} e^{(2\pi i/p)\text{Tr}[(k+b)^3 + v(k+b)]} |k\rangle, \quad (\text{A.6})$$

where $b \in \mathbb{F}_{p^n}$ and $|k\rangle$ are standard basis elements of $\mathbb{C}^{p^n}$. Together with the standard basis they form a set of $(p^n + 1)$ MU bases. The proof follows from a result on Weyl sums over finite fields, which is applicable only when p is odd.

A.4 Unitary operator bases

We now exploit the link between maximally commuting operator classes and MU bases (cf. Equivalence 5.4 in Sec. 5.4) to construct complete sets using the Heisenberg-Weyl group, following Bandyopadhyay *et al.*'s approach [31].

To recap, we require a unitary operator basis of $\mathbb{M}_d(\mathbb{C})$ with d^2 elements that partition into $(d+1)$ subsets, each containing a maximal set of commuting unitary matrices. One such candidate is the Heisenberg-Weyl group generated from the cyclic *shift* (modulo d) and *phase* operators X and Z , respectively, defined as

$$X|k\rangle = |k+1\rangle \quad \text{and} \quad Z|k\rangle = \omega^k |k\rangle, \quad (\text{A.7})$$

where $\omega = e^{2\pi i/d}$ is a d -th root of unity and $\{|k\rangle\}$ is the standard basis with $k = 0, \dots, d-1$. An overview of the role of this group in the context of MU bases can be found in Ref. [52].

For prime dimensions $d = p$, the group elements $X^k Z^l$ can be split into $(p+1)$ cyclic subgroups generated by the operators $Z, X, XZ, \dots, XZ^{p-1}$, which form the commuting subclasses required. The eigenstates of these operators provide the $(p+1)$ MU bases. Each basis can be written in a compact form, with the eigenstates of Z giving the standard basis $\{|0\rangle, \dots, |p-1\rangle\}$ and the remaining bases $\mathcal{B}_b = \{|v_b\rangle\}$ consisting of the eigenstates of $X(Z)^b$, for $0 \leq b, v \leq p-1$, as

$$|v_b\rangle = \frac{1}{\sqrt{p}} \sum_{k=0}^{p-1} (\omega^v)^{p-k} (\omega^{-b})^{s_k} |k\rangle, \quad (\text{A.8})$$

where $s_k = k + \dots + (p-1)$.

The generalisation to the case of prime powers, $d = p^n$, uses Heisenberg-Weyl unitary operators acting on the Hilbert space $\mathbb{C}^p \otimes \dots \otimes \mathbb{C}^p$, which are of the form

$$X(k_1 \dots k_n) Z(l_1 \dots l_n) \equiv X^{k_1} Z^{l_1} \otimes \dots \otimes X^{k_n} Z^{l_n}, \quad (\text{A.9})$$

where $k_j, l_j \in \mathbb{F}_p$. The elements $\omega^j X(k_1 \dots k_n) Z(l_1 \dots l_n)$ form the Heisenberg-Weyl group (or generalised Pauli group $\mathbb{P}_j(p, n)$) of unitary operators on $\mathbb{C}^p \otimes \dots \otimes \mathbb{C}^p$ for some integer $j > 0$.

One can form a unitary operator basis of the set of $p^n \times p^n$ complex matrices $\mathbb{M}_{p^n}(\mathbb{C})$ from the elements of (A.9). These operators split into commuting classes $\mathcal{C}_1, \dots, \mathcal{C}_d$, and we associate

with each class a $(n \times n)$ matrix A_b over $\mathbb{Z}_p$ with $b = 1, \dots, p^n$. By extending each matrix to a matrix $(\mathbb{I}_n, A_b)$ of size $(n \times 2n)$, with $\mathbb{I}_n$ the identity, the rows of $(\mathbb{I}_n, A_b)$ are chosen to represent the exponents $(k_1, \dots, k_n, l_1, \dots, l_n)$ of the operators (A.9) in class $\mathcal{C}_b$. Thus, each class contains n operators.

The MU bases are built by making use of the following result: let A_b and $A_{b'}$ be a symmetric pair of $(n \times n)$ matrices over $\mathbb{Z}_p$ such that $\det(A_b - A_{b'}) \not\equiv 0 \pmod{p}$, then A_b and $A_{b'}$ correspond to a pair of MU bases in $\mathbb{C}^{p^n}$. Thus, by including the standard basis, a set of matrices $\{A_1, \dots, A_{p^n}\}$ satisfying these properties corresponds to a complete set of MU bases. To construct these matrices we require n symmetric nonsingular matrices $B_1, \dots, B_n \in \mathbb{M}_n(\mathbb{C})$ such that the matrix $\sum_{j=1}^n b_j B_j$ is nonsingular for every nonzero vector $(b_1, \dots, b_n) \in \mathbb{Z}_p^n$. Then, the p^n matrices $A_b = \sum b_j B_j$, $(b_1, \dots, b_n) \in \mathbb{Z}_p^n$, form a set of matrices $(0_n, \mathbb{I}_n), (\mathbb{I}_n, A_1), \dots, (\mathbb{I}_n, A_{p^n})$ which yield the $(p^n + 1)$ MU bases.

A general method to find the symmetric nonsingular matrices $B_1, \dots, B_n$ has been given by Wootters in [401]. In particular, let $\gamma_1, \dots, \gamma_n$ be a basis of $\mathbb{Z}_p^n$ as a vector space over $\mathbb{Z}_p$ (i.e. any element $c \in \mathbb{Z}_p^n$ can be expressed as $c = \sum_i c_i \gamma_i$ where $c_i \in \mathbb{Z}_p$). Then, any element $\gamma_i \gamma_j \in \mathbb{Z}_p^n$ can be written uniquely as $\gamma_i \gamma_j = \sum_{l=1}^n b_{ij}^l \gamma_l$, with b_{ij}^l the ij -th element of B_l .

Unsurprisingly, this approach fails for dimensions $d \notin \mathbb{P}\mathbb{P}$, as some of the required properties no longer hold. For example, symmetric matrices satisfying $\det(A_b - A_{b'}) \not\equiv 0 \pmod{p}$ no longer correspond to pairs of MU bases in $\mathbb{C}^{p^n}$. At best, one can construct $(p_1^{n_1} + 1)$ MU bases of $\mathbb{C}^d$ in this way, where $p_1^{n_1}$ is the smallest prime-power factor of d . In Ref. [52], the Heisenberg-Weyl group and its commuting subclasses are described in terms of flowers and their petals.

A.5 Discrete geometries

Affine planes display structural similarities to sets of MU bases. These discrete geometric structures consist of points and lines that satisfy the following three axioms: (i) any two points have exactly one line in common; (ii) for any line and additional point there is a unique line through this point and disjoint (parallel) from the given line; and finally: (iii) there exist at least three non-collinear points. This being the case, an affine

plane of order d contains d^2 points and $d(d+1)$ lines, with each line containing d points. The lines of an affine plane can be partitioned into $(d+1)$ sets, called *striations*, each containing d parallel lines. Any two non-parallel lines intersect at only one point.

An affine plane can also be represented by a set of orthogonal Latin squares. A Latin square of order d is an array of $d \times d$ integers ranging from 0 to $(d-1)$ such that each number appears exactly once in each row and column. Two Latin squares L and L' are orthogonal if all ordered pairs of elements (L_{ij}, L'_{ij}) are distinct. Pairs of orthogonal Latin squares exist for all $d > 2$ and $d \neq 6$. For every prime and prime-power d , there exist $(d-1)$ mutually orthogonal (MO) Latin squares, a consequence of the existence of affine planes [126]. When the order d of an affine plane equals either $(1 \pmod{4})$ or $(2 \pmod{4})$, the Bruck-Ryser theorem imposes the restriction that d must be the sum of two squares [82]. In this way, the existence of affine planes in an infinite number of composite dimensions, including orders 6 and 14, can be ruled out. Furthermore, a computation-based proof has shown there is no affine plane of order 10 [245, 246].

A set of ℓ mutually orthogonal Latin squares can be extended to an *augmented* set of MO Latin squares which include two additional (non-Latin) squares A and B defined via $A_{ij} = i$ and $B_{ij} = j$. An example of an augmented set of MO Latin squares in $d = 3$ is given by

$$\begin{array}{ccc|ccc|ccc} 0 & 1 & 2 & 0 & 0 & 0 & 0 & 1 & 2 & 0 & 1 & 2 \\ 0 & 1 & 2 & 1 & 1 & 1 & 2 & 0 & 1 & 1 & 2 & 0 \\ 0 & 1 & 2 & 2 & 2 & 2 & 1 & 2 & 0 & 2 & 0 & 1 \end{array} \quad (\text{A.10})$$

where the last two squares are Latin and all four are mutually orthogonal. Each square from an augmented set of MO Latin squares corresponds to a striation of an affine plane, with the points on a line corresponding to distinct integers.

An augmented set of orthogonal Latin squares of size $(\ell + 2)$ is equivalent to a combinatorial design known as a *net*. An algorithm which translates an augmented set of $(\ell + 2)$ MO Latin squares to a *net design* is given in [306]. The resulting net design can be written as a table with $(\ell + 2)$ rows containing d^2 integers, split into d cells of size d . The numbers contained in one cell of a given row are distributed evenly among all cells of any other row. Then, a correspondence

between MU bases and net designs emerges from linking the cells and rows of the net to the exponents of the Heisenberg-Weyl group elements generated by the shift and phase operators X and Z , respectively, defined in Eq. (A.7). Each row of the net corresponds to a subclass of commuting operators from the Heisenberg-Weyl group, and the common eigenstates associated with each commuting set form $(d+1)$ MU bases, as described in Appendix A.4.

Since affine planes also exist in prime-power dimensions, one can generalise the algorithm to construct MU bases for these cases too [306]. However, it was pointed out in [178] that this approach only works for *some* sets of MO Latin squares, and the construction is ultimately based on Galois fields. In particular, it reproduces the method based on Wigner functions described by Gibbons *et al.* [154]. Thus, evidence suggests the link between MU bases and affine planes is due to their association with Galois fields rather than any other, possibly deeper, underlying connection.

The process of constructing MO Latin squares from sets of MU bases can also be reversed, an idea is developed in [177], where complete sets of MU bases for odd prime-powers are used to generate complete sets of MO Latin squares. Two methods are highlighted, one using linear combinations of vectors from MU bases to construct MO Latin squares, while the other one relies on so-called *planar* functions. More similarities between MU bases and affine planes are discussed briefly in Appendix C. Latin and *Quantum* Latin squares, which are related to maximally entangled MU bases in square dimensions [291, 292], are considered in Sec. 6.9.

A.6 Relative difference sets

Relative difference sets (defined below) are a tool from discrete geometry which can be used to construct MU bases. We will summarise results by Godsil and Roy [157] using relative (d, μ, d, λ) -difference sets to obtain $(\mu+1)$ MU bases in $\mathbb{C}^d$.

A difference set D of a group G is a subset in which every element of G (excluding the identity) can be expressed as a difference $d_1 - d_2$ of elements of D in exactly λ ways. A *relative* difference set is defined as follows.

Definition A.1. Let G be a group, N a normal subgroup of G , and R a subset of G such that $|G| = \mu d$, $|N| = \mu$ and $|R| = r$. Then R is a *relative (d, μ, r, λ) -difference set* if there exists λ such that

$$|\{r_{1,2} \in R : r_1 - r_2 = b\}| = \begin{cases} d\mu, & b = 0 \\ 0, & b \in N \setminus \{0\} \\ \lambda, & b \in G \setminus N. \end{cases}$$

A relative difference set is *semi-regular* if $d = r$. A theorem has been established that links semi-regular relative (d, μ, d, λ) -difference sets with MU bases.

Theorem A.1. *The existence of a semi-regular (d, μ, d, λ) -relative difference set in an Abelian group implies the existence of a set of $(\mu+1)$ MU bases of $\mathbb{C}^d$*

By taking a particular finite commutative semi-field of order d , relative difference sets with parameters $(d, d, d, 1)$ can be constructed. The characters of the group G , restricted to the set R , lead to a set of $(d+1)$ MU bases in $\mathbb{C}^d$, as shown in [157]. A relative $(d, d, d, 1)$ -difference set exists only if d is a prime-power [63], thus, this method only finds complete sets for $d = p^n \in \mathbb{PP}$.

The relation of relative difference sets to complete sets of MU bases is also discussed in [45], as well as a link to other combinatorial structures such as planar functions.

A.7 Graph-theoretic constructions

Complete sets of MU bases can be built from *graph-states* generated from a set of graphs, or equivalently, their *adjacency matrices* [348]. A set of p graph-states $|G_b\rangle \in \mathbb{C}^{p^n}$, $b \in \mathbb{Z}_p$, are defined by p different n -vertex graphs (or $n \times n$ adjacency matrices). A graph-state basis is constructed from a state $|G_b\rangle$ by taking as the basis vectors $|G_b(m_1, \dots, m_n)\rangle = Z^{m_1} \otimes \dots \otimes Z^{m_n} |G_b\rangle$ where $m_i \in \mathbb{Z}_p$.

The adjacency matrices which correspond to the MU bases are the same symmetric matrices over $\mathbb{Z}_p$ which appear in the construction of a unitary operator basis (see Sec. A.4). Therefore, the graph-state bases corresponding to A_b and $A_{b'}$ are mutually unbiased if $\det(A_b - A_{b'}) \neq 0 \pmod{p}$. To construct complete sets of MU bases one takes the p^n graph-state bases formed from the graph-states $|G_b\rangle \in \mathbb{C}^{p^n}$ together with

the computational basis. Thus, p^n adjacency matrices $\{A_1, \dots, A_{p^n}\}$ must be found that satisfying the determinant condition. This is exactly the same requirement given by Bandyopadhyay *et al.* [31], and the construction given by Wootters and Fields [401] can be used.

An alternative method to construct matrices A_b using powers and sums of powers of a single symmetric matrix is presented in [348]. In particular, it is possible to find an $n \times n$ symmetric matrix Q over $\mathbb{Z}_p$ such that its characteristic polynomial is irreducible and primitive; this property implies that the set $S = \{Q^i\}_{i=0}^{p^n-2} \cup \{O_n\}$ is a matrix representation of the field $\mathbb{F}_{p^n}$, with respect to matrix addition and multiplication. Here, O_n is the zero matrix of order n .

Since S is a matrix representation of the field $\mathbb{F}_{p^n}$, it contains the required property of the set $\{A_1, \dots, A_{p^n}\}$ that the difference of any two matrices from S is an invertible matrix, i.e. $\det(A_b - A_{b'}) \neq 0 \pmod{p}$. Two methods to construct the matrix Q are provided in [348]: a construction via symmetrised companion matrices which works for any prime-power, and a construction via tridiagonal matrices which works when $d = 2^n$.

Other graph-theoretical constructions of MU bases exist involving clique finding problems in Cayley graphs [8, 424], for example.

A.8 Other constructions and inequivalent complete sets

We now point the curious reader to a few more alternative approaches to construct complete sets of MU bases. Gow [160] establishes a method based on the existence of a unitary matrix whose powers generate MU bases. Gibbons *et al.* [154] start from Wigner functions defined on discrete phase spaces, which are constructed using a two-dimensional phase space (p, q) , taking the coordinates to be elements of the field $\mathbb{F}_d$, with $d \in \mathbb{PP}$ a prime-power. The phase space induces a geometrical way to construct MU bases, with the technique sharing similarities to an earlier construction based on generalised Pauli matrices, maximally commuting classes and finite fields [311]. A distinct feature of the Wigner function approach is that it works for all finite fields, regardless of p being an even or an odd prime.

In 1997, Calderbank *et al.* [92] constructed complete sets using symplectic spreads and

$\mathbb{Z}_4$ -Kerdock codes. An interesting feature here is that *inequivalent* complete sets of MU bases come into play (see Sec. 3.13). In the construction of Calderbank *et al.*, a complete set of MU bases is associated with a symplectic spread, and two such sets are equivalent if and only if their symplectic spreads can be mapped to each other via a symplectic transformation. *Inequivalent* symplectic spreads, which appear in [213, 216], are then used to build inequivalent MU bases, e.g., when $d = 2^n$ and $n > 3$ is odd. Kantor describes this association in [212], and he presents more details on inequivalent MU bases, including examples for $d = p^n$, with odd $p \in \mathbb{P}$. Other constructions of MU bases from symplectic spreads have been developed in [3, 234].

As pointed out in [157], all known complete sets of MU bases (including those derived here) are covered by the construction of Calderbank *et al.* in Ref. [92]. In particular, for odd prime-powers, Wootters' complete set, i.e. Eq. (A.2), is equivalent to Alltop's complete set in Eqs. (A.6) and the set from Bandyopadhyay *et al.*, in Eq. (A.9). For $d = 2^n$, the Klappenecker and Rötteler set in Eq. (A.4) is equivalent to those constructed by Wootters and Fields, and Bandyopadhyay *et al.* The bases from relative $(d, d, d, 1)$ -difference sets are equivalent to the sets found by Klappenecker and Rötteler.

Later, Abdukhalikov [3] studied the relations between various constructions and remarks that "essentially there are only three types of constructions up to now", by which he means those from symplectic spreads, planar functions over fields of odd characteristic, and Gow's construction [160] of cyclic MU bases from a unitary matrix. The latter, he remarks, "seems to be isomorphic to the classical one". A new construction of MU bases from (pseudo-) planar functions over fields of characteristic two is also given, which is shown to relate to symplectic spreads by means of a commutative presemifield.

B Complex Hadamard matrices

First we define the notion of equivalence between complex Hadamard matrices and compare this to the equivalence of MU pairs. For Hadamard matrices, the ordering of the columns and their overall phase factors are not important. Therefore, we can multiply a Hadamard H from the left

by a permutation matrix P_1 and a unitary diagonal matrix D_1 , and the resulting matrix HD_1P_1 is regarded as equivalent to H . Similarly, equivalence is also maintained if we multiply H from the left with permutation and diagonal matrices.

Definition B.1. Two Hadamard matrices H and K are *equivalent*, i.e. $H \sim K$, if they satisfy $H = P_1D_1KD_2P_2$.

It is not known to us whether this mathematical notion of inequivalence has a simple physical interpretation.

A Hadamard matrix is usually expressed in its dephased form with the first row and column having elements $H_{i1} = H_{1j} = 1/\sqrt{d}$. Importantly, if two Hadamard matrices H and K are equivalent, the resulting pairs of MU bases $\{\mathbb{I}, H\}$ and $\{\mathbb{I}, K\}$ are also equivalent (see Sec. 3.13 for the equivalence relations of MU bases). However, two inequivalent Hadamard matrices *may* form equivalent pairs of MU bases. For example, the Fourier matrix and its transpose, F and F^T , are inequivalent but the MU pairs $\{\mathbb{I}, F\}$ and $\{\mathbb{I}, F^T\}$ are equivalent.

One challenge is to deduce whether two Hadamard matrices are equivalent. A useful test involves constructing the Haagerup set $\Lambda(H)$ of the complex Hadamard matrix H defined as

$$\Lambda(H) = \{H_{pq}H_{qr}^*H_{rs}H_{sp}^* : p, q, r, s = 1, \dots, d\}, \quad (\text{B.1})$$

where H_{ij}^* denotes the complex conjugation of the matrix element H_{ij} [174]. The Haagerup set is invariant under equivalence transformations so that two matrices H and K with *different* Haagerup sets are necessarily *inequivalent*.

A Hadamard matrix H can be *isolated*, which means that all Hadamard matrices in its immediate neighbourhood are equivalent to it [361]. Otherwise, H is a member of a family of Hadamard matrices depending on continuous parameters. Different types of parameter dependence can be distinguished.

Definition B.2. An *affine* family of Hadamard matrices is a set $H(\mathcal{R})$ stemming from a Hadamard matrix H of order d , where

$$H(\mathcal{R}) = \{H \circ \text{EXP}(i \cdot R) : R \in \mathcal{R}\}, \quad (\text{B.2})$$

and $\mathcal{R}$ is a subspace of all real matrices of order d with zeros in the first row and column.

Here the notation $\circ$ is the entry-wise product of matrices known as the Hadamard (or Schur) product, and $\text{EXP}(\cdot)$ is the entry-wise exponential function acting on a matrix. Families not of the form (B.2) are called *non-affine*.

An upper bound on the number of free parameters for the set of matrices stemming from H is given by the *defect* $\text{def}(H)$ of the matrix, introduced in Ref. [361]. It is defined by multiplying the elements of the *core* of the matrix with free phase factors and solving the unitary condition on H to first order; the core consists of all elements different from the first row and column.

Definition B.3. The defect $\text{def}(H)$ of a complex Hadamard matrix H equals the dimension of the solution space of the real linear system of equations with respect to a matrix variable $R \in \mathbb{R}^{d \times d}$:

$$\sum_{\ell=1}^d H_{j\ell}H_{k\ell}^*(R_{j\ell} - R_{k\ell}) = 0, \quad 1 \leq j < k \leq d, \quad (\text{B.3})$$

and $R_{11} = R_{1s} = R_{s1} = 0$ for $s = 2 \dots d$.

Ref. [49] provides an instructive example. When d is large a computer program is usually necessary to determine the value of $\text{def}(H)$. The defect is useful to identify *isolated* Hadamard matrices [361].

Lemma B.1. A dephased Hadamard matrix H is isolated if its defect is zero.

The *span condition* [299] represents an alternative method to determine if a matrix is isolated: For a given $d \times d$ Hadamard matrix H , the dimension of the vector space $\text{span}\{uv - vu : u \in \mathcal{D}, v \in H^*\mathcal{D}H\}$ must equal $(d-1)^2$, where $\mathcal{D}$ is the algebra of diagonal matrices. It is presently unknown if isolation is equivalent to the span condition or if there exist matrices with non-zero defect that are not part of any family.

The defect provides an upper bound on the dimensionality of families of Hadamard matrices but is not necessarily sharp. Including higher order equivalents of Def. B.3 (which is based on the first order calculation (B.3)) can lead to sharper upper bounds [38]. As an example, the Fourier matrix F_d , with $F_{ij} = \omega^{ij}/\sqrt{d}$ and $\omega = e^{2\pi i/d}$, has defect

$$\text{def}(F_d) = \sum_{n=1}^{d-1} (\text{gcd}(n, d) - 1). \quad (\text{B.4})$$

This gives an upper bound on any smooth (dephased) family of Hadamard matrices travelling through F_d . The bound is saturated when d is a prime-power. However, the dimension of the largest smooth family stemming from F_d is strictly *less* than the defect for $6 < d \leq 100$ when d is not a prime or prime-power [38]. The $d = 6$ case seems to be special: the defect of F_6 is four and there exists of a four-parameter family which is likely to contain F_6 [38, 345] (cf. Sec. 7.1).

Furthermore, it seems that the bound on the dimension of a smooth family stemming from the Fourier matrix depends on the prime decomposition of d . It has so far not been possible to find an exact bound for arbitrary d —we have to make do with a conjecture: if $d = p_1 p_2^2$ then there is a family of Hadamard matrices stemming from F_d which has $(3p_1 p_2^2 - 3p_1 p_2 - 2p_2^2 + p_2 + 1)$ free parameters [38]. Since we know that Hadamard matrices correspond to pairs of complementary bases, this result is another indication that the geometry of the quantum state space depends heavily on the number theoretic properties of the dimension d .

C MU bases and affine planes

In Appendix A.5 we discussed constructions of MU bases based on affine planes. It is known that affine planes of order d exist if d is a prime or a prime-power; for certain composite dimensions such as $d = 6$, however, affine planes do not exist. In fact, the Bruck-Ryser theorem states that no affine plane of order d exists if $(d - 1)$ or $(d - 2)$ is divisible by four and d is not the sum of two squares [82]. Numerical computations also ruled out their existence for $d = 10$ [245].

These results bear a striking resemblance to the MU existence problem which has led to a conjecture establishing a possible link with projective planes [326]:

Conjecture C.1. *The non-existence of a projective plane of order d implies that there are fewer than $(d + 1)$ MU bases in the corresponding Hilbert space $\mathbb{C}^d$, and vice versa.*

A projective rather than an affine plane is used here, but the two objects are essentially the same in the current context. One can construct an affine plane from a projective plane by removing a single line along with all the points it contains. A

potential link between MU bases and affine planes was perhaps first mentioned in [229].

While no rigorous association between affine planes and MU bases is known, it has been suggested by Wootters [403] to associate lines λ with projection operators P_λ , projecting onto orthogonal quantum states. A set of d parallel lines then corresponds to a basis of d orthogonal projection operators satisfying $\sum_\lambda P_\lambda = 1$, and two non-parallel lines with associated projection operators P_λ and P_ν satisfy $\text{Tr}[P_\lambda P_\nu] = 1/d$. In this way, the $(d + 1)$ *striations* of an affine plane correspond to a set of $(d + 1)$ MU bases. An obvious question arises about the role of the d^2 points in such a correspondence. In [403], a point α is chosen to represent a Hermitian operator A_α/d such that (i) $\text{Tr}[A_\alpha/d] = 1/d$; (ii) $\text{Tr}[A_\alpha A_\beta/d^2] = \delta_{\alpha\beta}/d$; and (iii) $\sum_{\alpha \in \lambda} (A_\alpha/d) = P_\lambda$ hold. Unfortunately, in this scheme the existence of $(d + 1)$ striations does not imply the existence of a complete set of MU bases since it is not known how to construct the operators A_α .

Caution, however, should be taken with the similarities between affine planes and MU bases since some unexpected differences appear between them [389]. A mismatch arises when considering mutually unbiased *constellations*, that is, sets of vectors which are either orthogonal or mutually unbiased (see Sec. 8.3). A numerical search is unable to find a MU constellation consisting of three MU bases together with four orthogonal states [78]. On the other hand, the largest *affine constellation* contains three striations, each with six lines, and an additional set of four parallel lines. An affine constellation is defined as a set of points and lines such that any two lines within a set do not intersect, and any pair of lines from different sets have one point in common. Thus, if an affine constellation does not exist, then neither will an affine plane. If there is a connection between affine planes and MU bases such that parallel lines correspond to orthonormal bases and intersecting ones to MU states, as suggested by Wootters [403], one would expect the structure of affine and MU constellations to be similar, if not identical—which seems not to be the case.

Another discrepancy appears when considering the behaviour of MU bases and affine planes in the limit of ever larger dimensions, $d \rightarrow \infty$. It was shown by Chowla *et al.* [115] that the number of

mutually orthogonal Latin squares approaches infinity as $d \rightarrow \infty$, while only three MU bases (with basis-independent overlaps) have been found in the infinite-dimensional Hilbert space $L^2(\mathbb{R})$ [390] (cf. Sec. 9.13).