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# Entanglement Patterns in Mutually Unbiased Basis Sets for $N$ Prime-state Particles

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## Abstract

A few simply-stated rules govern the entanglement patterns that can occur in mutually unbiased basis sets (MUBs), and constrain the combinations of such patterns that can coexist (*ie*, the stoichiometry) in full complements of  $(p^N + 1)$  MUBs. We consider Hilbert spaces of prime power dimension (as realized by systems of  $N$  prime-state particles, or *qupits*), where full complements are known to exist, and we assume only that MUBs are eigenbases of generalized Pauli operators, without using a particular construction. The general rules include the following: 1) In any MUB, a particular qupit appears either in a pure state, or totally entangled, and 2) in any full MUB complement, each qupit is pure in  $(p+1)$  bases (not necessarily the same ones), and totally entangled in the remaining  $(p^N - p)$ . It follows that the maximum number of product bases is  $p + 1$ , and when this number is realized, all remaining  $(p^N - p)$  bases in the complement are characterized by the total entanglement of every qupit. This “standard distribution” is inescapable for two qupits (of any  $p$ ), where only product and generalized Bell bases are admissible MUB types. This and the following results generalize previous results for qubits [13, 17] and qutrits [16], drawing particularly upon Ref. [17]. With three qupits there are three MUB types, and a number of combinations  $(p+2)$  are possible in full complements. With  $N = 4$ , there are 6 MUB types for  $p = 2$ , but new MUB types become possible with larger  $p$ , and these are essential to realizing full complements. With this example, we argue that new MUB types, showing new entanglement characteristics, should enter with every step in  $N$ , and when  $N$  is a prime plus 1, also at critical  $p$  values,  $p = N - 1$ . Such MUBs should play critical roles in filling complements.

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## I. INTRODUCTION

Mutually unbiased basis sets are known to provide an optimal basis for quantum tomography [1, 2], to play key roles in quantum cryptography [3–6], and to be instrumental in solving the mean king problem in prime power dimensions [7]. The generalized Pauli operators associated with MUB’s include the stabilizers of quantum error correcting codes [8–10], and serve as entanglement witnesses [11] for the MUB states. Of interest for the foundations of quantum physics, the MUB concept sharpens the concept of complementarity [12, 13], and raises the question of existence in composite dimensions. An excellent comprehensive review of MUBs has recently appeared [14].

We deal here with Hilbert spaces of prime power dimensions ( $d = p^N$ ), where  $d + 1$  MUBs are known to exist [2]. This is both the largest possible number, and also the number required for a complete operator basis (in representing the density matrix, for example). So, while each MUB is a complete orthonormal basis in the Hilbert space, the set of  $d + 1$  MUBs is a complete (nonorthogonal) basis in the space of all operators, which has dimension  $d^2 = p^{2N}$ . Regarding terminology, to avoid reference to a “complete set of complete sets,” and prompted by the fact that different MUBs (or the observable sets associated with them) are maximally complementary [12], I will use the term “full complement,” or sometimes just “complement,” to denote the set of all  $d + 1$  MUBs. Partial MUB sets have been discussed in connection with composite dimensions and referred to as “constellations” [15].

The natural systems to which MUBs apply consist of  $N$   $p$ -state objects (*qupits*). In such systems, while MUB complements exhibit only a single entanglement type for  $N = 2$  (and all  $p$ ), the number of distinct types proliferates with increasing  $N$ . The variety is illustrated in a number of recent discussions, mostly on multiple qubit systems but also multiple qutrit systems [6, 13, 16–20]. In particular, a systematic study by Romero and collaborators [17] illustrates a broad range of entanglement patterns that occur naturally in a construction scheme for full MUB complements. Such complements are catalogued for up to 4 qubits. Wieśniak and collaborators [18] have developed a construction scheme aimed at experimental implementation and discussed the total entanglement content of full MUB complements of bipartite systems.

With the general MUB problem in mind, our purpose here is to develop a general framework, independent of construction schemes, for exploring MUB entanglement patterns for

all  $p$  and  $N$ . The project begins by proving three general theorems (the “rules”) that underlie and lead quickly to an array of more specific results. Many of the latter apply to all  $p$ , but are  $N$ -specific, as each step in  $N$  introduces further richness. All results refer to one of two levels - that of individual MUBs and that of full complements. At the individual level, MUB types are characterized by first specifying the *separation pattern* - How many, and how big, are the irreducible subsets of qubits defined by the factorization of the wavefunction? - and next, by describing the *entanglement pattern* - What is the nature of the entanglement within each irreducible subset? At the level of the full complement, we ask about the possible *MUB distributions* - What combinations of MUB types can coexist within full complements. At the first level, we will show that all conceivable separation patterns are possible, and we will show with examples how to describe the entanglement within the nonseparable factors. At the level of the full complement, we will show how to deduce constraints on the possible MUB distributions. For  $N = 2$  and  $3$ , surprisingly, the general global constraints mentioned in the abstract suffice to determine all MUB distributions for all  $p$ . The  $N = 4$  case is considerably more complex and requires the derivation of more detailed constraint equations.

Let us begin with a review of basic concepts and notation in Section II. In Section III we prove the three general theorems. These rules are applied in Section IV to obtain the entanglement patterns of individual MUBs, and to deduce constraints on their possible distributions within full complements, taking the  $N = 2 - 4$  cases in turn. In Section V we summarize results and comment on unresolved questions.

## II. BACKGROUND CONCEPTS AND DEFINITIONS

In Hilbert spaces of dimension  $d$ , two orthonormal bases ( $K$  and  $Q$ ) are mutually unbiased if any state  $|K, k\rangle$  in basis  $K$  has uniform probability of being found in any state  $|Q, q\rangle$  in basis  $Q$ ; that is, if

$$|\langle K, k | Q, q \rangle|^2 = 1/d. \quad (1)$$

Thus, measurements in the two bases provide no redundant information. Since measurements in any basis provide  $d - 1$  independent probabilities, and since  $d^2 - 1$  real parameters are needed to determine an unknown quantum state (its density matrix  $\rho$ ), it follows that  $d + 1$  MUB's are required. In this way the MUB projectors form a complete nonorthog-

onal basis in operator space. This required number of MUBs is (only) known to exist in power-of-prime dimensions.

There is an intimate connection between MUBs and generalized Pauli operators (hereafter called simply “Pauli operators”) which underlies several construction schemes (Ref. [14] provides a comprehensive listing [21]). These operators are conventionally written in the form of a tensor product,

$$\mathcal{O}_{n,m} = X^n Z^m \equiv X_1^{n_1} X_2^{n_2} \dots X_N^{n_N} Z_1^{m_1} \dots Z_N^{m_N}, \quad (2)$$

whose factors, acting on individual qupits, are powers of the generalized  $(p \times p)$  Pauli matrices,

$$Z = \sum_{k=0}^{p-1} |k\rangle \omega^k \langle k| \quad \text{and} \quad X = \sum_{k=0}^{p-1} |k+1\rangle \langle k|, \quad (3)$$

where  $\omega = e^{2\pi i/p}$ , and  $X$  is the raising operator of  $Z$ . The powers  $n$  and  $m$  are  $p$ -nary numbers, *eg*,  $n = (n_1, \dots, n_N)$ , whose digits take the values  $0, 1, \dots, p-1$ . Thus, there are  $p^{2N}$  operators  $\mathcal{O}_{n,m}$  (including the identity  $\mathcal{I} = \mathcal{O}_{o,o}$ ), which make up a complete and orthonormal basis in operator space (with the trace operation as inner product). The desired connection with MUB’s is described in Ref. [22]: The  $\mathcal{O}_{n,m}$  partition into  $p+1$  internally-commuting subsets, each consisting of  $p-1$  traceless operators (excluding  $\mathcal{I}$ ). The corresponding eigenbases then form a complete complement of MUB’s.

The above are standard definitions and conventions. It will be useful to adopt a couple of more special conventions for use throughout this paper. First, the operator set  $\mathcal{O}_{n,m}$  does not form a group, because multiplication generates irreducible phase factors. However, for odd  $p$  the set  $\mathcal{O}_{n,m} \otimes (1, \omega, \dots, \omega^{p-1})$  does form a group, of order  $p^{2N+1}$ , and for  $p=2$  the analogous set  $\mathcal{O}_{n,m} \otimes (\pm 1, \pm i)$  forms a group of order  $2^{2N+2}$ . These are called discrete Heisenberg-Weyl, or generalized Pauli groups [14, 23]. We shall not make direct use of them, but we shall take advantage of the freedom to redefine the phases of the  $\mathcal{O}_{n,m}$  in the original set: We choose phases so that the compatible subsets form groups, and we call these *compatibility groups*. They are all isomorphic to those consisting of  $X^n$  and  $Z^m$ , each of which is generated by the  $N$  independent elements,  $X = (X_1, \dots, X_N)$  and  $Z = (Z_1, \dots, Z_N)$ , respectively. Thus, to construct another compatibility group, we may choose a generator set  $G = (G_1, \dots, G_N)$  that consists of any  $N$  elements in the original compatible subset that do not form a subgroup,

and write the resulting group elements as

$$G^n \equiv G_1^{n_1} G_2^{n_2} \dots G_N^{n_N}. \quad (4)$$

Thus, all of the compatibility groups are representations of the same group - the abelian group of order  $p^N$  generated by  $N$  elements. A simple example of a compatibility group so generated is

$$Y^n = (X_1 Z_1)^{n_1} (X_2 Z_2)^{n_2} \dots (X_N Z_N)^{n_N}. \quad (5)$$

Note that phase factors are introduced with respect to the original Pauli operators because, *eg*,  $(X_i Z_j)^2 = \omega^{\delta_{ij}} X_i^2 Z_j^2$ .

The generator set  $G$ , by itself, completely determines the states of the basis ( $G$ ) in the Hilbert space, through the eigenvalue equations  $G_i |G, k\rangle = \omega^{k_i} |G, k\rangle$ , where  $k = (k_1, k_2, \dots, k_N)$  is a  $p$ -nary representation of the state index  $k$ . The eigenvalues of a general group element are then given by

$$G^n |G, k\rangle = \omega^{n \cdot k} |G, k\rangle, \quad (6)$$

where  $n \cdot k = n_1 k_1 + n_2 k_2 + \dots + n_N k_N$ , and the spectral representation of  $G^n$  is therefore just the Fourier transform [24]

$$G^n = \sum_k |G, k\rangle \omega^{n \cdot k} \langle G, k| \equiv \sum_k \omega^{n \cdot k} \mathcal{P}(G, k), \quad (7)$$

where  $\mathcal{P}(G, k)$  is the projector onto state  $k$  in basis  $G$ . This MUB projector is then given by the inverse transform,

$$\mathcal{P}(G, k) = p^{-N} \sum_n \omega^{-n \cdot k} G^n. \quad (8)$$

The existence of these simple transform relationships between every compatibility group and its corresponding MUB projector set is a consequence of defining the former to be a group. The only remaining arbitrary phases are those of the generators.

### III. GENERAL RESULTS ON ENTANGLEMENT

In this section we establish the general rules that will form the basis for the rest of the work. For ease of reference and completeness I will state and prove these results as three separate numbered theorems. For transparency, here, in plain English, is what they will

say about MUB states: (I) A given qupit is perfectly pure or totally entangled, (II) The distribution of one-qupit operator factors in the compatibility group correlates with this purity,..., and (III) In any full MUB complement, every qupit appears pure  $p + 1$  times, and totally entangled  $p^N - p$  times.

These theorems and the results that follow from them rely on the assumption that MUB states are eigenstates of Pauli operators. While this is restrictive for individual MUB pairs, it is not restrictive for known MUB complements or known construction schemes [21, 25], allowing for unitary equivalence. An example may help to illustrate. Consider the standard basis in 4D, and another related to it by the unitary transformation  $U_{n,m} = (i)^{nm}/2$  (where  $n, m = 0, 1, 2, 3$ ), which is not an eigenbasis of the Pauli operators of Eq. 2. The two bases are MU, but a full complement cannot be completed containing both of them. However, full complements can be found containing either basis without the other: Starting with the well-known full complement containing the standard basis, one could apply  $U_{n,m}$  to each of its bases to obtain another full complement. The latter are not eigenbases of the original Pauli operators, but clearly they *are* eigenbases of transformed Pauli operators, which may be thought of as corresponding to redefined parts (and redefined quantization axes). The results of this paper then apply with reference to these redefined parts. Regarding the existence of a MUB complement outside of this equivalence - I believe that this question also remains unresolved [25]. We will return to these points in the conclusions.

As a brief preliminary, one-qupit states within the  $N$ -qupit system are defined by the reduced density matrices,

$$\rho_i = \text{Tr}^{(i)} \rho, \quad (9)$$

where  $\text{Tr}^{(i)}$  denotes the partial trace over states of all but the  $i$ -th qupit. Perfect purity means that  $\rho_i = \rho_i^2$  is a projector, while total impurity means that  $\rho_i = \mathcal{I}/p$ . One can define the purity of the state  $\rho_i$  as

$$P_i = (p \text{Tr} \rho_i^2 - 1)/(p - 1), \quad (10)$$

which takes its extremal values, 1 and 0, in the respective cases.

**Theorem I:** If the system is in a pure eigenstate of Pauli operators (a generator set  $G$ ), then any individual qupit must exist in a state of either perfect purity, or total impurity, the same for all eigenstates of  $G$ .

**Proof:** The generators produce a compatibility group, and the  $N$ -qupit density matrix

representing a pure eigenstate,  $\rho = \mathcal{P}(G, k)$ , may be expanded as in Eq. 8. Considering now the Pauli matrix factors that act on just the  $i$ th qubit, the generator set  $G$  must fall into one of two categories: Only one Pauli matrix, say  $Z_i$  (and possibly powers of it), appears in the generator set, or more than one appear (including, say,  $X_i$  and  $Y_i$ ), that are not powers of one another. Consider the latter case, which is simpler: Let  $G_1$  and  $G_2$  be generators that contain the factors  $X_i$  and  $Y_i$ . No operator of the form  $U_i \mathcal{I}$  (where  $U_i$  is any one-qubit Pauli matrix) commutes with both  $G_1$  and  $G_2$ , and all such operators are thereby excluded from the compatibility group. As a result, the only operator with a nonvanishing partial trace  $\text{Tr}^{(i)}$  is the global identity  $\mathcal{I}$ . Since  $\mathcal{I}$  enters the summation (8) with the coefficient  $p^{-N}$ , and  $\text{Tr}^{(i)}$  produces a factor of  $p^{(N-1)}$ , the reduced density matrix for the  $i$ th qubit is

$$\rho_i = p^{-1} \mathcal{I}_i, \quad (11)$$

indicating that the  $i$ th qubit is totally impure.

Now turn to the other case: If only  $Z_i$  (and possibly powers) appear in the generator set, then only  $Z_i$  and its powers can appear in the compatibility group (again referring only to those factors that act on the  $i$ th qubit). Since the “one-body” operators  $Z_i^{n_i} \mathcal{I}$  commute with all of these, they must belong to the compatibility group. These one-body operators are the only ones that survive the partial trace. Since each of them enters the summation (Eq. 8) with coefficient  $p^{-N} \omega^{-n_i k_i}$ , and since  $\text{Tr}^{(i)}$  produces a factor of  $p^{(N-1)}$  in each term, we find in this case that

$$\rho_i = p^{-1} \sum_n \omega^{-n_i k_i} Z_i^{n_i} = |Z_i, k_i\rangle \langle Z_i, k_i|. \quad (12)$$

This shows that  $\rho_i$  is a projector onto the eigenstate of  $Z_i$  whose eigenvalue is  $\omega^{k_i}$ , that is,

$$\rho_i^2 = \rho_i \quad \text{and} \quad Z_i \rho_i = \omega^{k_i} \rho_i. \quad (13)$$

This proof is independent of the choice of the eigenstate  $k = (k_1 \dots k_N)$  in the basis  $G$ , and so clearly the  $i$ th qubit is perfectly pure for all eigenstates in this basis.

Here is a related more detailed theorem on the distribution of one-qubit matrices associated with a single qubit.

**Theorem II:** In any compatibility group of  $N$ -qubit Pauli operators, the distribution of one-qubit factors acting on the  $i$ th qubit must be one of two types: (i) Only a single Pauli matrix and its powers occur, and each power occurs an equal number ( $p^{N-1}$ ) of times, or (ii) every Pauli matrix occurs, and each occurs an equal number ( $p^{N-2}$ ) of times.



**Proof:** Consider any set  $G$  of  $N$  generators of the compatibility group. This set must be one of the two types considered in the foregoing proof: Suppose first that only one Pauli matrix (say  $Z_i$ ), and possibly powers of  $Z_i$  appear. Let  $G_1$  be a generator containing  $Z_i$  as a factor, and let  $G_2, G_3, \dots, G_N$  be the rest.  $G_1$  by itself generates a cyclic subgroup containing all powers of  $Z_i$ . Then,  $G_1$  and  $G_2$  by themselves generate a subgroup of order  $p^2$  in which, by virtue of the rearrangement theorem, every power of  $Z_i$  appears  $p$  times (no matter which power of  $Z_i$  is present in  $G_2$ ). One may repeat this argument, multiplying the order of the subgroup by  $p$  at each stage, until the full compatibility group is generated, with each power of  $Z_i$  being produced  $p^{N-1}$  times.

In the other case, let  $G_1$  and  $G_2$  be generators containing the  $X_i$  and  $Y_i$  factors, respectively. These two generators, by themselves, generate a subgroup of order  $p^2$  in which every Pauli matrix factor  $U_i$  appears once and only once. (To see this, note that  $X_i$  and  $Y_i$ , by themselves, generate the one-qubit Pauli group [26], but since  $G_1$  and  $G_2$  commute, the multiplicity of phase factors is absent.) Now, by including a third generator,  $G_3$ , one generates a subgroup of order  $p^3$  in which, by the rearrangement theorem, each Pauli matrix factor appears  $p$  times. Repeating the process through  $G_N$ , one generates the full compatibility group with each Pauli matrix factor appearing  $p^{N-2}$  times.

The second result is particularly striking in light of the fact that the nature of the entanglement of the  $i$ th qubit may vary widely, in the sense that its entanglement may be shared with any number of other qubits in the system. Nevertheless, only two kinds of Pauli matrix distributions, with the corresponding purities, are possible.

We use both of the foregoing theorems to deduce the total entanglement content - as measured by the one-qubit purities - of a full complement of MUB's. This total content is constrained by the requirement that the two types of one-qubit Pauli matrix distributions be consistent with the set of all Pauli operators, which must appear in the full complement.

**Theorem III:** Within any full complement of  $p^N + 1$  MUB's, every qubit is perfectly pure in  $p + 1$  basis sets, and totally entangled in the remaining  $p^N - p$ .

**Proof:** Consider the  $i$ th qubit. Recall that the total number of Pauli operators (excluding  $\mathcal{I}$ ) is  $p^{2N} - 1$ , and that these exactly accommodate the  $p^N + 1$  compatibility groups containing  $p^N - 1$  traceless operators each. Each Pauli matrix factor  $U_i$  appears in  $p^{2N-2}$  Pauli operators, except for  $\mathcal{I}_i$  which appears in  $p^{2N-2} - 1$  because we are not counting  $\mathcal{I}$  in the individual groups. This number must equal the sum of  $\mathcal{I}_i$  factors appearing in all of the compatibility

groups. According to the previous theorem, there are  $p^{N-1} - 1$  such factors in compatibility groups in which the  $i$ th qupit is pure, and  $p^{N-2} - 1$  such factors in all other compatibility groups. If  $\nu_S$  is the number of compatibility groups (or basis sets) in which it is pure, then, in order to account for all  $\mathcal{I}_i$  factors, we must have

$$p^{2N-2} - 1 = \nu_S(p^{N-1} - 1) + (p^N + 1 - \nu_S)(p^{N-2} - 1). \quad (14)$$

Solving this equation, we find the number of basis sets in which the  $i$ th qupit is pure,

$$\nu_S = p + 1, \quad (15)$$

and consequently, the number of basis sets in which it is totally entangled,

$$\nu_E = p^N - p. \quad (16)$$

The following corollary arises when all qupits take their pure states simultaneously:  
**Corollary:** The maximum number of product MUBs is  $p + 1$ , and in any MUB complement where this number is realized, all of the remaining MUBs ( $p^N - p$ ) must be totally entangled (in the sense that every qupit is totally entangled) [27]. This is the standard distribution.

Note that the probability of finding the  $i$ th qupit pure in a MUB state picked at random from any full complement is equal to the averaged purity (Eq. 10),

$$\langle P_i \rangle_{comp} = \frac{\nu_S}{\nu_S + \nu_E} = \frac{p + 1}{p^N + 1}, \quad (17)$$

which vanishes exponentially with  $N$ .

#### IV. ENTANGLEMENT PATTERNS AND THEIR STOICHIOMETRIES

We discuss the  $N = 2 - 4$  cases in turn. The first two are simpler, and we find that Theorems I and III are sufficient to determine all possible MUB distributions, although II provides useful insights. With  $N = 4$ , we require Theorem II in deriving more detailed constraints that apply to individual qupits.

##### bipartite systems

Clearly, if one qupit is pure, then so must be the other. In light of Theorem I, then, both purities must be unity, or both zero. Because these purities coincide, the corollary of

Theorem III applies: There are  $p + 1$  product bases and  $p^2 - p$  totally entangled bases - the standard distribution is inevitable.

We shall refer to all of the entangled bases as generalized Bell bases, because they share the common property that their compatibility groups consist solely of two-body operators, *ie*, those containing no  $I_k$  factors [28]. To see the consequences of this, write one of the two generators as  $G_1 = UV$ . The most general eigenstates of  $G_1$  may then be written as  $p$ -term expansions in the product basis of  $IV$  and  $UI$ ,

$$|\psi\rangle = \frac{1}{\sqrt{p}} \sum_k C_k |k\rangle_u |q - k\rangle_v, \quad (18)$$

where the eigenvalues of  $UV$  are  $\omega^q$  and the coefficients  $C_k$  are determined by the other generator, call it  $G_2 = ST$ . Commutativity demands that both  $S \neq U$  and  $T \neq V$ , so  $G_2$  induces cyclic permutations (of order  $p$ ) in the product states  $|k\rangle_u |q - k\rangle_v$ . Therefore the  $C_k$  are unimodular, and the  $p$  eigenvalues ( $\omega^r$ ) of  $G_2$  are nondegenerate, like those of  $G_1$ . This confirms explicitly what we know from Theorem I - namely, that measurements of one-qupit properties (*eg*,  $IV$  or  $UI$ ) must produce random distributions over all possible outcomes.

The generalized Bell states defined above are contained within a broader class definitions given elsewhere [29, 30]. The more restrictive definition given here - defining classes of states by the Pauli operators of which they form eigenbases - applies nonetheless to all MUBs that are compatible with known full complements, and we shall employ such definitions throughout this work as we proceed to larger  $N$ .

We note for future reference that the precise form of the product state expansion (18) depends on the choice of basis. A bad choice would require a  $p^2$ -term expansion, but even a good choice could look slightly different. For example, if eigenstates of  $UV^{-1}$  were expanded in the same product basis used in Eq. 18, one would find sums of  $|k\rangle_u |q + k\rangle_v$ .

As a final note on Bell states, our working definition may be given in words alone: A generalized Bell state is any totally entangled two-qupit eigenstate of Pauli operators (since total entanglement requires that the two Pauli operators be of the form  $UV$  and  $ST$ ).

### tripartite systems

The standard MUB complement has  $p + 1$  product bases and  $p^3 - p$  totally entangled bases. We shall refer to all of *these* totally entangled bases as generalized GHZ, or  $G$ -bases, because they have common properties describable as follows:

Let us first illustrate with a specific example that generalizes a standard choice of generators for qubits [31],

$$G \equiv (G_1, G_2, G_3) = (XXY, XYX, YXX), \quad (19)$$

to arbitrary  $p$ . To identify an optimal product basis for an expansion, replace the latter two generators by  $G'_2 = G_2 G_1^{-1}$  and  $G'_3 = G_3 G_1^{-1}$ . Recalling the usual definition  $Y_i = X_i Z_i$  on the  $i$ th qupit (modulo possible phase factors), the result is

$$G' = (XXY, IZZ^{-1}, ZIZ^{-1}). \quad (20)$$

Clearly the most general joint eigenstates of  $G'_2$  and  $G'_3$  are  $p$ -term expansions in the standard basis,

$$|\psi\rangle = \frac{1}{\sqrt{p}} \sum_k C_k |k+q\rangle |k+r\rangle |k\rangle, \quad (21)$$

where  $\omega^r$  and  $\omega^q$  are the eigenvalues of  $G'_2$  and  $G'_3$ , respectively, and the  $C_k$  are determined by  $G_1$ . The  $C_k$  are again unimodular because  $G_1$  generates a cyclic group of order  $p$ , of which the  $p$  product states form a basis. This again illustrates the randomness of one-qupit properties in totally entangled states.

To demonstrate the commonality of all totally entangled three-qupit bases, we note that at least one generator must be a three-body operator (having no  $I_k$  factors), which we write in complete generality as  $G_1 = UVW$ . Now, according to Theorem II, the inverse of each factor occurs  $p$  times in the compatibility group, once with the inverse of  $G_1$  itself, and  $p-1$  times in other three-body operators in which it is the only inverse (footnote [28]). Choosing two from the latter category, one containing  $U^{-1}$  and the other containing  $V^{-1}$ , and multiplying  $G_1$  by each in turn, we obtain the generator set

$$G = (UVW, IBC, AIC), \quad (22)$$

where compatibility requires that  $C$  is common to  $G_2$  and  $G_3$  as indicated. Clearly,  $A$ ,  $B$ , and  $C$  define the product basis for the  $p$ -term expansions,

$$|\psi\rangle = \frac{1}{\sqrt{p}} \sum_k C_k |q-k\rangle_a |r-k\rangle_b |k\rangle_c, \quad (23)$$

and each of  $A$ ,  $B$ , and  $C$  must differ from corresponding factors that appear in three-body operators of the compatibility group. In other words, every three-body operator in the

compatibility group induces cyclic permutations of the states composing the product basis. The similarity of generator sets shows that all totally entangled three-qubit bases have  $p$ -term expansions in some special product basis, and that all of their compatibility groups (of the same  $N$  and  $p$ ) have the same numbers of three-body and two-body operators.

Again, a purely verbal definition is possible: A generalized GHZ state is any totally entangled 3-qubit eigenstate of Pauli operators. A general statement for  $N \geq 4$  is possible but less categorical.

The new aspect of MUBs that enters with  $N = 3$  is the appearance of a third (nonstandard) MUB type, and with it, the possibility of composing a full complement with varying combinations. The third type is biseparable, and thereby nonsymmetric with respect to qubits - one qubit separates, leaving the other two in a Bell state. We shall refer to these as “separable-Bell” bases, with the shorthand notation  $SB$  (or  $S_iB$  if we wish to identify the pure qubit). Such MUB bases are known for  $p = 2$  and 3 (Refs. [13, 16]), and to describe them for arbitrary  $p$ , we consider a generator set

$$S_1B = (IIA, UVI, STI), \quad (24)$$

where  $UV$  and  $ST$  are commuting two-body operators acting on qubits 2 and 3. The  $p^3$  joint eigenstates of this set may be written as

$$|S_1B : k, q, p\rangle = |A_1 : k\rangle |B_{2,3} : q, p\rangle, \quad (25)$$

which describes qubit 1 in the  $k$ th eigenstate of  $A$ , and qubits 2 and 3 in the Bell state denoted by the eigenvalues  $q$  and  $p$  of  $UV$  and  $ST$ , respectively. Similarly, the compatibility group of  $S_1B$  is a tensor product of that associated with qubit 1 ( $I_1, A_1, \dots, A_1^{p-1}$ ) and that of the Bell basis of qubits 2 and 3. The tensor product is a common characteristic of all separable MUBs, and the eigenstates of a particular MUB all have the same character - the separation pattern involves the same entangled subsets of qubits, and the nature of the entanglement within each subset is the same.

The three MUB types discussed above, including the three variations of the SB bases, exhaust all of the possibilities for three qubits.

The remaining question now is, what combinations the three types of bases may appear in the full complement? One can answer this question simply by conserving the number of pure qubits while conserving the number of basis sets. We then find that we can remove a

(a) three qubits					(b) three qutrits					
$\Pi$	3	2	1	0	$\Pi$	4	3	2	1	0
$SB$	0	3	6	9	$SB$	0	3	6	9	12
$G$	6	4	2	0	$G$	24	22	20	18	16

(c) three qubits				
$\Pi$	$p + 1$	$p$	$\dots$	0
$SB$	0	3	$\dots$	$3(p + 1)$
$G$	$p^3 - p$	$p^3 - p - 2$	$\dots$	$p^3 - 3p - 2$

TABLE I: Numbers of product, separable-Bell, and GHZ bases coexisting for three particles.

single product basis ( $\Pi$ ) while adding three  $SB$  and removing two  $G$  bases:

$$\Pi + 2G \rightleftharpoons 3SB \quad (26)$$

Table I shows the possibilities for three particles with any  $p$ . The cases of  $p = 2$  and 3 dramatize the role of totally entangled states with increasing dimension of the Hilbert space. In fact, case (a), dimension  $d = 8$ , is the only multiparticle MUB dimension in which a complement can be found with no totally entangled bases. And more typically, a majority of MUBs are totally entangled: In case (b) at least 4/7 of all bases are  $G$  bases, and even for *two* qutrits, 6 of the 10 bases are Bell bases. For  $N = 3$  and general  $p$ , the minimum number of  $G$  bases is given by  $N_{min}(G) = p^3 - 3p - 2$ , an ever-increasing fraction of the total number of bases as  $p$  increases.

It is noteworthy that  $SB$  bases can be introduced only in steps of three, reflecting the condition that the three variations  $S_i B$  must balance in the full complement, since the other MUB types are symmetric with respect to permutations of qubits. This condition follows from the conservation of pure states for each qubit separately.

#### quadrapartite systems

The  $N = 4$  case is more complex in a number of respects. Most importantly, new MUB types enter with increasing  $p$ . But even with  $p = 2$ , the number of distinct MUB types exceeds the number of separation patterns. Figure 1 shows the five separation patterns that

characterize all  $p$ , and lists seven MUB types, six of which account for all  $p = 2$  options, and a seventh which represents, but is not exhaustive for  $p \geq 3$ . Let us first discuss the MUB types for general  $p$ , and later specialize to particular cases for constraints and stoichiometries.

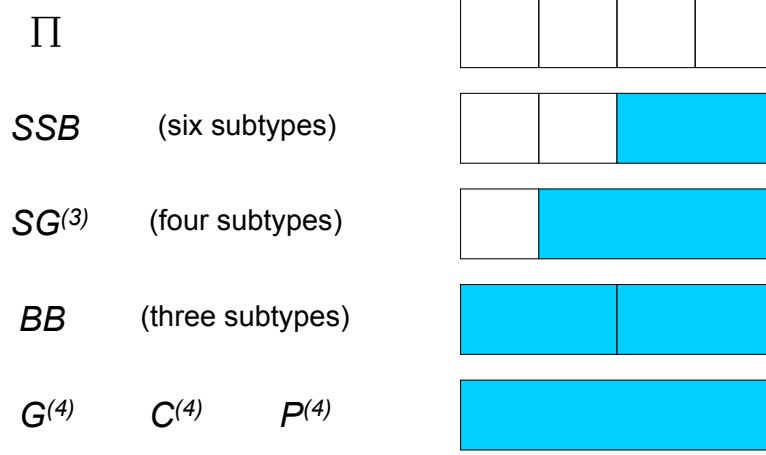


FIG. 1: Seven MUB types listed with 5 separation patterns for 4 qubits.

The separable MUBs' compatibility groups are tensor products of those of their constituent MUBs, and their generator sets may be constructed accordingly. With  $SG^{(3)}$ , a single generator is associated with the separating particle (for example  $IIIA$ ), while three generators (each of the form  $UVWI$  or their alternatives) are associated with the three particles forming  $G^{(3)}$  states. There are four variations on this pattern corresponding to the choices of the separating particle. In the  $BB$  case, one could pick two generators of the form  $IIUV$ , and two of the form  $STII$ . There are three variations on this separation pattern, corresponding on the three ways of picking the two entangled pairs, as compared with six variations on the  $SSB$  pattern from the six ways of picking a single entangled pair.

Let us discuss the nonseparable bases in somewhat more detail beginning with four-particle GHZ bases ( $G^{(4)}$ ). These are straightforward generalizations of the three-particle bases  $G^{(3)}$ , and a standard generator set [31] consists of the four operators

$$G^{(4)} = (XXXY, XXYX, XYXX, YXXX). \quad (27)$$

From an alternative generator set,  $(XXXY, IIZZ^{-1}, IZIZ^{-1}, ZIIZ^{-1})$ , it is apparent that eigenstates may again be written as superpositions of  $p$  product states in the standard basis. A more general characterization of GHZ states is provided in the Appendix.

Cluster bases ( $C^{(4)}$ ) were introduced in connection with measurement-based, one-way

quantum computation [32], and in fact both cluster and GHZ states are special cases of a broad class of  $N$ -qubit states, called graph states, which form the basis of this [33]. Ref. [20] has shown that graph states may be classified in terms of curves in phase space, which provides a further connection with the MUB problem. Cluster bases are defined here, for all  $p$ , by generator sets of which a standard example, introduced for the qubit case [32], is

$$C^{(4)} = (XZXI, ZXIX, XIXZ, IXZX). \quad (28)$$

Cluster states have stronger entanglement links between smaller groupings of particles, making their entanglement more robust against decoherence [19] than GHZ entanglement, which is shared equally among all particles. This is reflected in the fact that  $C^{(4)}$  has only two 2-body operators in its compatibility group, as compared with three in the  $G^{(4)}$  case. For this reason, its generator set can only be simplified to  $(XZXI, ZIZ^{-1}I, IZ^{-1}IZ, IXZX)$ , and as a result, the eigenstate expansions can be reduced to no less than  $p^2$  terms in the standard basis. A general characterization of  $C^{(4)}$  accompanies that of  $G^{(4)}$  in the Appendix, which then goes on to show that these, together with the four separable bases, exhaust all MUB possibilities for four qubits.

As a final example, I have found that a new type of basis, one that has no counterpart for qubits, is necessary for the existence of full MUB complements when  $p > 2$ , for reasons that will become apparent. A generator set giving rise to such a basis is

$$P^{(4)} = (ZXYW, XZWY, WYXZ, YWZX), \quad (29)$$

where standard definitions  $Y = XZ$  and  $W = XZ^2$  are followed. The essential point is that the generators are tensor products of four noncommuting one-body matrices, which rules out qubits, but makes possible the elimination of 2-body operators from the compatibility groups for  $p \geq 3$ . Less essential is that the four generators are related by pairwise permutations of operators (hence the notation  $P^{(4)}$ ). The eigenstates have Bell correlations between all pairs of particles, not just the chosen pairs as in  $BB$  states. So, unlike cluster or  $BB$  states, the entanglement is shared equally among all four particles, but unlike GHZ states, the entanglement is robust. One can perform measurements on any two particles, in any two different bases, and produce a Bell state of the other two.

To show that the  $P^{(4)}$  basis does not exhaust the possibilities for  $p \geq 3$ , we mention another generator set involving cyclic permutations,  $(ZXYW, XYWZ^{-1}, YWZX, WZ^{-1}XY)$ ,



where the  $Z^{-1}$  factors are inserted for compatibility. The corresponding basis could play a role similar to that of  $P^{(4)}$  in filling MUB complements for  $p \geq 5$ , although it turns out to be relatively inconsequential when  $p = 3$ . In any case, since it would needlessly complicate the discussion without changing our conclusions, we exclude this example from the analysis.

It is interesting to note in passing, that despite the differences in appearance among the generator sets of the four (five) totally entangled bases, the total numbers of  $I_k$  factors appearing in their compatibility groups must be the same, namely  $4(p^2 - 1)$ , in accordance with Theorem II. This has consequences for stoichiometry, in particular for the standard distributions, and justifies classifying  $BB$  bases as totally entangled.

Let us now turn to questions of stoichiometry. While in previous cases we were able to deduce the allowed entanglement patterns from global constraints alone (those involving total numbers of pure and entangled qubits in MUB complements), with  $N \geq 4$  this is no longer the case. The existence of multiple totally entangled basis types requires that we consider more microscopic constraints associated with the distributions of  $I_k$  factors, as was done for qubits in Ref. [17]. To this end, we define a quantity that is capable of distinguishing among all MUB types under consideration.

The “ $n$ -body profile” of a particular MUB is the distribution of  $n$ -body operators ( $n = 1, 2, \dots, N$ ) in its compatibility group, where (as implied earlier)  $n$ -body operators are those with  $N - n$  identity factors,  $I_k$ . This distribution is normalized to the total number of operators in the compatibility group,  $p^N - 1$ . Examples of  $n$ -body profiles are given in Table II, where we include the  $N = 2$  and 3 cases both for comparison with  $N = 4$ , and also to show how global information is recovered. The number of operators in each category, summed over all MUBs, must equal the numbers listed at the bottom of each column. The latter represent the  $n$ -body profile of the set of all Pauli operators, and are thus independent of the particular MUB choices. They are determined by generating all of the Pauli operators as expansions in the tensor products,

$$(I_1, Z_1, X_1, \dots, X_1 Z_1^{(p-1)}) \otimes \dots \otimes (I_N, Z_N, X_N, \dots, X_N Z_N^{(p-1)}). \quad (30)$$

Thus, the total number of  $n$ -body operators is  $\binom{N}{n}(p - 1)^n$ , as shown. The condition that the MUB sums equal these bottom lines, column by column, provides  $(N - 1)$  independent constraint equations. (In the exceptional case of  $N = 2$ , both equations are independent.)

It is immediately apparent from all of the first columns that the maximum number of  $\Pi$

(a) $N = 2$			(b) $N = 3$			
	1-body	2-body		1-body	2-body	3-body
$\Pi$	$2(p-1)$	$(p-1)^2$	$\Pi$	$3(p-1)$	$3(p-1)^2$	$(p-1)^3$
$B$	0	$p^2-1$	$SB$	$p-1$	$p^2-1$	$(p-1)(p^2-1)$
all	$2(p^2-1)$	$(p^2-1)^2$	$G$	0	$3(p-1)$	$(p-1)^2(p+2)$
			all	$3(p^2-1)$	$3(p^2-1)^2$	$(p^2-1)^3$

(c) $N = 4$				
	1-body	2-body	3-body	4-body
$\Pi$	$4(p-1)$	$6(p-1)^2$	$4(p-1)^3$	$(p-1)^4$
$S^2B$	$2(p-1)$	$2p(p-1)$	$2(p-1)(p^2-1)$	$(p-1)^3(p+1)$
$SG^{(3)}$	$p-1$	$3(p-1)$	$(p-1)^2(p+5)$	$(p-1)^3(p+2)$
$BB$	0	$2(p^2-1)$	0	$(p^2-1)^2$
$G^{(4)}$	0	$6(p-1)$	$4(p-1)(p-2)$	$p^4-4p^2+6p-3$
$C^{(4)}$	0	$2(p-1)$	$4p(p-1)$	$p^4-4p^2+2p+1$
$P^{(4)}$	0	0	$4(p^2-1)$	$p^4-4p^2+3$
all	$4(p^2-1)$	$6(p^2-1)^2$	$4(p^2-1)^3$	$(p^2-1)^4$

TABLE II:  $n$ -body profiles for all MUBs under discussion. The bottom lines (“all”) are the  $n$ -body profiles of the set of all Pauli operators.

bases is always given by  $p+1$ , the number that defines the standard MUB complement. Part (a) confirms that this is the only choice for  $N = 2$ , and its second column then determines the number of Bell bases  $(p^2 - p)$ , in accordance with the required total number of MUBs. Part (b) reproduces all  $N = 3$  results, as were summarized on Table I. The three columns provide three equations, but only two are linearly independent: The first column determines all possible combinations of  $\Pi$  and  $SB$  bases, and the second column then determines the number of  $G^{(3)}$  bases, which is again consistent with the required total number of MUBs,  $p^3 + 1$ . The third column provides no further constraint.

Proceeding to the case of  $N = 4$ , the calculation of the  $n$ -body profiles for the separable bases is straightforward, since their compatibility groups are tensor products of those whose profiles have already been calculated. The new nonseparable bases require more thought.

	1-body	2-body	3-body	4-body
$\Pi$	4	6	4	1
$S^2B$	2	4	6	3
$SG^{(3)}$	1	3	7	4
$BB$	0	6	0	9
$G^{(4)}$	0	6	0	9
$C^{(4)}$	0	2	8	5
all	12	54	108	81

TABLE III: Specific  $n$ -body profile for four qubits.

We found that the more symmetrical generator sets listed in Eqs. 27-29 were helpful in working out the profiles for general  $p$ .

One can see by inspection of Table II(c) that there is a qualitative difference between  $N = 4$  and the other cases. Consider just the first 6 MUB types, which represent all possibilities for  $p = 2$ . Looking at the 3-body factors in column (iii), we can see that as  $p$  increases, the number of  $G^{(4)}$  and/or  $C^{(4)}$  MUBs would have to increase as  $\sim p^4$  in order to satisfy just Eq. (iii). But then they could not satisfy Eq. (ii), for they would produce too many two-body operators. Clearly, one eventually needs a basis which, like  $P^{(4)}$ , has no two-body operators. This need makes itself felt already with  $p = 3$ , and becomes urgent with  $p = 5$ . With these differences in mind, let us consider the  $p = 2, 3$  and  $5$  cases sequentially, to show how the general picture evolves with increasing  $p$ .

#### four qubits

The  $n$ -body profiles for  $p = 2$  are shown on Table III. To explore stoichiometries, consider the three equations (i, ii, and iii) represented by the first three columns, respectively. Equation (i), by itself, determines all possible combinations of the first three MUB types,

$$4N(\Pi) + 2N(S^2B) + N(SG^{(3)}) = 12. \quad (31)$$

Next, notice that we can isolate the  $BB$  and  $G^{(4)}$  MUBs because of their simple profiles. Indeed, by simply adding (i) and (iii) we obtain the sum of all *other* MUBs,

$$N(\Pi) + N(S^2B) + N(SG^{(3)}) + N(C^{(4)}) = 15. \quad (32)$$

	$(p = 2)$		$(p = 3)$		$(p = 5)$	
$\Pi$	3	0	4	0	6	0
$SG^{(3)}$	0	12	0	16	0	24
$BB$	2	2	0	0	0	0
$C^{(4)}$	12	3	72	66	360	396
$P^{(4)}$	–	–	6	0	260	206
all	17	17	82	82	626	626

TABLE IV: Examples of MUB distributions for four qubits with  $p = 2, 3$ , and  $5$ . First, third, and fifth columns show standard distributions that maximize the numbers of totally entangled bases, while even columns show nonstandard distributions that minimize this number. Examples are chosen to minimize the number of  $P^{(4)}$  MUBs in all of the  $p = 3$  and  $5$  cases.

Since there are 17 MUBs in total we know immediately that

$$N(BB) + N(G^{(4)}) = 2, \quad (33)$$

a result which also follows from  $2(\text{ii}) + (\text{iii}) - (\text{i})$ , which reproduces the total number.

There are 16 ways to satisfy Eq. 31, with  $N(C^{(4)})$  determined in each case by Eq. 32. For each of these combinations, there are 3 ways to satisfy Eq. 33, for a total of 48 possible MUB distributions. To illustrate the range, a standard and a nonstandard distribution are shown in the two leftmost columns of Table IV. These examples are chosen to show the maximum and minimum numbers of the new (nonseparable)  $C^{(4)}$  MUBs, which make up a majority of MUBs in 30 of the 48 possible distributions. The dominance of  $C^{(4)}$  MUBs is related to the large number of 3-body operators in their profile. Similar complements were found in Ref. [17] through an explicit construction, except that the  $G^{(4)}$  MUBs were not produced, so that 16 combinations were obtained with 2  $BB$  MUBs present in all of them.

#### four qutrits

The  $n$ -body profiles for the  $p = 3$  case are shown in Table V. Again, the first column restricts the combinations of the first three MUB types,

$$4N(\Pi) + 2N(S^2B) + N(SG^{(3)}) = 16. \quad (34)$$

(a) $p = 3$				(b) $p = 5$			
	1-body	2-body	3-body		1-body	2-body	3-body
$\Pi$	8	24	32	$\Pi$	16	96	256
$S^2B$	4	12	32	$S^2B$	8	40	192
$SG^{(3)}$	2	6	32	$SG^{(3)}$	4	12	160
$BB$	0	16	0	$BB$	0	48	0
$G^{(4)}$	0	12	8	$G^{(4)}$	0	24	48
$C^{(4)}$	0	4	24	$C^{(4)}$	0	8	80
$P^{(4)}$	0	0	32	$P^{(4)}$	0	0	96
all	32	384	2048	all	96	3456	55296

TABLE V: The  $n$ -body profiles for four qutrits and four ququints.

The first and second columns together [(ii)–3(i)] restrict other combinations,

$$4N(BB) + 3N(G^{(4)}) + N(C^{(4)}) = 72, \quad (35)$$

and the inclusion of the third column [(iii)+2(ii)–6(i)] yields the total MUB count,

$$N(\Pi) + \dots + N(P^{(4)}) = 82. \quad (36)$$

There are 25 combinations of the first three MUB types that satisfy Eq. 34, as compared with 16 such combinations in the qubit case. But, in the absence of  $P^{(4)}$  MUBs, one cannot solve both Eqs. 35 and 36 for all of these combinations, and we find a total of only 11 MUB distributions. To trace the reasons, we subtract Eq. 35 from 36 and solve for  $P^{(4)}$ :

$$N(P^{(4)}) = 10 + 3N(BB) + 2N(G^{(4)}) - [N(\Pi) + N(SSB) + N(SG^{(3)})]. \quad (37)$$

Without  $P^{(4)}$  MUBs the left side vanishes, and there can be solutions only if the quantity in square brackets is 10 or larger. This condition fails for the standard distribution, for which this number is  $N(\Pi) = 4$ . In this case, the minimum number of  $P^{(4)}$  MUBs is 6, as shown on Table IV. The other entry maximizes the quantity in square brackets at  $N(SG^{(3)}) = 16$ . In both entries we then minimize the number of  $P^{(4)}$  MUBs by maximizing the number of  $C^{(4)}$  MUBs. One can increase the number of  $P^{(4)}$  MUBs over these minima by adding  $BB$  and/or  $G^{(4)}$  and subtracting  $C^{(4)}$  MUBs. Although its numbers can be small, the  $P^{(4)}$  MUBs

play a critical role in maintaining the balance of 3-body operators (Table V) at no cost in two-body operators.

With  $P^{(4)}$  MUBs included, the multiplicity of each of the 25 solutions of Eq. 34 is large (we estimate more than 200), for a total of probably more than 5000 solutions. We cannot argue that all of these solutions represent realizable MUB distributions, because we cannot rule out the possibility of more subtle constraints. Such concerns are beyond the scope of the present paper.

#### four ququints

Again consulting Table V for the  $p = 5$  case, it is striking to see how three simple equations can again emerge from appropriate combinations. The first column gives us directly

$$4N(\Pi) + 2N(S^2B) + N(SG^{(3)}) = 24, \quad (38)$$

the combination [(iii)+8(ii)−64(i)] relates the other four quantities,

$$8N(BB) + 5N(G^{(4)}) + 3N(C^{(4)}) + 2N(P^{(4)}) = 1600, \quad (39)$$

and still another combination [(iii)+2(ii)−22(i)] yields the total MUB count,

$$N(\Pi) + \dots + N(P^{(4)}) = 626. \quad (40)$$

There are 49 combinations of the first three MUB types that satisfy Eq. 38, but in the absence of the  $P^{(4)}$  MUBs, *none* of these admits solutions of Eqs. 39 and 40. To see how this situation arises, solve the latter two equations for  $N(P^{(4)})$  while eliminating  $N(C^{(4)})$ :

$$N(P^{(4)}) = 278 + 5N(BB) + 2N(G^{(4)}) - 3[N(\Pi) + N(SG^{(3)}) + N(SSB)]. \quad (41)$$

The quantity in square brackets has minimum and maximum values of 6 (the standard distribution) and 24, as shown on Table V, corresponding to lower bounds on  $N(P^{(4)})$  of 260 and 206, respectively. The latter is the absolute minimum number of  $P^{(4)}$  MUBs in any full complement. Again, one can add  $P^{(4)}$  MUBs by removing  $C^{(4)}$  and adding  $BB$  and/or  $G^{(4)}$  MUBs, so that  $P^{(4)}$  can be the majority MUB type in some complements. While  $P^{(4)}$  is critical for both  $p = 3$  and 5 cases, it plays a considerably more dominant role here. The underlying reason is that the ratio of the numbers of 3-body to 2-body operators increases considerably in going from  $p = 3$  to 5, as shown in Table V.

We estimate the total number of solutions of Eqs. 38-40 to be in excess of  $10^6$ , but again, we cannot argue that all such solutions represent realizable MUB distributions, or provide a revised estimate, without a further study of possible constraints.

The examples of this section have shown us that with every step in  $N$ , and with some steps in  $p$ , full complements require not only those MUB types generated from smaller systems, but also new, nonseparable MUB types that exhibit new entanglement characteristics inaccessible to smaller systems. In the step from  $N = 2$  to 3,  $G^{(3)}$  MUBs are required for the standard distribution, although a nonstandard distribution ( $SB$  only) is possible with  $p = 2$ . With the step to  $p = 3$ , no MUB complement exists without  $G^{(3)}$ . In the step to  $N = 4$ , the  $C^{(4)}$  MUBs are indispensable to all MUB distributions with  $p = 2$ . With the step to  $p = 3$ , the new  $P^{(4)}$  MUBs become possible, and they in turn make possible the standard distribution. At  $p = 5$ , the  $P^{(4)}$  MUBs become indispensable to all distributions.

Projecting to larger systems, the distinguishing feature of the  $P^{(4)}$  generator set is that a different (noncommuting) Pauli matrix factor is associated with each qupit. The number of such factors in general is  $p + 1$ , and when this is equal to the number of qupits, a new type of entanglement becomes possible. Thus we predict that when  $N$  is equal to any prime plus 1, then that prime ( $p_N = N - 1$ ) is a critical value for the emergence of new entangled states as  $p$  is increased at fixed  $N$ . These states should play critical roles in filling MUB complements for  $p$  equal to or slightly greater than  $p_N$ .

## V. CONCLUSIONS AND OPEN QUESTIONS

We have exploited the connections between MUBs and Pauli operators to develop a general framework for investigating both the entanglement properties of individual MUBs, and the combinations of such MUBs that can be found in full complements. We began by proving general theorems regarding MUBs as eigenbases of Pauli operators: We showed that the purities of individual qupits in such eigenbases must be either 0 or 1, that the purity alone dictates the distribution of Pauli matrix factors (including  $I_k$ ) in the compatibility groups of these MUBs, and that every qupit must adopt these special purities the same number of times within any MUB complement:  $(p + 1)$  times pure, and  $(p^N - p)$  times totally entangled. An immediate corollary is that one may have at most  $p + 1$  product MUBs in a full complement, and when one does, all remaining MUBs must be totally entangled. This

defines the standard distribution.

Armed with these theorems and the general properties of Pauli operators, one quickly obtains more specific results: When  $N = 2$ , only product and generalized Bell bases are possible, for any  $p$ , and the standard MUB distribution is inevitable. With  $N = 3$ , the unique totally entangled bases are generalized GHZ bases, but a third MUB type becomes possible, namely separable-Bell bases. This makes possible  $p+2$  distinct MUB distributions. With  $N = 4$  and  $p = 2$  there are six MUB types, including two nonseparable bases and a third ( $BB$ ) that is separable but totally entangled. There are 48 possible MUB distributions, with cluster bases making up the majority of MUBs in most of these. With  $N = 4$  and larger  $p$ , further MUB types exist, and at least one such MUB type ( $P^{(4)}$ ) is essential to forming a standard MUB complement with  $p = 3$ , and to forming *any* MUB complement with  $p = 5$ .

Several results have emerged in the course of working the above examples, and it seems useful to synthesize these in one place: (1) A MUB can exist in any separation pattern. (2) All states in a particular MUB have common separation and entanglement patterns - the generator set contains all information about the nature of the entanglement, while the eigenvalues specify the states. (3) Compatibility groups of separable bases are tensor products of those of the nonseparable constituent bases. It follows that (4) within nonseparable groupings of qupits, those with two qupits must be in generalized Bell states, those with three qupits - generalized GHZ states. Those with 4 qupits have the same broader array of options available to 4-qupit systems.

Perhaps the most important lesson to be drawn from the present examples is that, although it is easy to construct MUBs from those found at lower  $N$ , either as tensor products, or as larger- $N$  counterparts such as  $G^{(N)}$ , the more interesting challenge is to find the new nonseparable MUB types, with no counterparts at smaller  $N$  (or sometimes  $p$ ), that make full complements possible. It may be a general feature that such MUBs tend to dominate MUB distributions near the  $N$  and  $p$  values where they first emerge, only to be superceded by other MUB types as the system size increases. In this sense, every  $N$  is critical, but not every  $p$ . We predict that when  $N$  is a prime plus 1 (*eg*,  $N = 6, 8, \dots$ ), there will be a critical value,  $p_N = N - 1$ , for the introduction of new entangled states that will play critical roles in MUB distributions.

Closing thoughts on the existence question: The intimate connection between MUBs



and entanglement for  $N \geq 2$  highlights the way in which all known MUB complements take advantage of the symmetry associated with equivalent parts, unique to dimensions  $p^N$  [34]. Theorem I, which makes no reference to dimension, cannot hold in (at least some) composite dimensions: In the simplest counterexample, 6 dimensions, the qubit can be totally entangled, but the qutrit cannot be. Yet, the import of Theorem I is that for all known MUB complements, there exists a factorization into parts (represented by some set of generalized Pauli operators), in terms of which Theorem I (and the others) hold. Thus, in addition to the existence question in composite dimensions, there is also an existence question in  $p^N$  dimensions - Do MUB complements exist that violate Theorem I? Perhaps entanglement considerations such as the present ones will help in answering these persistent questions.

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## APPENDIX

First, we write general definitions of  $G^{(4)}$  and  $C^{(4)}$  bases in terms of generator sets, and then we show that these are the only possible nonseparable bases for four qubits.

To generalize Eqs. 27 and 28 with maximum transparency, we follow the alternative forms written in the text and define  $G^{(4)}$  bases by the generator set

$$G^{(4)} = (ABII, AICI, AIID, STUV), \quad (42)$$

where every four-body factor must differ from its two-body counterpart ( $S \neq A$ , etc.). The two-body operators provide the special product basis for the  $p$ -term expansion. The generalization to  $N$ -qubit GHZ states is apparent.

The  $C^{(4)}$  bases are best defined in a similar way, although a bit less transparently because there are only two independent two-body operators,

$$C^{(4)} = (AICI, IBID, SBUI, ITCV). \quad (43)$$

Again, the two-body operators provide a product basis for the expansion, which in this case requires  $p^2$  terms. Individual factors in the three-body operators must differ from corresponding factors in the two-body operators, except where their equality is explicit.

It should be noted that there are two variations on the  $C^{(4)}$  generator set, corresponding to the other ways of pairing the two-body factors. One such variation is  $(ABII, IICD, STCI, IBUV)$ . The three alternatives are mathematically equivalent, although one can make a physical distinction based on entanglement links between pairs. The stronger entanglement links in a system represented by Eq. 43 are between neighbors in the sequence (1-2-3-4-1). In the variation given above, the sequence is (1-3-2-4-1), and in the other possible variation it is (1-2-4-3-1). The various possibilities are not unphysical, as one can imagine unlike particles with tetrahedral coordination.

### Completeness for qubits

We now argue that the two bases defined above are the only nonseparable options for qubits. We first argue that both are the unique nonseparable representatives of their respective  $n$ -body profiles as shown on Table III. We then show that other profiles cannot exist for qubits.

It is straightforward to verify that the  $G^{(4)}$  generators produce six two-body operators involving the same factors,  $A - D$ . These exhaust all 12 of the available  $I_k$  factors (Theorem II demands three  $I_k$  factors per qubit), so that all remaining operators are 4-body operators, as shown in the table. The only other basis that can share this profile is  $BB$ , in which the two-body operators have factors that do not commute individually. But, by virtue of this fact, the  $BB$  basis has four independent two-body operators, so that these can compose the generator set. The separability of the basis is then obvious.

Turning to the  $C^{(4)}$  case, it is straightforward to show that the generators of Eq. 43 produce no further two-body operators beyond the two shown, so that remaining  $I_k$  factors must appear with the 8 three-body operators. One might wonder whether a different basis could be found with the same profile by using four-body generators in place of the three-body generators. The answer is no - It is easy to show that this would generate only  $G^{(4)}$  or  $BB$  bases, depending upon whether one of the four-body generators shares factors with one of the two-body generators.

The remaining point is to rule out other four-qubit profiles. It suffices to consider just the two-body operators, whose maximum number is six. We will show that the numbers 4 and 0 are impossible for qubits. The former case is very simple - it is impossible to find four commuting two-body operators that do not generate two more (and these will immediately identify themselves as belonging to either a  $G^{(4)}$  or  $BB$  compatibility group).

As to the latter case, assume that there are no two-body operators. Then all 12 of the  $I_k$  factors must appear in one-body operators, making three appearances on each qubit (Theorem II). Consider any two of these operators that have their  $I_k$  factors on the same qubit. Commutativity demands that they have exactly one other factor in common, so that their product is a two-body operator. This forms a contradiction and shows that there is no profile without two-body operators.

To briefly summarize the results of this appendix, the 6 MUB types listed on Table III exhaust the possibilities for four qubits. The 5 corresponding  $N$ -body profiles are also exhaustive; in particular, a  $P^{(4)}$ -like profile does not exist for qubits.

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