A new proof for the existence of mutually unbiased bases^{*}

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Abstract

We develop a strong connection between maximally commuting bases of orthogonal unitary matrices and mutually unbiased bases. A necessary condition of the existence of mutually unbiased bases for any finite dimension is obtained. Then a constructive proof of the existence of mutually unbiased bases for dimensions that are powers of primes is presented. It is also proved that in any dimension d the number of mutually unbiased bases is at most d + 1. An explicit representation of mutually unbiased observables in terms of Pauli matrices are provided for $d = 2^m$.

1 Introduction

A *d*-level quantum system is described by a density operator ρ that requires $d^2 - 1$ real numbers for its complete specification. A maximal orthogonal quantum test performed on such a system has, without degeneracy, *d* possible outcomes, providing d - 1 independent probabilities. It follows that in principle one requires at least d + 1 different orthogonal measurements for complete state determination.

Since the quantum mechanical description of a physical system is characterized in terms of probabilities of outcomes of conceivable experiments consistent with quantum formalism, in order to obtain full information about the system under consideration we need to perform measurements on a large number of identically prepared copies of the system. The different measurements are performed on several subensembles. However, there may be redundancy in the measurement results as the probabilities will

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not, in general, be independent of each other unless a minimal set of measurements satisfying appropriate criteria is specified. This minimal set need not be necessarily optimal in the sense it may not serve the best way to ascertain the quantum state. However, intuitively speaking, a minimal set of measurements can be reasonably close to an optimal set if they mutually differ as much as possible, thereby ruling out possible overlaps in the results which become crucial in case of error prone measurements. The characterization and proving the existence of such a minimal set of measurements for complete quantum state determination is therefore of fundamental importance.

It has been shown that measurements in a special class of bases, i.e. mutually unbiased bases, not only form a minimal set but also provide the optimal way of determining a quantum state. Mutually unbiased measurements (MUM), loosely speaking, correspond to measurements that are as different as they can be so that each measurement gives as much new information as one can obtain from the system under consideration. In other words the MUM operators are maximally noncommuting among themselves. If the result of one MUM can be predicted with certainty, then all possible outcomes of every other measurement, unbiased to the previous one are equally likely.

As noted earlier mutually unbiased bases (MUB) have a special role in determining the state of a finite dimensional quantum system. Ivanovic [10] first introduced the concept of MUB in the context of quantum state determination, where he proved the existence of such bases when the dimension is a prime by an explicit construction. Later Wootters and Fields [16] showed that measurements in MUB provide the minimal as well as optimal way of complete specification of the density matrix. The optimality is understood in the sense of minimization of statistical errors in the measurements. By explicit construction they showed the existence of MUB for prime power dimensions and proved that for any dimension *d* there can be at most d + 1 MUB. However the existence of MUB for other composite dimensions which are not power of a prime still remains an open problem.

In this paper we give a constructive proof of the results earlier obtained by Ivanovic, Wootters, and Fields [10, 16] with a totally different method. The two distinct features of our new proof are:

- Our approach is based on developing an interesting connection between maximal commuting bases of orthogonal unitary matrices and mutually unbiased bases, whereby we find a necessary condition for existence of MUB in any dimension. We then provide a constructive proof of existence of MUB in composite dimensions which are power of a prime. This allows us to connect encryption of quantum bits [3], which uses unitary bases of operators, to quantum key distribution, which uses mutually unbiased bases of quantum systems.
- Another advantage of our method is that we provide an explicit construction of the MUB observables (operators) as tensor product of the Pauli matrices for dimensions $d = 2^m$. This answers a critical related question: how can these mutually unbiased measurements be actually performed and

what are the observables to which these measurements correspond to. When d = 2 the mutually unbiased operators are the three Pauli matrices, but unfortunately this observation cannot be generalized in a straightforward way to higher dimension. In addition to the obvious importance of mutually unbiased bases in the context of quantum state determination and foundations of quantum mechanics, recently it has also found useful applications in quantum cryptography where it has been demonstrated that using higher dimensional quantum systems for key distribution has possible advantages over qubits, and mutually unbiased bases play a key role in such a key distribution scheme [1, 2]. Thus the fact that we provide an explicit construction of the MUB observables can turn out to be crucial in the application of MUB in quantum cryptography with systems with more than two states.

Before continuing it is useful to provide a formal definition of mutually unbiased bases.

Definition. Let $B_1 = \{|\varphi_1\rangle, \dots, |\varphi_d\rangle\}$ and $B_2 = \{|\psi_1\rangle, \dots, |\psi_d\rangle\}$ be two orthonormal bases in the *d* dimensional state space. They are said to be **mutually unbiased bases** (**MUB**) if and only if $|\langle \varphi_i | \psi_j \rangle| = \frac{1}{\sqrt{d}}$, for every $i, j = 1, \dots, d$. A set $\{\mathcal{B}_1, \dots, \mathcal{B}_m\}$ of orthonormal bases in \mathbb{C}^d is called a *set of mutually unbiased bases* (a set of MUB) if each pair of bases \mathcal{B}_i and \mathcal{B}_j are mutually unbiased.

The simplest example of a complete set of MUB is obtained in the case of spin 1/2 particle where each unbiased basis consists of the normalized eigenvectors of the three Pauli matrices respectively. However, the analysis of a set of MUB corresponding to a two level quantum system does not capture one of the basic features of MUB, i.e., its importance in determining the quantum state. In the case of two level systems, the density operator has three independent parameters and almost any choice of the three measurements is sufficient to have the complete knowledge of the system. This is not true in general for any other dimension greater than two, where the existence of MUB becomes more crucial in the context of minimal number of required measurements for quantum state determination.

In Section 2 we show the existence of p + 1 MUB in the space \mathbb{C}^p , for any prime p. This result first shown by Ivanovic [10] by explicitly defining the mutually unbiased bases. Here we show that these bases are in fact bases each consists of eigenvectors of the unitary operators

$$Z, X, XZ, \ldots, XZ^{d-1},$$

where X and Z are generalizations of Pauli operators to the quantum systems with more than two states (see, e.g., [8, 9]).

In Section 3 we show that there is a useful connection between mutually unbiased bases and special types of bases for the space of the square matrices. These bases consist of orthogonal unitary matrices which can be grouped in maximal classes of commuting matrices. As a result of this connection we show that every MUB over \mathbb{C}^d consists of at most d + 1 bases.

Finally, in Section 4 we present our construction of MUB over \mathbb{C}^d when d is a prime power. The basic idea of our construction is as follows. When $d = p^m$, imagine the system consists of m subsystems each of dimension p. Then the total number of measurements on the whole system, viewed as performing measurement on every subsystem in their respective MUB is $(p + 1)^m$. We show that these $(p + 1)^m$ operators fall into $p^m + 1$ maximal noncommuting classes where members of each class commute among themselves. The bases formed by eigenvectors of each such mutually noncommuting class are mutually unbiased. It should be mentioned that the operators in each maximal commuting class have the same structure as the **stabilizers** of *additive quantum error correcting codes* (see, e.g., [4, 6, 8]).

One of the referees has brought to our attention that there is a close connection between the MUB problem and the problem of determining arrangements of lines in the Grassmannian spaces so that they are as far apart as possible [5] (see also [7]). This problem (and some other combinatorial problems discussed in [5]) can be related to the problem of finding the maximum number of lines through the origin of \mathbb{C}^d that are either perpendicular or are at angle θ , where $\cos \theta = 1/\sqrt{d}$. Any MUB \mathcal{M} defines such a line–set: consider all lines through the origin defined by all vectors in the bases of \mathcal{M} . In [5], for the case of $d = 2^m$, with an approach similar to the one presented in this paper, such line–sets are constructed.

Notation. Let $\mathbb{M}_d(\mathbb{C})$ be the set of $d \times d$ complex matrices. In a natural way, the set $\mathbb{M}_d(\mathbb{C})$ is a d^2 -dimensional linear space. Each matrix A in $\mathbb{M}_d(\mathbb{C})$ can be also naturally considered as a d^2 -dimensional complex vector $|v_A\rangle$, where the entries of the matrix A being regarded as the components of the vector $|v_A\rangle$. In this way, for matrices $A, B \in \mathbb{M}_d(\mathbb{C})$ we can define the inner product $\langle A, B \rangle$ of matrices as the inner product $\langle v_A | v_B \rangle$ of vectors. It is easy to check that

$$\langle A, B \rangle = \operatorname{Tr}(A^{\dagger}B).$$

We say the matrices $A, B \in \mathbb{M}_d(\mathbb{C})$ are **orthogonal** if and only if $\langle A, B \rangle = 0$.

2 Construction of sets of MUB for prime dimensions

Ivanovic [10] for the first time showed that for any prime dimension d, there is a set of d + 1 mutually unbiased bases. In that paper the bases are given explicitly. Here we show that there is a nice symmetrical structure behind these bases, and their existence can be derived as a consequence of properties of Pauli operators on d-state quantum systems. The core of our construction is the following theorem.

Theorem 2.1 Let $\mathcal{B}_1 = \{ |\varphi_1\rangle, \dots, |\varphi_d\rangle \}$ be an orthonormal basis in \mathbb{C}^d . Suppose that there is a unitary operator V such that $V |\varphi_j\rangle = \beta_j |\varphi_{j+1}\rangle$, where $|\beta_j| = 1$ and $|\varphi_{d+1}\rangle = |\varphi_1\rangle$; i.e., V applies a cyclic shift modulo a phase on the elements of the basis \mathcal{B}_1 . Assume that the orthonormal basis $\mathcal{B}_2 = \{ |\psi_1\rangle, \dots, |\psi_d\rangle \}$ consists of eigenvectors of V. Then \mathcal{B}_1 and \mathcal{B}_2 are MUB.

Proof. Assume that $V |\psi_k\rangle = \lambda_k |\psi_k\rangle$. Then $|\lambda_k| = 1$. Now, for every $k = 1, \ldots, d$, we have

$$\begin{aligned} |\langle \psi_k | \varphi_1 \rangle| &= |\lambda_k^* \langle \psi_k | V | \varphi_1 \rangle| \\ &= |\beta_1 \langle \psi_k | \varphi_2 \rangle| \\ &= |\langle \psi_k | \varphi_2 \rangle|. \end{aligned}$$

A similar argument shows

$$|\langle \psi_k | \varphi_1 \rangle| = |\langle \psi_k | \varphi_2 \rangle| = \cdots = |\langle \psi_k | \varphi_d \rangle|.$$

Therefore,

$$|\langle \psi_k | \varphi_j \rangle|^2 = \frac{1}{d}, \qquad 1 \le j \le d.$$

Thus \mathcal{B}_1 and \mathcal{B}_2 are MUB.

Throughout this section, we suppose that d is a prime number, and *all algebraic operations are modulo* d. We consider $\{ |0\rangle, |1\rangle, \ldots, |d-1\rangle \}$ as the standard basis of \mathbb{C}^d . We define the unitary operators X_d and Z_d over \mathbb{C}^d , as a natural generalization of Pauli operators σ_x and σ_z :

$$X_d |j\rangle = |j+1\rangle, \qquad (1)$$

$$Z_d \left| j \right\rangle = \omega^j \left| j \right\rangle, \tag{2}$$

where ω is a d^{th} root of unity; more specifically $\omega = \exp(2\pi i/d)$. We are interested in unitary operators of the form $X_d (Z_d)^k$. Note that

$$X_d \left(Z_d \right)^k \left| j \right\rangle = \left(\omega^k \right)^j \left| j + 1 \right\rangle.$$

Theorem 2.2 For $0 \le k, \ell \le d-1$, the eigenvectors of $X_d (Z_d)^k$ are cyclically shifted under the action of $X_d (Z_d)^{\ell}$.

Proof. The eigenvectors of $X_d (Z_d)^k$ are

$$\left|\psi_{t}^{k}\right\rangle = \frac{1}{\sqrt{d}} \sum_{j=0}^{d-1} \left(\omega^{t}\right)^{d-j} \left(\omega^{-k}\right)^{s_{j}} \left|j\right\rangle, \qquad t = 0, \dots, d-1,$$
(3)

where $s_j = j + \dots + (d-1)$. Then $|\psi_t^k\rangle$ is an eigenvector of $X_d (Z_d)^k$ with eigenvalue ω^t , because

$$\begin{aligned} X_{d} \left(Z_{d} \right)^{k} \left| \psi_{t}^{k} \right\rangle &= \frac{1}{\sqrt{d}} \sum_{j=0}^{d-1} \left(\omega^{t} \right)^{d-j} \left(\omega^{-k} \right)^{s_{j}} \left(\omega^{k} \right)^{j} \left| j+1 \right\rangle \\ &= \frac{1}{\sqrt{d}} \sum_{j=0}^{d-1} \left(\omega^{t} \right)^{d-j} \left(\omega^{-k} \right)^{s_{j+1}} \left| j+1 \right\rangle \\ &= \frac{1}{\sqrt{d}} \sum_{j=0}^{d-1} \left(\omega^{t} \right)^{d-j+1} \left(\omega^{-k} \right)^{s_{j}} \left| j \right\rangle \\ &= \omega^{t} \left| \psi_{t}^{k} \right\rangle. \end{aligned}$$

The action of $X_d \, (Z_d)^\ell$ on $\left| \psi^k_t \right\rangle$ is as follows:

$$X_{d} (Z_{d})^{\ell} \left| \psi_{t}^{k} \right\rangle = \frac{1}{\sqrt{d}} \sum_{j=0}^{d-1} (\omega^{t})^{d-j} (\omega^{-k})^{s_{j}} (\omega^{\ell})^{j} \left| j + 1 \right\rangle$$

$$= \frac{1}{\sqrt{d}} \sum_{j=0}^{d-1} (\omega^{t})^{d-j+1} (\omega^{-k})^{s_{j-1}} (\omega^{\ell})^{j-1} \left| j \right\rangle$$

$$= \frac{\omega^{t-\ell}}{\sqrt{d}} \sum_{j=0}^{d-1} (\omega^{t})^{d-j} (\omega^{-k})^{s_{j}} (\omega^{-k})^{j-1} (\omega^{\ell})^{j} \left| j \right\rangle$$

$$= \frac{\omega^{t+k-\ell}}{\sqrt{d}} \sum_{j=0}^{d-1} (\omega^{t})^{d-j} (\omega^{-k})^{s_{j}} (\omega^{\ell-k})^{j} \left| j \right\rangle$$

$$= \frac{\omega^{t+k-\ell}}{\sqrt{d}} \sum_{j=0}^{d-1} (\omega^{t+k-\ell})^{d-j} (\omega^{-k})^{s_{j}} \left| j \right\rangle$$

$$= \omega^{t+k-\ell} \left| \psi_{t+k-\ell}^{k} \right\rangle.$$

Note that the standard basis $\{ |0\rangle, |1\rangle, \dots, |d-1\rangle \}$ is the set of the eigenvectors of Z_d . From (3) it follows that the $|\langle j | \psi_t^k \rangle|^2 = \frac{1}{d}$. Therefore, we have proved the following construction.

Theorem 2.3 For any prime d, the set of the bases each consisting of the eigenvectors of

$$Z_d, X_d, X_d Z_d, X_d (Z_d)^2, \dots, X_d (Z_d)^{d-1},$$

form a set of d + 1 mutually unbiased bases.

Example d = 2. By Theorem 2.3, the eigenvectors of the operators σ_z , σ_x , and $\sigma_x \sigma_z$ form a set of mutually unbiased bases; i.e., the following set

$$\begin{split} \left\{ \begin{vmatrix} 0 \rangle \,, \lvert 1 \rangle \right\}, \\ \left\{ \frac{\lvert 0 \rangle + \lvert 1 \rangle}{\sqrt{2}}, \frac{\lvert 0 \rangle - \lvert 1 \rangle}{\sqrt{2}} \right\}, \\ \left\{ \frac{\lvert 0 \rangle + i \lvert 1 \rangle}{\sqrt{2}}, \frac{\lvert 0 \rangle - i \lvert 1 \rangle}{\sqrt{2}} \right\}. \end{split}$$

Example d = 3. The set of the eigenvectors of the following unitary matrices form a set of MUB (here $\omega = \exp(2\pi i/3)$):

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \qquad \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}, \qquad \begin{pmatrix} 0 & 0 & \omega^2 \\ 1 & 0 & 0 \\ 0 & \omega & 0 \end{pmatrix}, \qquad \begin{pmatrix} 0 & 0 & \omega \\ 1 & 0 & 0 \\ 0 & \omega^2 & 0 \end{pmatrix}.$$

3 Bases for unitary operators and MUB

In this section we study the close relation between MUB and a special type of bases for $\mathbb{M}_d(\mathbb{C})$. Here we are dealing with classes of commuting unitary matrices. The following lemma shows that the maximum size of such class is d.

Lemma 3.1 There are at most d pairwise orthogonal commuting unitary matrices in $\mathbb{M}_d(\mathbb{C})$.

Proof. Let A_1, \ldots, A_m be pairwise orthogonal commuting unitary matrices in $\mathbb{M}_d(\mathbb{C})$. Then there is a unitary matrix U such that the matrices B_1, \ldots, B_m , where $B_j = U A_j U^{\dagger}$, are diagonal. Moreover, $\langle B_j, B_k \rangle = \langle A_j, A_k \rangle$; so B_j and B_k are orthogonal for $j \neq k$. Let $|\mathbf{b}_j\rangle \in \mathbb{C}^d$ be the diagonal of B_j . Then $\langle B_j, B_k \rangle = \langle \mathbf{b}_j | \mathbf{b}_k \rangle$. So the vectors $|\mathbf{b}_1\rangle, \ldots, |\mathbf{b}_m\rangle$ are mutually orthogonal; therefore, $m \leq d$.

Let $\mathcal{B} = \{U_1, U_2, \dots, U_{d^2}\}$ be a *basis of unitary* matrices for $\mathbb{M}_d(\mathbb{C})$. Without loss of generality, we can assume that $U_1 = \mathbb{1}_d$, the identity matrix of order d. We say that the basis \mathcal{B} is a **maximal commuting basis** for $\mathbb{M}_d(\mathbb{C})$ if \mathcal{B} can be partitioned as

$$\mathcal{B} = \{\mathbf{1}_d\} \bigcup \mathcal{C}_1 \bigcup \cdots \bigcup \mathcal{C}_{d+1},\tag{4}$$

where each class C_j contains exactly d - 1 commuting matrix from \mathcal{B} . Note that $\{\mathbb{1}_d\} \bigcup C_j$ is a set of d commuting orthogonal unitary matrices, which by Lemma 3.1 is maximal.

Theorem 3.2 If there is a maximal commuting basis of orthogonal unitary matrices in $\mathbb{M}_d(\mathbb{C})$, then there is a set of d + 1 mutually unbiased bases.

Proof. Let \mathcal{B} be a maximal commuting basis of orthogonal unitary matrices in $\mathbb{M}_d(\mathbb{C})$, where (4) provides the decomposition of \mathcal{B} into maximal classes of commuting matrices. For any $1 \leq j \leq d+1$, let

$$C_j = \{ U_{j,1}, U_{j,2}, \dots, U_{j,d-1} \}.$$

We also define $U_{j,0} = 1_d$; then

$$C'_{j} = \{ U_{j,0}, U_{j,1}, U_{j,2}, \dots, U_{j,d-1} \}$$

is a maximal set of commuting orthogonal unitary matrices. Thus for each $1 \le j \le d + 1$, there is an orthonormal basis

$$\mathbb{T}_{j} = \left\{ \left| \psi_{1}^{j} \right\rangle, \left| \psi_{2}^{j} \right\rangle, \dots, \left| \psi_{d}^{j} \right\rangle \right\}$$

such that every matrix $U_{j,t}$ (for $0 \le t \le d-1$) relative to the basis T_j is diagonal. Let

$$U_{j,t} = \sum_{k=1}^{d} \lambda_{j,t,k} \left| \psi_k^j \right\rangle \left\langle \psi_k^j \right|.$$
(5)

Let M_j be a $d \times d$ matrix whose k^{th} row is the diagonal of the right-hand side matrix of (5); i.e.,

$$M_{j} = \begin{pmatrix} \lambda_{j,0,1} & \lambda_{j,0,2} & \dots & \lambda_{j,0,d} \\ \lambda_{j,1,1} & \lambda_{j,1,2} & \dots & \lambda_{j,1,d} \\ \vdots & \vdots & \ddots & \vdots \\ \lambda_{j,d-1,1} & \lambda_{j,d-1,2} & \dots & \lambda_{j,d-1,d} \end{pmatrix}$$

Then M_j is a *unitary* matrix. Note that the first row of M_j is the constant vector (1, 1, ..., 1). We consider the classes \mathcal{C}_1 and \mathcal{C}_2 . Then for $0 \le s, t \le d - 1$, the orthogonality condition implies

$$\operatorname{Tr}\left(U_{1,s}^{\dagger} U_{2,t}\right) = d\,\delta_{s,0}\,\delta_{t,0}.$$

But, since $\operatorname{Tr}\left(\left|\psi_{k}^{1}\right\rangle\left\langle\psi_{\ell}^{2}\right|\right) = \left\langle\psi_{k}^{1}\left|\psi_{\ell}^{2}\right\rangle^{*}$,

$$\operatorname{Tr}\left(U_{1,s}^{\dagger} U_{2,t}\right) = \operatorname{Tr}\left(\sum_{k=1}^{d} \sum_{\ell=1}^{d} \lambda_{1,s,k}^{*} \lambda_{2,t,\ell} \left|\psi_{k}^{1}\right\rangle \left\langle\psi_{k}^{1} \left|\psi_{\ell}^{2}\right\rangle \left\langle\psi_{\ell}^{2}\right|\right)\right)$$
$$= \sum_{k=1}^{d} \sum_{\ell=1}^{d} \lambda_{1,s,k}^{*} \lambda_{2,t,\ell} \left\langle\psi_{k}^{1} \left|\psi_{\ell}^{2}\right\rangle \operatorname{Tr}\left(\left|\psi_{k}^{1}\right\rangle \left\langle\psi_{\ell}^{2}\right|\right)\right)$$
$$= \sum_{k=1}^{d} \sum_{\ell=1}^{d} \lambda_{1,s,k}^{*} \lambda_{2,t,\ell} \left|\left\langle\psi_{k}^{1} \left|\psi_{\ell}^{2}\right\rangle\right|^{2}.$$

Therefore

$$\sum_{k=1}^{d} \sum_{\ell=1}^{d} \lambda_{1,s,k}^{*} \lambda_{2,t,\ell} \left| \left\langle \psi_{k}^{1} \left| \psi_{\ell}^{2} \right\rangle \right|^{2} = d \,\delta_{s,0} \delta_{t,0}, \qquad 0 \le s, t \le d-1.$$
(6)

The system of equations (6) can be written in the following matrix form

$$AP = \Lambda,$$

where

$$A = M_1^* \otimes M_2,$$

$$P = \left(\left| \left\langle \psi_1^1 \left| \psi_1^2 \right\rangle \right|^2, \left| \left\langle \psi_1^1 \left| \psi_2^2 \right\rangle \right|^2, \dots, \left| \left\langle \psi_d^1 \left| \psi_d^2 \right\rangle \right|^2 \right)^{\mathrm{T}}, \right.$$

$$\Lambda = (d, 0, 0, \dots, 0)^{\mathrm{T}}.$$

Note that A is a unitary matrix and its first row is the constant vector (1, 1, ..., 1). Then from $P = A^{-1}\Lambda$ it follows

$$\left|\left\langle \psi_s^1 \left| \psi_t^2 \right\rangle\right|^2 = \frac{1}{d}, \qquad 1 \le s, t \le d$$

By repeating the same argument for the classes C_j and C_k , we conclude that

 $\{\mathfrak{T}_1,\ldots,\mathfrak{T}_{d+1}\}$

is a set of MUB.

Before we continue, we prove the following useful simple lemma.

Lemma 3.3 For any integers m and n such that $0 < m \le n$ we have

$$\sum_{k=1}^{n} e^{2\pi i \frac{mk}{n}} = 0.$$

Proof. We have

$$\sum_{k=1}^{n} \left(e^{2\pi i \frac{m}{n}} \right)^k = e^{2\pi i \frac{m}{n}} \frac{\left(e^{2\pi i \frac{m}{n}} \right)^n - 1}{e^{2\pi i \frac{m}{n}} - 1} = 0.$$

The converse of Theorem 3.2, in the following sense, holds.

Theorem 3.4 Let $\mathcal{B}_1, \ldots, \mathcal{B}_m$ be a set of MUB in \mathbb{C}^d . Then there are m classes $\mathcal{C}_1, \ldots, \mathcal{C}_m$ each consisting of d commuting unitary matrices such that matrices in $\mathcal{C}_1 \bigcup \cdots \bigcup \mathcal{C}_m$ are pairwise orthogonal.

Proof. Suppose that

$$\mathcal{B}_j = \left\{ \left| \psi_1^j \right\rangle, \dots, \left| \psi_d^j \right\rangle \right\}.$$

Then

$$\left\langle \psi_s^j \left| \psi_t^j \right\rangle = \delta_{s,t}, \qquad 1 \le s, t \le d,$$

and

$$\left|\left\langle \psi_s^j \left| \psi_t^k \right\rangle\right|^2 = \frac{1}{d}, \qquad 1 \le j < k \le d, \ 1 \le s, t \le d.$$

We label the matrices in the class \mathbb{C}_j as

$$\mathcal{C}_{j} = \{ U_{j,0}, U_{j,1}, \dots, U_{j,d-1} \},\$$

where

$$U_{j,t} = \sum_{k=1}^{d} e^{2\pi i \frac{tk}{d}} \left| \psi_k^j \right\rangle \left\langle \psi_k^j \right|, \qquad 0 \le t \le d-1.$$

Note that $U_{j,0} = \mathbb{1}_d$. Then $U_{j,s}$ and $U_{j,t}$ are commuting, because both are diagonal relative to the basis \mathcal{B}_j . We now show that all these matrices are orthogonal. First we note that

$$\begin{array}{lll} \langle U_{j,s}, U_{k,t} \rangle &=& \operatorname{Tr} \left(U_{j,s}^{\dagger} U_{k,t} \right) \\ &=& \displaystyle \sum_{x=1}^{d} \sum_{y=1}^{d} e^{2\pi i \frac{ty-sx}{d}} \operatorname{Tr} \left(\left| \psi_{x}^{j} \right\rangle \left\langle \psi_{y}^{j} \left| \psi_{y}^{k} \right\rangle \left\langle \psi_{y}^{k} \right| \right) \\ &=& \displaystyle \sum_{x=1}^{d} \sum_{y=1}^{d} e^{2\pi i \frac{ty-sx}{d}} \left| \left\langle \psi_{x}^{j} \left| \psi_{y}^{k} \right\rangle \right|^{2}. \end{array}$$

Thus, by Lemma 3.3, if j = k, then

$$\langle U_{j,s}, U_{j,t} \rangle = \sum_{x=1}^{d} \sum_{y=1}^{d} e^{2\pi i \frac{ty-sx}{d}} \delta_{x,y}$$
$$= \sum_{x=1}^{d} e^{2\pi i \frac{x(t-s)}{d}}$$
$$= d \, \delta_{s,t}.$$

If $j \neq k$ and $(s, t) \neq (0, 0)$, then

$$\langle U_{j,s}, U_{k,t} \rangle = \sum_{x=1}^{d} \sum_{y=1}^{d} e^{2\pi i \frac{ty-sx}{d}} \frac{1}{d}$$

$$= \frac{1}{d} \left(\sum_{x=1}^{d} e^{2\pi i \frac{sx}{d}} \right)^* \left(\sum_{y=1}^{d} e^{2\pi i \frac{ty}{d}} \right)$$

$$= 0. \blacksquare$$

As an immediate corollary of the above theorem, we have the following upper bound on the size of a set of MUB.

Theorem 3.5 Any set of mutually unbiased bases in \mathbb{C}^d contains at most d + 1 bases.

Proof. If a set of MUB contains m bases, then by Theorem 3.4, there are at least 1 + m(d-1) pairwise orthogonal matrices in the d^2 -dimensional space $\mathbb{M}_d(\mathbb{C})$. Therefore, $1+m(d-1) \leq d^2$, thus $m \leq d+1$.

4 Construction of a set of MUB for prime powers

4.1 The Pauli group

To construct a maximal set of MUB in $\mathcal{H} = \mathbb{C}^{p^m}$, where p is a prime number, we consider the Hilbert space \mathcal{H} as tensor product of m copies of \mathbb{C}^p ; i.e.,

$$\mathcal{H} = \underbrace{\mathbb{C}^p \otimes \cdots \otimes \mathbb{C}^p}_{m \text{ times}}.$$

Like the case of \mathbb{C}^p , we build a set of MUB as the sets of eigenvectors of special types of unitary operators on the background space \mathcal{H} . On the space \mathbb{C}^p we considered the generalized Pauli operators X_p and Z_p , defined by equations (1) and (2). On the space \mathcal{H} , we consider the tensor products of operators X_p and Z_p .

We denote the finite field $\{0, 1, \dots, p-1\}$ by \mathbb{F}_p . Let $\omega = e^{2\pi i/d}$ be a primitive p^{th} root of unity. Then

$$Z_p X_p = \omega X_p Z_p.$$

Therefore, if $U_1 = (X_p)^{k_1} (Z_p)^{\ell_1}$ and $U_2 = (X_p)^{k_2} (Z_p)^{\ell_2}$ then

$$U_2 U_1 = \omega^{k_1 \ell_2 - k_2 \ell_1} U_1 U_2. \tag{7}$$

We are interested on unitary operators on $\mathcal{H} = \mathbb{C}^p \otimes \cdots \otimes \mathbb{C}^p$ (the tensor product of *m* copies of \mathbb{C}^p) of the form

$$U = M_1 \otimes \cdots \otimes M_m, \quad \text{where } M_j = (X_p)^{k_j} (Z_p)^{\ell_j}, 0 \le k_j, \ell_j \le p - 1.$$
(8)

To describe an operator of the form (8) it is enough to specify the powers k_j and ℓ_j . So we represent an operator (8) by the following vector of length 2m over the field \mathbb{F}_p :

$$(k_1,\ldots,k_m\,|\,\ell_1,\ldots,\ell_m),$$

or equivalently as

$$X_p(k_1,\ldots,k_m) Z_p(\ell_1,\ldots,\ell_m).$$

If we let $\alpha = (k_1, \ldots, k_m)$ and $\beta = (\ell_1, \ldots, \ell_m)$, then $\alpha, \beta \in \mathbb{F}_p^m$ and we denote the corresponding operator by

$$X_p(\alpha) Z_p(\beta).$$

The **Pauli group** $\mathbb{P}(p,m)$ is the group of all unitary operators on $\mathcal{H} = \mathbb{C}^p \otimes \cdots \otimes \mathbb{C}^p$ (the tensor product of *m* copies of \mathbb{C}^p) of the form

$$\omega^j X_p(\alpha) Z_p(\beta), \tag{9}$$

for some integer $j \ge 0$ and vectors $\alpha, \beta \in \mathbb{F}_p^m$, where $\omega = \exp(2\pi i/p)$. In this section we are mainly interested in the subset $\mathbb{P}_0(p,m)$ of $\mathbb{P}(p,m)$ of the operators of the form (9) with j = 0. Note that $\mathbb{P}_0(p,m)$ is not a subgroup, but generators of subgroups of the Pauli group can always be considered as subsets of $\mathbb{P}_0(p,m)$.

If the operators U and U' in $\mathbb{P}_0(p, m)$ are represented by the vectors

$$(k_1, \ldots, k_m | \ell_1, \ldots, \ell_m)$$
 and $(k'_1, \ldots, k'_m | \ell'_1, \ldots, \ell'_m)$,

respectively, then U and U' are commuting if and only if

$$\sum_{j=1}^m k_j \ell'_j - \sum_{j=1}^m k'_j \ell_j = 0 \mod p.$$

We can state this condition equivalently in the following form.

Lemma 4.1 If $U = X_p(\alpha) Z_p(\beta)$ and $U' = X_p(\alpha') Z_p(\beta')$, for $\alpha, \beta, \alpha', \beta' \in \mathbb{F}_p^m$, then U and U' are commuting if and only if

$$\alpha \cdot \beta' - \alpha' \cdot \beta = 0 \mod p. \tag{10}$$

A set $X_p(\alpha_1) Z_p(\beta_1), \ldots, X_p(\alpha_t) Z_p(\beta_t)$ of operators in $\mathbb{P}_0(p, m)$ is represented by the $t \times (2m)$ matrix

$$\left(\begin{array}{c|c} \alpha_1 & \beta_1 \\ \vdots & \vdots \\ \alpha_t & \beta_t \end{array}\right).$$

Before we continue, we would like to get an explicit formula for the action of a $\mathbb{P}_0(p,m)$ operator $X_p(\alpha) Z_p(\beta)$. Let $\alpha = (\alpha_1, \ldots, \alpha_m)$ and $\beta = (\beta_1, \ldots, \beta_m)$. The standard basis of the Hilbert space $\mathcal{H} = \mathbb{C}^p \otimes \cdots \otimes \mathbb{C}^p$ consists of the vectors $|j_1 \cdots j_m\rangle$, where $(j_1, \ldots, j_m) \in \mathbb{F}_p^m$. Then

$$X_p(\alpha) Z_p(\beta) |j_1 \cdots j_m\rangle = \omega^{j_1 \beta_1 + \cdots + j_m \beta_m} |(j_1 + \alpha_1) \cdots (j_m + \alpha_m)\rangle$$

Equivalently,

$$X_p(\alpha) Z_p(\beta) |a\rangle = \omega^{a \cdot \beta} |a + \alpha\rangle, \qquad a \in \mathbb{F}_p^m,$$
(11)

$$X_p(\alpha) Z_p(\beta) = \sum_{a \in \mathbb{F}_p^m} \omega^{a \cdot \beta} |a + \alpha\rangle \langle a|, \qquad (12)$$

where the operations are in the field \mathbb{F}_p .

Theorem 4.2 Let $U = X_p(\alpha) Z_p(\beta)$ and $U' = X_p(\alpha') Z_p(\beta')$ be operators in $\mathbb{P}_0(p, m)$. If $U \neq U'$, i.e., $(\alpha, \beta) \neq (\alpha', \beta')$, then the operators U and U' are orthogonal.

Proof. We have

$$\begin{array}{lll} \left\langle U, U' \right\rangle &=& \mathrm{Tr} \left(U^{\dagger} \ U' \right) \\ &=& \mathrm{Tr} \left(\sum_{a \in \mathbb{F}_p^m} \sum_{b \in \mathbb{F}_p^m} \omega^{\beta' \cdot b - \beta \cdot a} \left| a \right\rangle \left\langle a + \alpha \left| b + \alpha' \right\rangle \left\langle b \right| \right) \\ &=& \sum_{a \in \mathbb{F}_p^m} \omega^{\beta' \cdot b - \beta \cdot a} \left\langle a + \alpha \left| a + \alpha' \right\rangle . \end{array}$$

If $\alpha \neq \alpha'$, then $\langle a + \alpha | a + \alpha' \rangle = 0$, for every $a \in \mathbb{F}_p^m$. Thus in this case $\langle U, U' \rangle = 0$. If $\alpha = \alpha'$ and $\beta \neq \beta'$ then, by Lemma 3.3,

$$\langle U, U' \rangle = \sum_{a \in \mathbb{F}_p^m} \omega^{(\beta' - \beta) \cdot a}$$

= 0.

4.2 The general construction

Our scheme for constructing a set of MUB is based on Theorem 3.2. The maximal commuting orthogonal basis for $\mathbb{M}_{p^m}(\mathbb{C})$ with partition of the form (4) is such that each class $\{\mathbb{1}_p\} \bigcup \mathcal{C}_j$, in the following sense, is a *linear* space of operators in the Pauli group $\mathbb{P}(p, m)$. Let

$$X_p(\alpha_1) Z_p(\beta_1), \ldots, X_p(\alpha_{p^m}) Z_p(\beta_{p^m})$$

be the operators in the class $\{1_p\} \bigcup C_j$. We say that this class is **linear** if the set of the vectors

$$\mathcal{E}_j = \{ (\alpha_1 | \beta_1), \dots, (\alpha_{p^m} | \beta_{p^m}) \}$$

form an *m*-dimensional subspace of \mathbb{F}_p^{2m} . In this case, to specify a linear class, it is enough to present a basis for the subspace \mathcal{E}_j . Such a basis can be represented by an $m \times (2m)$ matrix. So instead of listing all operators in the classes $\mathcal{C}_1, \ldots, \mathcal{C}_{p^m+1}$, we could simply list the $p^m + 1$ matrices representing the bases of these classes.

More specifically, the bases of linear classes of operators in our construction are represented by the matrices

$$(0_m|\mathbf{1}_m), (\mathbf{1}_m|A_1), \ldots, (\mathbf{1}_m|A_{p^m}),$$

where 0_m is the all-zero matrix of order m and each A_j is an $m \times m$ matrix over \mathbb{F}_p . It easy to see what conditions should be imposed on the matrices A_j so that the requirements of Theorem 3.2 satisfied. The following lemma gives a simple necessary and sufficient condition for operators in each class commuting. Note that in a linear class of operators, if the basic operators are commuting then any pair of operators in these class will commute.

Lemma 4.3 Let S be a set of m operators in $\mathbb{P}_0(p, m)$, and S be represented by the matrix $(\mathbb{1}_m|A)$, where $\mathbb{1}_m$ is the identity matrix of order m and A is an $m \times m$ matrix over \mathbb{F}_p . Then the operators in S are pairwise commuting if and only if A is a symmetric matrix.

Proof. Let $A = (a_{jk})$. Then, by (10), S is a set of commuting operators if and only if $a_{jk} - a_{kj} = 0 \mod p$, for every $1 \le j < k \le m$. Since $a_{jk} \in \mathbb{F}_p$, S is a set of commuting operators if and only if A is symmetric.

The other condition is that the classes C_j and C_k should be disjoint. This condition is met if the span of the matrices $(\mathbb{1}_m | A_j)$ and $(\mathbb{1}_m | A_k)$ are disjoint. The last condition is equivalent to $\mathbf{x}A_j \neq \mathbf{x}A_k$, for every non-zero $\mathbf{x} \in \mathbb{F}_p^m$. The last condition is equivalent to $\det(A_j - A_k) \neq 0$. Thus we can summarize our construction in the following theorem. **Theorem 4.4** Let $\{A_1, \ldots, A_\ell\}$ be a set of symmetric $m \times m$ matrices over \mathbb{F}_p such that $\det(A_j - A_k) \neq 0$, for every $1 \leq j < k \leq \ell$. Then there is a set of $\ell + 1$ mutually unbiased bases on \mathbb{C}^{p^m} .

More specifically, the $\ell + 1$ bases of the above theorem are represented by the matrices

$$(0_m|\mathbf{1}_m), \quad (\mathbf{1}_m|A_1), \quad \dots, \quad (\mathbf{1}_m|A_\ell)$$

Example d = 4. The four matrices (over $\mathbb{F}_2 = \{0, 1\}$) which satisfy the conditions of Theorem 4.4 are

$$\begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}, \quad \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \begin{pmatrix} 0 & 1 \\ 1 & 1 \end{pmatrix}, \quad \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix}.$$
(13)

Therefore the classes of maximal commuting operators are

where

$$I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \qquad X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad Y = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} = XZ, \qquad Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

We represent this basis explicitly. To this end, we naturally represent each basis by a 4×4 matrix such that the j^{th} row of this matrix is the components of the j^{th} vector of the corresponding basis with respect to the standard basis $|00\rangle$, $|01\rangle$, $|10\rangle$, $|11\rangle$: the first matrix is $\mathcal{B}_0 = 1_4$, and

Note that, in this case, the mutually unbiasedness condition is equivalent to the condition that $\mathcal{B}_i \mathcal{B}_i^{\dagger} = 1_4$, for every $0 \le i \le 4$, and each entry of $\mathcal{B}_i \mathcal{B}_j^{\dagger}$, for $0 \le i < j \le 4$, has absolute value equal to $\frac{1}{2}$.

4.3 Construction for $d = p^m$

By Theorem 4.4, to construct $p^m + 1$ mutually unbiased bases in \mathbb{C}^{p^m} , we only need to find m symmetric nonsingular matrices $B_1, \ldots, B_m \in \mathbb{M}_m(\mathbb{C})$ such that the matrix $\sum_{j=1}^m b_j B_j$ is also nonsingular, for every *nonzero* vector $(b_1, \ldots, b_m) \in \mathbb{F}_p^m$. Because if this condition satisfied then the p^m matrices

$$\sum_{j=1}^{m} a_j B_j, \qquad (a_1, \dots, a_m) \in \mathbb{F}_p^m,$$

satisfy the condition of Theorem 4.4.

Example d = 8. The following eight 3×3 matrices determine a set 9 mutually unbiased bases on \mathbb{C}^8 . Let $A_1 = \mathbf{0}_3$ (the zero matrix), $A_2 = \mathbf{1}_3$, and

$$A_{3} = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 1 & 1 \\ 0 & 1 & 1 \end{pmatrix} \qquad A_{4} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 1 \\ 1 & 1 & 0 \end{pmatrix} \qquad A_{5} = \begin{pmatrix} 1 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$$
$$A_{6} = \begin{pmatrix} 1 & 0 & 1 \\ 0 & 0 & 1 \\ 1 & 1 & 1 \end{pmatrix} \qquad A_{7} = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 0 \\ 1 & 0 & 1 \end{pmatrix} \qquad A_{8} = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}$$

Note that these matrices are of the following general form:

$$a_1 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} + a_2 \begin{pmatrix} 0 & 1 & 0 \\ 1 & 1 & 1 \\ 0 & 1 & 1 \end{pmatrix} + a_3 \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 1 \\ 1 & 1 & 0 \end{pmatrix}, \qquad a_1, a_2, a_3 \in \mathbb{F}_2.$$

Wootters and Fields [16] have found the following general construction for the matrices B_1, \ldots, B_m . Let $\gamma_1, \ldots, \gamma_m$ be a basis of \mathbb{F}_{p^m} as a vector space over \mathbb{F}_p . Then any element $\gamma_i \gamma_j \in \mathbb{F}_{p^m}$ can be written uniquely as

$$\gamma_i \gamma_j = \sum_{\ell=1}^m b_{ij}^\ell \gamma_\ell$$

Then $B_{\ell} = \left(b_{ij}^{\ell}\right)$; i.e., the $(i, j)^{\text{th}}$ entry of B_{ℓ} is b_{ij}^{ℓ} .

4.3.1 A set of MUB for the case $d = p^2$

We would like to mention here that for the case $d = p^2$, there is a more explicit construction. We find p^2 matrices A_1, \ldots, A_{p^2} over \mathbb{F}_p which satisfy the conditions of Theorem 4.4. For this purpose, we let

$$A_j = \begin{pmatrix} a_j & b_j \\ b_j & sa_j + tb_j \end{pmatrix}, \qquad a_j, b_j \in \mathbb{F}_p,$$

where $s, t \in \mathbb{F}_p$ are two constants which their value need to be determined. By construction, the matrix A_j is symmetric, so we have to choose the values of the parameters s and t such that $\det(A_j - A_k) \neq 0$, for every $1 \le j < k \le p^2$. Let $\alpha = a_j - a_k$ and $\beta = b_j - b_k$. Then $(\alpha, \beta) \ne (0, 0)$, and we have

$$\det(A_j - A_k) = D(\alpha, \beta) = \begin{vmatrix} \alpha & \beta \\ \beta & s\alpha + t\beta \end{vmatrix} = s\alpha^2 + t\alpha\beta - \beta^2.$$

If $\alpha = 0$, then $D(\alpha, \beta) = -\beta^2 \neq 0$. Suppose now that $\alpha \neq 0$, and let $\beta/\alpha = \gamma$. Then

$$D(\alpha,\beta) = -\alpha^2(\gamma^2 - t\gamma - s)$$

Thus $D(\alpha, \beta) \neq 0$ if the quadratic polynomial $\gamma^2 - t\gamma - s$ is irreducible over \mathbb{F}_p . Since for every prime p there is at least one irreducible quadratic polynomial over \mathbb{F}_p , it is possible to choose the parameters $s, t \in \mathbb{F}_p$ such that $D(\alpha, \beta) \neq 0$, for every $\alpha, \beta \in \mathbb{F}_p$.

Example d = 4. The four matrices (13) are obtained from the irreducible polynomial $x^2 + x + 1$ over \mathbb{F}_2 . Therefore, all those matrices are of the following form

$$\begin{pmatrix} a & b \\ a & a+b \end{pmatrix}, \qquad a,b \in \mathbb{F}_2.$$

Example d = 9. The polynomial $x^2 + x + 2$ is irreducible over \mathbb{F}_3 . Therefore, the matrices A_j are of the general form of

$$\begin{pmatrix} a & b \\ b & a+2b \end{pmatrix}.$$

So the nine matrices are

$$\begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}, \qquad \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \qquad \begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix},$$

$$\begin{pmatrix} 0 & 1 \\ 1 & 2 \end{pmatrix}, \qquad \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \begin{pmatrix} 0 & 2 \\ 2 & 1 \end{pmatrix},$$

$$\begin{pmatrix} 1 & 2 \\ 2 & 2 \end{pmatrix}, \qquad \begin{pmatrix} 2 & 1 \\ 1 & 1 \end{pmatrix}, \qquad \begin{pmatrix} 2 & 2 \\ 2 & 0 \end{pmatrix}.$$

5 Conclusion

In this paper we partially solved the problem of existence of sets of MUB in composite dimensions. We formulated an interesting connection between maximal commuting basis of orthogonal unitary matrices

and sets of MUB. We obtained the necessary condition for the existence of sets of MUB in any dimension. Using these we proved the existence of sets of MUB for dimensions which are prime power. We provided a sharp upper bound on the size of any MUB for any dimension. We expressed the sets of MUB observables as tensor products of Pauli matrices. However we could not apply this method when the dimension d is a product of different primes instead of being a prime power (the simplest case that belongs to this category is when d = 6) because if we do so the convenient properties of the case $d = p^m$ no longer remain valid. For instance Theorem 4.4 does not hold in this case.

A useful application of our result is in secure key distribution using higher dimensional quantum systems. Specifically we note that the protocol suggested by Bechmann–Pasquinucci and Tittel [2] using four dimensional quantum system will become more efficient if all the five mutually unbiased bases are used in the protocol instead of only two as suggested by the authors.

Note added: After we submitted our paper for this journal and posted it on the Los Alamos quant-ph web site, a related paper [12] was posted on that e-print server. In that paper, with an approach similar to that introduced by us in this paper, in the case of $d = 2^m$, the authors discuss the relationship between MUB and the commuting bases of unitary matrices, similar to what we have presented in this paper.

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