## Unextendible Mutually Unbiased Bases in Prime-Squared Dimensions

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Two orthonormal bases  $\mathcal{A} = \{|a_i\rangle, i = 1, ..., d\}$  and  $\mathcal{B} = \{|b_j\rangle, j = 1, ..., d\}$  of a *d*-dimensional Hilbert space  $\mathbb{C}^d$  are said to be **mutually unbiased** if for all basis vectors  $|a_i\rangle \in \mathcal{A}$  and  $|b_j\rangle \in \mathcal{B}$ ,

$$|\langle a_i|b_j\rangle| = \frac{1}{\sqrt{d}}, \forall i, j = 1, \dots, d.$$

In other words, if a physical system is prepared in an eigenstate of basis  $\mathcal{A}$  and measured in basis  $\mathcal{B}$ , all outcomes are equally probable. A set of orthonormal bases  $\{\mathcal{B}_1, \mathcal{B}_2, \ldots, \mathcal{B}_m\}$  in  $\mathbb{C}^d$  is called a set of mutually unbiased bases (MUBs) if every pair of bases in the set is mutually unbiased.

MUBs form a minimal and optimal set of orthogonal measurements for quantum state tomography [1, 2]. Such bases play an important role in our understanding of complementarity in quantum mechanics [3] and are central to quantum information tasks such as entanglement detection [4], information locking [5], and quantum cryptography [6, 7]. MUBs correspond to measurement bases that are most 'incompatible', as quantified by uncertainty relations [8] and other incompatibility measures [9, 10], and, the security of quantum cryptographic tasks relies on this property of MUBs. In particular, protocols based on higher-dimensional quantum systems with larger numbers of unbiased basis sets can have certain advantages over those based on qubits [11, 12]. It is therefore important for cryptographic applications to identify sets of MUBs in higher-dimensional systems that satisfy strong uncertainty relations.

The maximum number of MUBs that can exist in a *d*-dimensional Hilbert space is d + 1 and explicit constructions of such complete sets are known when *d* is a prime power [2, 13, 14]. One such construction is based on forming *mutually disjoint maximal commuting classes* from a unitary operator basis. Specifically, consider a set  $\mathcal{U}$  of  $d^2$  unitary operators that forms a basis for the space of  $d \times d$  complex matrices. If there exist subsets  $\{\mathcal{C}_1, \mathcal{C}_2, \ldots, \mathcal{C}_L | \mathcal{C}_j \subset \mathcal{U} \setminus \{\mathcal{I}\}\}$  of size  $|\mathcal{C}_j| = d - 1$  such that, (a) the elements of  $\mathcal{C}_j$  commute for all  $1 \leq j \leq L$  and (b)  $\mathcal{C}_j \cap \mathcal{C}_k = \emptyset$ for all  $j \neq k$ , then, it was shown in [13] that the common eigenbases of L such disjoint maximal commuting classes form a set of L mutually unbiased bases.

When the unitary basis is comprised of the generalized Pauli operators, this approach provides a construction of a complete set of d+1 MUBs in prime-power dimensions  $(d = p^n)$ . In terms of the computational basis  $\{|j\rangle, j = 1, ..., p\}$ , the generalized Pauli operators  $\mathcal{X}_p, \mathcal{Z}_p$  (also the generators of the Weyl-Hiesenberg group) in *p*-dimensions are given by

$$\mathcal{X}_p|j\rangle = |(j+1)mod p\rangle; \quad \mathcal{Z}_p|j\rangle = e^{i2\pi j/p}|j\rangle.$$

Now, let  $\mathcal{U}_{p,n}$  be the set of unitaries in dimension  $d = p^n$  that are generated as *n*-fold tensor products of products of  $\mathcal{X}_p$  and  $\mathcal{Z}_p$ . Then, it was shown that the set  $\mathcal{U}_{p,n}/\{\mathbb{I}\}$  can always be partitioned into such a set of d + 1 maximal commuting classes in  $d = p^n$  dimensions, their common eigenbases forming a complete set of d + 1 MUBs [13].

However, in non-prime-power dimensions, the question of whether a complete set of MUBs exists remains unresolved. Related to the question of finding complete sets of MUBs is the important concept of unextendible sets of MUBs. A set of MUBs  $\{\mathcal{B}_1, \mathcal{B}_2, \ldots, \mathcal{B}_m\}$  in  $\mathbb{C}^d$  is said to be unextendible if there does not exist another basis in  $\mathbb{C}^d$  that is unbiased with respect to all the bases  $\mathcal{B}_j, j = 1, \ldots, m$ . Examples of such unextendible sets are known in the literature. In dimension d = 6, the three eigenbases of  $\mathcal{X}_6, \mathcal{Z}_6$  and  $\mathcal{X}_6\mathcal{Z}_6$  were shown to be an unextendible set of MUBs [15]. This has the important consequence that the eigenbases of Weyl-Hiesenberg generators will not lead to a complete set of 7 MUBs in d = 6. In fact, several distinct families of unextendible triplets of MUBs have been constructed in d = 6 [16–18]. Moving away from six dimensions, the set of three MUBs obtained in d = 4 using Mutually Orthogonal Latin Squares (MOLS) [19] is an example of an unextendible set of MUBs in prime-power dimensions [20].

More recently, a systematic construction of such smaller sets that are unextendible to a complete set was obtained for two- and three-qubit systems [21]. Specifically, it was shown that there exist smaller sets of  $k = \frac{d}{2} + 1$  commuting classes  $\{C_1, C_2, \ldots, C_k\}$  in  $d = 2^n$  that are *unextendible* in the following sense—no more maximal commuting classes can be formed out of the remaining *n*-qubit Pauli operators that are not contained in  $C_1 \cup C_2 \ldots \cup C_k$ . The eigenbases of  $\{C_1, \ldots, C_k\}$ thus constitute a **weakly unextendible** set of *k* MUBs which cannot be extended to a complete set of d + 1 MUBs using Pauli classes. While an explicit construction of such unextendible classes was provided for d = 4, 8, their existence was conjectured for  $d = 2^n (n > 3)$ . This conjecture has been further improved upon [22] using a correspondence between unextendible sets of MUBs and maximal partial spreads of the polar space formed by the *n*-qubit Pauli operators [23].

Here, we show the existence of weakly unextendible sets of MUBs in prime-squared dimensions  $d = p^2$ , where p is prime. Each basis is realized as the common eigenbasis of a maximal commuting class of tensor products of the generalized Pauli operators. While the existence of unextendible sets of classes in  $d = p^2$  has been shown recently using the geometry of symplectic polar spaces [22], we provide an algebraic construction which makes it easier to visualize the corresponding bases. Our construction also brings to light an interesting connection between the existence of unextendible sets of p + 1 MUBs that saturate both a Shannon and a collision EUR in  $d = p^2$ . We merely state our results here and refer to the technical supplement [28] for further details and proofs.

## First Result: [Unextendible sets of $p^2 - p + 2$ classes in $d = p^2$ for $p \ge 3$ ]

Given  $\mathcal{U}_{p,2}$ , the set of unitaries in  $d = p^2$  generated by  $\mathcal{X}_p$  and  $\mathcal{Z}_p$ , we provide an explicit construction of unextendible sets of  $N(p) = p^2 - p + 2$  classes for  $p \ge 3$ . For the case of  $p \ge 3$ , our construction crucially relies on the following fact: there exist a set of p+1 classes that are a part of the complete set of  $p^2 + 1$  classes out of which, exactly 2 more maximal commuting classes can be formed. Therefore, these two new classes along with the remaining  $p^2 - p$  classes form an unextendible set of N(p) classes.

**Example in** p = 3, d = 9: Consider the following four maximal commuting classes which are part of a complete set of ten classes –  $\{C_1, C_2, \ldots, C_{10}\}$  – in  $d = 3^2$ :

Note that we describe each class  $C_i$  in terms of their generators – the remaining operators in the class are simply realized as higher powers and products of these [29]. From the elements of

$$\begin{array}{ll} \mathcal{C}_{I} &= \left\langle \ \mathcal{I} \otimes \mathcal{X}_{3} \mathcal{Z}_{3}^{2}, \ \mathcal{Z}_{3} \otimes \mathcal{X}_{3} \mathcal{Z}_{3}^{2} \ \right\rangle \\ \mathcal{C}_{II} &= \left\langle \ \mathcal{X}_{3} \mathcal{Z}_{3} \otimes \mathcal{I}, \ \mathcal{X}_{3} \mathcal{Z}_{3} \otimes \mathcal{X}_{3}^{2} \mathcal{Z}_{3}^{2} \ \right\rangle \end{array}$$

 $C_I, C_{II}$  contain exactly two elements from each of the four classes. Since no more maximal commuting classes can be formed using the elements of  $C_1, C_2, C_3, C_4$ , the new classes  $C_I, C_{II}$  along with the remaining classes  $\{C_5, C_6, \ldots, C_{10}\}$  constitute an unextendible set of 8 classes in  $d = 3^2$  dimensions. The common eigenbasis of such an unextendible set of maximal commuting classes form a weakly unextendible set of 8 MUBs in a nine dimensional space.

## Second Result: [Tightness of Shannon and $H_2$ EURs in $d = p^2$ ]

We further show that the existence of unextendible classes implies the tightness of an entropic uncertainty relation (EUR) for the Rényi entropy of order 2 -  $H_2$  (also known as the collision entropy [30]) in primesquared dimensions. In particular, given a set of p + 1 classes such that one more class  $C_I$  can be formed using the operators in the set, their common eigenbases  $\{\mathcal{B}_1, \mathcal{B}_2, \ldots, \mathcal{B}_{p+1}\}$  satisfy,

$$\frac{1}{p+1} \inf_{|\psi\rangle \in \mathbb{C}^{p^2}} \left[ \sum_{i=1}^{p+1} H_2(\mathcal{B}_i ||\psi\rangle) \right] = \log p = \frac{1}{2} \log d .$$
 (1)

Equality is attained for common eigenstates of the new class  $C_I$ . In other words, if the set of p + 1 classes corresponding to a given set of p + 1 MUBs are such that they give rise to an unextendible set of classes, then, the set of MUBs saturates the well known  $H_2$  EUR [8]. The minimum uncertainty is attained for states that "look alike" with respect to each of the p+1 MUBs [24]. Our result generalizes an earlier observation that the  $H_2$  EUR is tight for sets of 3 MUBs in d = 4 dimensions [21]. It further shows that the connection between the existence of unextendible classes and the tightness of this EUR which was earlier observed for only  $d = 2^2$  holds for any prime-squared dimensions.

Finally, we also note that such a set of p+1 classes – out of whose elements one more maximal commuting class can be formed – also leads to a tight Shannon EUR for the corresponding MUBs. In other words,  $\mathcal{B}_1, \mathcal{B}_2, \ldots, \mathcal{B}_{p+1}$  satisfy,

$$\frac{1}{p+1} \inf_{|\psi\rangle \in \mathbb{C}^{p^2}} \left[ \sum_{i=1}^{p+1} H_2(\mathcal{B}_i ||\psi\rangle) \right] = \log p = \frac{1}{2} \log d .$$

$$\tag{2}$$

Equality is again achieved by common eigenstates of the new class formed by picking a pair of elements from each of the p + 1 classes. Note that this lower bound on the average Shannon entropy is in fact a *trivial* consequence of the Maassen-Uffink bound [25] for a pair of bases. It has been noted earlier that there exist sets of upto p + 1 MUBs in prime-squared dimensions constructed using the generalized Pauli operators that saturate the lower bound [26] in Eq (2). However, the question of identifying such a set of MUBs that satisfy a trivial Shannon EUR remains unresolved [8]. Here, we make some progress towards answering this question.

**Applications:** Two simple corollaries follow from the tightness of the Shannon EUR. The fact that the set of p + 1 MUBs satisfies a weak lower bound implies that such a set of MUBs cannot give a better locking result than just using a pair of MUBs [5]. On the other hand, such MUBs can be used to witness entanglement in  $d \otimes d$  systems [27]. If a state  $|\psi\rangle \in \mathbb{C}^{p^2} \otimes \mathbb{C}^{p^2}$  violates the Shannon EUR lower bound in Eq. (2), then, it must be entangled. However, this is not a necessary condition for the state to be entangled: there could exist entangled state that satisfy the EUR bound.

**Conclusions:** We show by explicit construction the existence of unextendible sets of  $N(p) = p^2 - p + 2$  MUBs in prime squared  $(d = p^2)$  dimensions for  $p \ge 3$ . Our construction is based on grouping the generalized Pauli operators in these dimensions into sets of mutually disjoint, maximal commuting classes that are unextendible to a complete set of (d+1) classes. We further demonstrate a general connection between the existence of unextendible sets and the tightness of an entropic uncertainty relation.

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- [29] For example, the class  $C_i = \langle U_i, V_i \rangle$  in  $d = 3^2$  is comprised of the following set of d 1 = 8 operators:  $C_i = \{U_i, V_i, U_i^2, V_i^2, U_i V_i, (U_i)^2 V_i, U_i V_i^2, U_i^2 V_i^2\}$
- [30] The collision entropy  $H_2$  of the distribution obtained by measuring state  $|\psi\rangle$  in the measurement basis  $\mathcal{B}_i = \{|b_i^{(j)}\rangle: j = 1, ..., d\}$  is defined as,  $H_2(\mathcal{B}_i||\psi\rangle) = -\log \sum_{j=1}^d (|\langle b_i^{(j)}|\psi\rangle|^2)^2$ .