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Mutually unbiased bases: a group and graph theoretical approach

Gernot Alber[1] **and Christopher Charnes**

Institut für Angewandte Physik-Theorie, Hochschulstrasse 4a, D-6429 Darmstadt, Germany

E-mail: gernot.alber@physik.tu-darmstadt.de

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Abstract

In this contribution the main ideas underlying recent work aiming at the construction of mutually unbiased bases in finite dimensional Hilbert spaces are discussed. This approach relies on a systematic use of group and graph theoretical concepts announced by Charnes and Beth (2005 *ERATO Conf. on Quantum Information Science*) and extended significantly by Charnes (2018 in preparation) recently. A principal feature of this method is its independence of prime number restrictions thus distinguishing it from almost all previous constructions which have relied on finite fields and related concepts of finite geometry. This group and graph theoretical approach offers the possibility to gain new insight into the intricate relation between quantum theoretical complementarity as encoded in mutually unbiased bases and characteristic geometrical structures of the Hilbert space involved.

Keywords: mutually unbiased bases, group representations, graphs, quantum information

(Some figures may appear in colour only in the online journal)

1. Introduction

Mutually unbiased bases have interesting applications in quantum information processing ranging from quantum cryptography and quantum communication to applications in quantum tomography [1–8]. Since the seminal work of Wootters and Fields [4] which demonstrated that in a d-dimensional Hilbert space the maximum possible number of mutually unbiased bases is $(d + 1)$, numerous theoretical proposals have appeared for constructing maximal sets of mutually unbiased bases saturating this upper bound. Practically all these proposals are variants of the two constructions in odd and even characteristic finite fields developed by Wootters and Fields [4] which demonstrated that in Hilbert spaces, whose dimensions are prime powers, complete sets of mutually unbiased bases exist. With the help of these methods it has been shown constructively that the upper bound of $(d + 1)$ can be saturated for prime power Hilbert space dimensions.

Despite these interesting results and significant theoretical efforts these approaches still leave open numerous questions in particular as far as properties of mutually unbiased bases in Hilbert space dimensions are concerned which are not prime powers. Thus, it is still an open question, for example, whether the upper bound of $(d + 1) = 7$ can be saturated for Hilbert spaces with dimension $d = 6$.

Our contribution aims at describing and exploring the main ideas of a recently developed group and graph theoretical approach [9, 10] targeting the construction of large sets of mutually unbiased bases systems systematically and to demonstrate this group and graph theoretical approach by examples. Besides practical advantages this approach also offers novel conceptual advantages as it is independent of prime number conditions of previous approaches. With the help of this approach it can be demonstrated that the construction problem of mutually unbiased basis systems can be formulated as a clique finding problem in Cayley graphs of groups which are naturally associated with sets of mutually unbiased bases.

2. Mutually unbiased bases, unitary groups and Cayley graphs

Based on the early work of Charnes and Beth [9] in this section basic definitions are summarized which specify relations between mutually unbiases bases, their basis groups and associated Cayley graphs capable of encoding their characteristic features.

[1] Author to whom any correspondence should be addressed.

2.1. Mutually unbiased bases

Let us consider a d-dimensional Hilbert space $\mathcal{H}^d$ with a given scalar product, say $\langle .|.\rangle$, and with an ordered canonical orthonormal basis $(|\alpha\rangle;\ \alpha = 1,\cdots,\ d)$. By choosing a particular ordering every other orthonormal basis of this Hilbert space, say $B := (|B_i\rangle;\ i = 1,\cdots d)$, is characterized by its associated unitary matrix M_B with matrix elements $(M_B)_{i\alpha} = \langle B_i|\alpha\rangle^*$ and with $i,\ \alpha \in \{1,\cdots,\ d\}$. Correspondingly the unit matrix E_d is associated with the canonical basis itself. Furthermore, the group of unitary $d \times d$ matrices $U(d)$ acts transitively on the possible ordered bases of the Hilbert space $\mathcal{H}^d$, i.e. after the choice of a particular ordering of the states of each basis each pair of bases, say B and C, determines a unique unitary matrix $U \in U(d)$ mapping $B \to C$ by right multiplication, i.e. $M_B\, U = M_C$.

Two arbitrarily ordered orthonormal bases of this Hilbert space, say B and C, are defined to be mutually unbiased with respect to each other iff

$$|\langle B_i|C_j\rangle|^2 = |(M_C M_B^\dagger)_{ji}|^2 = \frac{1}{d} \tag{1}$$

for all $i,\ j \in \{1,\ \cdots,\ d\}$.

In physical terms this condition guarantees that a non-selective sequential quantum measurement of two observables, whose eigenbases are mutually unbiased, always results in the completely mixed (chaotic) state irrespective of the order in which these non-selective measurements are performed. Therefore, two mutually unbiased bases capture a characteristic feature of 'quantum complementarity'. They are capable of erasing all previous information about a quantum state by such a sequential non-selective measurement process. This characteristic property becomes apparent by denoting the Hermitian operators of these two observables by

$$\hat{B} = \sum_{i=1}^{d} b_i |B_i\rangle\langle B_i|,\quad \hat{C} = \sum_{j=1}^{d} c_j |C_j\rangle\langle C_j|. \tag{2}$$

A non-selective measurement, say first of observable $\hat{B}$ and subsequently of observable $\hat{C}$, changes an arbitrary initially prepared quantum state with density operator $\rho \geqslant 0$ and $\mathrm{Tr}(\rho) = 1$ into the completely mixed (chaotic) quantum state [11]

$$\rho' = \sum_{j=1}^{d} |C_j\rangle\langle C_j| \left(\sum_{i=1}^{d} |B_i\rangle\langle B_i|\rho|B_i\rangle\langle B_i| \right) \times |C_j\rangle\langle C_j| = \frac{1}{d}\sum_{j=1}^{d} |C_j\rangle\langle C_j| = \frac{1}{d}\mathbf{1}. \tag{3}$$

Thereby, the completeness relation $\mathbf{1} = \sum_{j=1}^{d} |C_j\rangle\ \langle C_j| = \sum_{i=1}^{d}\ |B_i\rangle\langle B_i|$ and the unit normalization condition of the quantum state ρ, i.e. $\mathrm{Tr}\ (\rho)\ = 1 = \sum_{i=1}^{d}\langle B_i|\ \rho|B_i\rangle\ = \sum_{j=1}^{d}\langle C_j|\ \rho|C_j\rangle$, have been used. The same result is obtained if the sequential measurement process is performed in the reverse order. It should also be pointed out that the introduction of an ordering within each basis system $B := (|B_i\rangle;\ i = 1,\cdots d)$ is physically relevant since each projector $|B_i\rangle\langle B_i|$ is associated with the physically observable eigenvalue b_i of the observable $\hat{B}$ of equation (2). Although each of these projectors is independent of phase changes of the various elements of this basis, such phase changes induced by a unitary operator diagonal in this basis are observable by their effect on arbitary pure quantum states which are linear superpositions of these basis states.

2.2. Unitary basis groups and their associated Cayley graphs

According to section 2.1 the group of unitary matrices $U(d)$ acts transitively on all possible ordered orthonormal bases of a d-dimensional Hilbert space by right multiplication. In order to capture characteristic structural features of a system of mutually unbiased bases it is useful to define the concept of an associated basis group. Accordingly, a basis group G of a set of (pairwise) mutually unbiased ordered bases, say $\{B^{(1)}, B^{(2)},\cdots, B^{(l)}\}$, of a d-dimensional Hilbert space is defined by the particular unitary subgroup of $U(d)$ generated by the unitary matrices associated with these mutually unbiased bases, i.e. $G := \langle M_{B^{(1)}},\cdots, M_{B^{(l)}}\rangle$. Consistent with our previous conventions, the elements of this basis group G act on themselves by right multiplication. It should be pointed out that in general not all pairs of elements of such a basis group are mutually unbiased and that in general there is no guarantee that the basis group of a set of mutually unbiased bases is finite. The structure of the mutually unbiased pairs generated by such a basis group G is captured conveniently by its associated basis Cayley graph $\Gamma(G, S)$. The vertices of this basis Cayley graph are the elements of the basis group G and its vertex x is directly connected to its vertex y, i.e. $x \to y$, iff $yx^{-1} \in S$. Thereby the set of edges S of this Cayley graph is defined by all those members of the basis group G which are mutually unbiased with respect to the canonical orthonormal basis represented by the unit matrix E_d.

In the following some basic properties of such a basis Cayleigh graph $\Gamma(G, S)$ are summarized:

- As the set S contains with each unitary basis matrix, say $M_{B^{(j)}}$, also its inverse $M_{B^{(j)}}^\dagger$ the basis Cayley graph $\Gamma(G, S)$ is undirected.
- Edge connectedness is defined by left multiplication and group multiplication within the unitary subgroup G by right multiplication. Therefore, group multiplication preserves the incidence relation. Consequently the basis group G is also a subgroup of the automorphism group $Aut(\Gamma(G, S))$ of the basis Cayley graph $\Gamma(G, S)$.
- As special instances of general Cayley graphs all basis Cayley graphs $\Gamma(G, S)$ are connected, i.e. there is an edge connected path between each possible pair of vertices.
- As special instances of general Cayley graphs all basis Cayley graphs $\Gamma(G, S)$ are regular, i.e. each vertex is connected to the same number of neighbors, i.e. it has the same valency.

From its definition it is apparent that the cliques of a basis Cayley graph $\Gamma(G, S)$, i.e. its completely connected subgraphs, are associated with mutually unbiased bases. As a consequence the search problem for maximal sets of mutually unbiased bases can be reformulated as a search problem for the largest clique of a basis Cayley graph $\Gamma(G, S)$, i.e. the size of its largest complete subgraphs. For a given dimension d of the Hilbert space this clique number cannot exceed the maximum possible number of mutually unbiased bases $(d + 1)$ [4].

3. Mutually unbiased bases and the structure of their basis Cayley graphs

In this section the main ideas underlying a recently established connection [10] between the structure of basis Cayley graphs and the existence of a maximum set of $(d+1)$ mutually unbiased bases in a d-dimensional Hilbert space are discussed.

According to section 2.2 a set of l mutually unbiased bases can be associated with a clique of size l, i.e. a completely connected subgraph with l vertices, of a basis Cayley graph $\Gamma(G, S)$. Therefore, it is of major interest to establish a quantitative relation between the clique number of basis Cayley graphs, i.e. the number of vertices of the largest possible completely connected subgraphs, and other characteristic features of Cayley graphs. It is a major recent result [10] that such a relation can be established for finite basis Cayley graphs which also restricts some of their structural properties.

In order to establish a general quantitative connection between the clique size of a basis Cayley graph Γ (G, S) and some of its other structural properties, we can take advantage of its regularity. If in addition, the basis Cayley graph under consideration is finite, advantage can be taken of powerful general relations which have already been established for regular finite graphs [12, 13]. For this purpose let us consider a general finite and regular graph of size n and valency k. A lower bound on the clique number of such a k-regular graph is given by $n/(n-k)$. This lower bound has been improved further by Wilf [12] with the help of spectral methods. Later Yildirim [13] derived closed form expressions for this lower bound and established that the clique number of a regular graph equals $n/(n-k)$ provided this regular graph is also complete multipartite, i.e. it can be partitioned into disjoint non empty sets, so called independent sets or 'colorings', so that there is an edge between every pair of vertices from different independent sets and that vertices of an independent set are not connected among themselves.

Based on these developments the following theorem has been established recently [10]:

Theorem. *Let G be a finite basis group of order $|G| = n$ whose basis Cayley graph has an edge generating set S of size $|S| = k$. If the condition*

$$\frac{n}{n-k} = d + 1 \tag{4}$$

is fulfilled the k-regular basis Cayley graph $\Gamma(G, S)$ has clique number $d+1$ and it is complete multipartite. This complete multipartite basis graph consists of $d+1$ independent sets and has $(n-k)^{d+1}$ maximum cliques each of size $d+1$.

According to this theorem the existence of a k-regular complete multipartite basis Cayley graph with n vertices fulfilling equation (4) is sufficient for the existence of $(n-k)^{d+1}$ cliques each of which contains a maximum set of $d+1$ mutually unbiased bases of a d-dimensional Hilbert space. As a consequence the construction of maximum sets of $d+1$ mutually unbiased bases in a d-dimensional Hilbert space requires the following steps:

- Select a finite edge generating set, say $S = \{M_{B^{(1)}}, \cdots, M_{B^{(k)}}\}$, so that the unitary matrices $M_B^{(l)}$ with $l = 1, \cdots, k$ are mutually unbiased with respect to the unit matrix E_d but not necessarily mutually unbiased among themselves;
- construct the group $G = \langle M_{B^{(1)}}, \cdots, M_{B^{(k)}}\rangle$ generated by these unitary matrices;
- choose the generating unitary matrices of the set S in such a way that G is finite, say of order n, and that the condition of equation (4) is fulfilled. As a result of the structure theorem the resulting Cayley graph $\Gamma(G, S)$ will be k regular and complete multipartite.

4. Examples of basis Cayley graphs associated with mutually unbiased bases

In this section examples of finite unitary basis groups acting in two and three dimensional Hilbert spaces are presented which generate sets of mutually unbiased bases and whose Cayley graphs are complete multipartite. These examples illustrate the general property formulated in the structure theorem of section 3. However, these examples also show that basis groups which do not generate maximum sets of mutually unbiased bases can also result in associated completely multipartite Cayley graphs and, moreover, that a complete multipartite graph can be the Cayley graph of different basis groups. These examples take advantage of the fact that unitary generators of finite orders, say U_1 and U_2 with $U_1^{n_1} = E_2 = U_2^{n_2}$, which are mutually unbiased with respect to the canonical basis represented by the unit matrix E_d and which imply that also their products are of finite orders, constitute convenient generators for basis groups.

4.1. Complete sets of mutually unbiased bases in d = 2

4.1.1. The complete tripartite graph $K_{1,1,1}$. The simplest complete multipartite graph associated with a maximum set of unbiased bases fulfilling equation (4) for $d = 2$ is a triangle with the characteristic parameters $(n, k, d) = (3, 2, 2)$ as depicted in figure 1. So it yields $(n-k)^{d+1} = 1$ set consisting of the maximum number of $d + 1 = 3$ mutually unbiased bases in a $d = 2$-dimensional Hilbert space.

This graph is a trivial example of a complete 3-partite graph denoted by $K_{1,1,1}$. It has 3 independent sets partitioning its vertices, and there is an edge between every pair of vertices from different independent sets. The notation $K_{1,1,1}$ indicates its 3-partite nature and the fact that each independent set contains a single vertex only. According to our previous discussion $K_{1,1,1}$ is a 2-regular 3-partite graph which can be interpreted as a basis Cayley graph $\Gamma(G, S)$ of a cyclic group $G := \langle M_B\rangle$ of order $n = 3$, i.e. its single generator fulfills the relation $M_B^3 = E_2$. This graph is isomorphic to the complete graph K_3 on three vertices and to the 1-skeleton of the simplex α_2, see [14].

According to the discussion of section 3 the set $S := \{M_B, M_B^\dagger\}$ is an edge set of this basis graph if and only if the pairs M_B and $M_B^\dagger$, and E_2 and M_B are both mutually unbiased. In the canonical basis the unitary 2×2-matrix M_B associated with the generating basis B has the most general form

$$M_B := \frac{e^{i\gamma}}{\sqrt{2}} \begin{pmatrix} e^{i\varphi} & e^{i\psi} \\ -e^{-i\psi} & e^{-i\varphi} \end{pmatrix}. \quad (5)$$

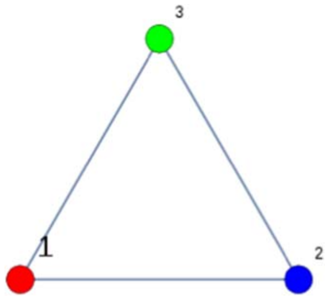

Figure 1. The complete 3-partite graph $K_{1,1,1}$ which forms a triangle: each vertex constitutes an independent set and all vertices are connected.

Consistent with the mutual unbiasedness of M_B, $M_B^\dagger$, and E_2 the periodicity condition requires either $\cos(\pi/3) = \cos\varphi/\sqrt{2}$ and $\gamma = \pi/3$ implying $\varphi = \pm\pi/4$ or $\cos(2\pi/3) = \cos\varphi/\sqrt{2}$ and $\gamma = 0$ implying $\varphi = \pm 3\pi/4$. In either case the phase ψ is arbitrary so that there exists a continuous family of different unitary cyclic basis groups $G := \langle M_B \rangle$ of order three for this particular basis Cayley graph.

A particular member of this continuous family is identified by the values of its phases $\psi \in [0, 2\pi)$, $\varphi \in \{\pm\pi/4, \pm 3\pi/4\}$ and the corresponding value of γ. The $d + 1$ elements of each of these groups form a maximum number of cyclic mutually unbiased bases in dimension $d = 2$. As these basis groups are Abelian all their two dimensional representations are equivalent.

4.1.2. The complete tripartite graph $K_{2,2,2}$—the octahedron. Another k-regular complete multipartite graph fulfilling equation (4) for $d = 2$ has the parameters $(n, k, d) = (6, 4, 2)$. It is a complete 3-partite graph denoted by $K_{2,2,2}$. This graph is the 1-skeleton of the regular octahedron or cross polytope β_3 in three dimensional Euclidean space [14, 15].

Each of its three independent coloring sets contains two vertices and as a consequence of its complete multipartite nature there is an edge connecting every pair of vertices from different color sets, while vertices within an independent set are unconnected. In view of this particular partitioning each vertex is the starting point of $k = 4$ edges. This 4-regular complete 3-partite graph can be interpreted as a basis Cayley graph $\Gamma(G, S)$ of various basis groups G of order $|G| = n = 6$. In the following we discuss two continuous families of such basis groups which can be associated naturally with the octahedron.

Let us denote the six vertices of the octahedron chosen in some order by the numbers $m = 1, \ldots, 6$. The first family of basis groups can be taken to be cyclic of order 6 so that each member of this family is characterized by a generating unitary 2×2-matrix M_A, i.e. $G := \langle M_A \rangle$, with $M_A^6 = E_2$. Thus, in the canonical basis the most general form of this generator is given by

$$M_A = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-i\pi/4} & e^{i\psi_A} \\ -e^{-i\psi_A} & e^{i\pi/4} \end{pmatrix} \quad (6)$$

with the arbitrary phase $\psi_A \in [0, 2\pi)$.

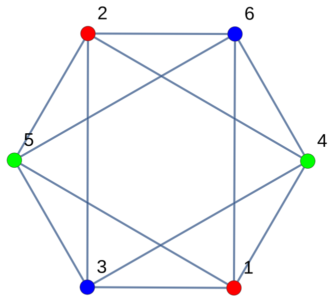

Figure 2. The complete 3-partite graph $K_{2,2,2}$: the 1-skeleton of the regular octahedron or cross polytope β_3.

The graph of figure 2 can be interpreted as the basis Cayley graph $\Gamma(G, S)$ of this cyclic group with the edge generating set $S := \{M_A, M_A^\dagger = M_A^5, M_A^2, M_A^{\dagger 2} = M_A^4\}$ by choosing a mapping of ordered orthonormal basis systems to the vertices such as

$$M_A^6 \to 1,\ M_A^3 \to 2,\ M_A^4 \to 3,\ M_A^2 \to 4,$$
$$M_A^5 \to 5,\ M_A \to 6. \quad (7)$$

In this way a continuous one-parameter family of basis groups is obtained whose members are identified by a particular value of the phase $\psi_A \in [0, 2\pi)$. According to equation (6) $M_A^m = -M_A^{m+3}$ for $m \in \{1, 2, 3\}$ so that the basis vectors of pairs of ordered orthonormal bases systems associated with m and $m + 3$ differ by a single global phase only. These three pairs form the three independent sets with different colors of the complete 3-partite graph $K_{2,2,2}$. They can be associated with the three cosets $[E_2]$, $[M_A]$, $[M_A^2]$ of the normal subgroup $C_2 = \{E_2, M_A^3\}$ in $G = \langle M_A \rangle$, i.e. $[M^i] := \{g \in G | g = M^i h$ for all $h \in C_2\}$ with $i = 0, 1, 2$.

As every pair of vertices from different independent sets is connected by an edge and vertices within each independent set are unconnected this complete multipartite graph can be simplified by collapsing each of these independent sets to a single (structured) vertex using for example the map

$$\{1, 2\} \to 1, \{3, 6\} \to 2, \{4, 5\} \to 3.$$

In this way the octahedron can be regarded as a triangle in which each (structured) vertex is formed by a pair of ordered orthonormal bases whose members differ by a single global phase only. This triangle captures the fact that apart from this single global phase there are only 3 mutually unbiased bases generated by this cyclic basis group of order 6. These bases are represented by the cosets $[E_2]$, $[M_A]$, $[M_A^2]$.

An example of a non-cyclic basis group of order 6 whose Cayley graph is the 1-skeleton of the regular octahedron is generated by the two non-commuting unitary 2×2-matrices

$$M_C := \frac{1}{\sqrt{2}}\begin{pmatrix} -1 & i \\ -i & 1 \end{pmatrix} = M_C^\dagger,$$
$$M_D := (-1)\begin{pmatrix} 0 & \mathrm{e}^{\mathrm{i}\pi/4} \\ \mathrm{e}^{-\mathrm{i}\pi/4} & 0 \end{pmatrix} = M_D^\dagger. \tag{8}$$

It is apparent that both generators are of order 2, i.e. $M_C^2 = M_D^2 = E_2$, their product is of order 3, i.e. $(M_C M_D)^3 = E_2$ with

$$M_C M_D = \frac{1}{\sqrt{2}}\begin{pmatrix} \mathrm{e}^{-3\mathrm{i}\pi/4} & \mathrm{e}^{\mathrm{i}\pi/4} \\ -\mathrm{e}^{-\mathrm{i}\pi/4} & \mathrm{e}^{3\mathrm{i}\pi/4} \end{pmatrix} \tag{9}$$

and $M_D M_C = (M_C M_D)^2$. The resulting non-Abelian group $G := \langle M_C, M_D\rangle \equiv \langle M_C, M_C M_D\rangle$ has order 6 and is isomorphic to the symmetric group S_3. Its group multiplication table is summarized in the appendix.

The graph of figure 2 can be interpreted as the basis Cayley graph $\Gamma(G, S)$ of this symmetric group S_3 with the edge generating set $S := \{M_D M_C M_D = (M_D M_C M_D)^\dagger, M_C, M_C M_D, (M_C M_D)^\dagger = M_D M_C = (M_C M_D)^2\}$. The mapping between ordered orthonormal basis systems and the vertices of the octahedron can be defined by

$$M_D \to 1,\ E_2 \to 2,\ M_C M_D \to 3,$$
$$(M_C M_D)^2 \to 4,\ M_C \to 5,\ M_D M_C M_D \to 6, \tag{10}$$

for example. The basis group $G := \langle M_C, M_D\rangle$ is a two dimensional irreducible representation of S_3.

By slightly changing the generators of equation (9) basis groups are obtained which do not generate maximum sets of mutually unbiased bases in $d = 2$. Nevertheless, their associated Cayley graphs are complete multiparite. As an example consider the group $G := \langle M_C, M_{\tilde{D}}\rangle$ with the generator M_C of equation (8) and with

$$M_{\tilde{D}} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \tag{11}$$

Despite the similarity between M_D of equation (8) and $M_{\tilde{D}}$ of equation (11) the groups $G := \langle M_C, M_D\rangle$ and $G := \langle M_C, M_{\tilde{D}}\rangle$ are very different. The group $G := \langle M_C, M_{\tilde{D}}\rangle$ is isomorphic to the dihedral group D_8 of order 8. This group has center $\{E_2, (M_C M_{\tilde{D}})^2 \equiv -E_2\}$. M_C and $M_{\tilde{D}}$ are of order two and $M_C M_{\tilde{D}}$ generates a subgroup of order 4. The Cayley graph of this group with respect to the edge generating set

$$S = \{M_C = M_C^\dagger, -M_C, M_C M_{\tilde{D}}, -M_C M_{\tilde{D}}$$
$$= (M_C M_{\tilde{D}})^\dagger\} \tag{12}$$

is depicted in figure 3. A mapping from the vertices to the group elements is given by

$$M_C M_{\tilde{D}} \to 1,\ -M_C M_{\tilde{D}} \to 2,\ M_C \to 3,\ -M_C \to 4,$$
$$M_{\tilde{D}} \to 5,\ E_2 \to 6,\ -M_{\tilde{D}} \to 7,\ -E_2 \to 8, \tag{13}$$

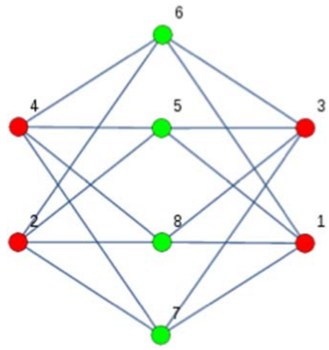

Figure 3. Cayley graph $\Gamma(G, S)$ of the dihedral basis group of order 8.

for example. This Cayley graph is complete 2-partite with the two independent sets $\{1, 2, 3, 4\}$ and $\{5, 6, 7, 8\}$. Its parameters $(n, k, d) = (8, 4, 2)$ satisfy the relation $n/(n-k) = 8/4 = 2$ and do not saturate the upper bound of $(d+1) = 3$ for complete sets of mutually unbiased bases in $d = 2$. Nevertheless this Cayley graph is complete multipartite.

4.2. The complete tripartite graph $K_{16,16,16}$

A more complex complete multipartite graph fulfilling equation (4) for $d = 2$ is the complete 3-partite graph $K_{16,16,16}$ characterized by the parameters $(n, k, d) = (48, 32, 2)$. Each of its three independent coloring sets contains 16 vertices and in view of its complete multipartite nature there is an edge connecting every pair of vertices from different independent sets so that there all vertices within each of the independent sets are unconnected. Therefore, each vertex is the starting point of $k = 32$ edges. This complete multipartite graph can be interpreted as the Cayley graph $\Gamma(G, S)$ of a basis group $G := \langle M_C, M_E\rangle$ of order $|G| = 48$ generated by the unitary 2×2 matrices M_C of equation (8) and

$$M_E = \frac{1}{\sqrt{2}}\begin{pmatrix} \mathrm{e}^{3\mathrm{i}\pi/4} & \mathrm{e}^{\mathrm{i}\pi/4} \\ -\mathrm{e}^{-\mathrm{i}\pi/4} & \mathrm{e}^{-3\mathrm{i}\pi/4} \end{pmatrix}. \tag{14}$$

Despite the fact that the matrices M_E of equation (14) and $M_C\, M_D$ of equation (9) differ only slightly in their phases the groups generated by these matrices are very different. The group $G := \langle M_A, M_E\rangle$ is of order 48. It is isomorphic to the direct product group $Q_8 \times D_6$, involving the quaternion group Q_8 of order 8 and the dihedral group D_6 of order 6 which is also isomorphic to S_3.

For convenience we summarize in the appendix the basic properties of these groups together with their representations which appear in the two dimensional matrix group $G := \langle M_C, M_E\rangle$. From these representations it is apparent that the bases associated with the 2×2 matrices representing the quaternion group are not mutually unbiased. This property also holds for all 6 possible cosets of Q_8 in G. Denoting these cosets by $[R_j] := \{g \in G = \langle M_C, M_E\rangle | g = R_j h, h \in Q_8\}$ with $j = 1, \ldots, 6$ representatives of these cosets are given by

$$R_1 = E_2,\ R_2 = R_2^\dagger = M_D,\ R_3 = M_C M_D,$$
$$R_4 = R_4^\dagger = M_D M_C M_D,$$
$$R_5 = R_3^\dagger = (M_C M_D)^2,\ R_6 = R_6^\dagger = M_C. \tag{15}$$

As Q_8 is a normal subgroup these cosets also form a group, namely the dihedral group D_6 of order 6. Their representatives $\{R_1,\cdots, R_6\}$ form an irreducible two dimensional representation of D_6. Some characteristic features of D_6 are summarized in the appendix. In terms of these cosets the edge generating set S of the Cayley graph $\Gamma(G, S)$ is given by

$$S = \{[R_3], [R_4], [R_5], [R_6]\}. \tag{16}$$

Associating each of the 6 cosets of equation (15) with a (structured) vertex of the octahedron of figure 2 a simplified description of the complete multipartite structure of the mutually unbiased bases is obtained. The underlying 3-partite structure of these mutually unbiased bases becomes even more apparent by defining three (structured) vertices with the help of the mapping

$$\{[R_1], [R_2]\} \to 1,\ \{[R_3], [R_4]\} \to 2,\\ \{[R_5], [R_6]\} \to 3 \tag{17}$$

and associating these three vertices with the vertices of the triangle of figure 1. Each of the vertices of this triangle represents one of the three independent sets of $K_{16,16,16}$ each of which contains 16 (unstructured) vertices whose associated bases are not mutually unbiased. Furthermore, every pair of these (unstructured) vertices belonging to different independent sets is connected by an edge as their associated ordered orthonormal bases are mutually unbiased.

4.3. Maximal sets of mutually unbiased bases in d = 3

Let $\omega \coloneqq \exp(\frac{2\pi i}{3})$ and

$$M_1 \coloneqq \frac{1}{3}\begin{pmatrix} -\omega + \omega^2 & -\omega - 2\omega^2 & -\omega - 2\omega^2 \\ 2\omega + \omega^2 & -\omega - 2\omega^2 & 2\omega + \omega^2 \\ 2\omega + \omega^2 & 2\omega + \omega^2 & -\omega - 2\omega^2 \end{pmatrix},$$

$$M_2 \coloneqq \frac{1}{3}\begin{pmatrix} \omega - \omega^2 & -2\omega - \omega^2 & -2\omega - \omega^2 \\ \omega + 2\omega^2 & -2\omega - \omega^2 & \omega + 2\omega^2 \\ \omega + 2\omega^2 & \omega + 2\omega^2 & -2\omega - \omega^2 \end{pmatrix},$$

$$M_3 \coloneqq \frac{1}{3}\begin{pmatrix} \omega - \omega^2 & \omega - \omega^2 & \omega - \omega^2 \\ \omega - \omega^2 & -2\omega - \omega^2 & \omega + 2\omega^2 \\ \omega - \omega^2 & \omega + 2\omega^2 & -2\omega - \omega^2 \end{pmatrix}.$$

These three matrices M_i together with E_3 form a maximum set of $d + 1 = 4$ mutually unbiased bases in $\mathcal{H}^3$. The entries of $3M_1$, $3M_2$, and $3M_3$ are the Eisenstein integers of squared norm 3. (Eisenstein integers have the form $a + b\omega$ where a and b are rational integers, and the squared norm is $a^2 - ab + b^2$.)

The quaternion group Q_8 is naturally associated with these mutually unbiased bases. If we take as the generating set of the basis group to be M_2 and M_3 we obtain Q_8. In this group the M_i belong to the three conjugacy classes of elements of order 4. Calculating the character multiplicities from the Q_8 character table [16] shows that this 3-dimensional representation of Q_8 splits into irreducible constituents as $3 = 1 \oplus 2$, i.e. the identity representation and the 2-dimensional unit quaternion representation (compare with equation (20)). As a corollary of Maschke's theorem there exists a fixed matrix T such that all the matrices M_j of this representation of the quaternion group Q_8 can be put into block diagonal form TM_jT^{-1} corresponding to this spliting.

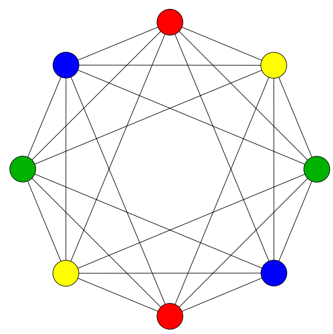

Figure 4. Cayley graph $\Gamma(G, S)$ of Q_8: the 1-skeleton of cross polytope β_4.

The Cayley graph $\Gamma(G, S)$ capturing the structural properties of the mutually unbiased bases of this representation of the quaternion group is depicted in figure 4. Its edge generating set is given by

$$S = \{M_2, M_3, M_3M_2, M_2^\dagger, M_3^\dagger, M_2^\dagger M_3^\dagger\}. \tag{18}$$

It has parameters $(n, k, d) = (8, 6, 3)$ and it is the 1-skeleton of a 16-cell or β_4 in four dimensional Euclidean space [14]. β_4 contains $(n - k)^{d+1} = 16$ simplices α_3 whose 1-skeletons are the maximum cliques K_4 of $\Gamma(G, S)$. The vertex set of every such K_4 is a maximum set of mutually unbiased bases in $\mathcal{H}^3$.

5. Conclusions and outlook

We have discussed and explored a recently developed group and graph theoretical approach aiming at the construction of maximum sets of mutually unbiased bases in finite dimensional Hilbert spaces. Contrary to previously developed approaches it is independent of prime number restrictions. The construction of systems of mutually unbiased bases is reformulated as a clique finding problem in Cayley graphs of finite basis groups naturally associated with these basis systems. Besides offering the possibility to enlarge and possibly complete previously known systems of mutually unbiased basis systems, this approach elucidates the intricate relation between quantum mechanical complementarity as encoded in systems of mutually unbiased bases and their underlying symmetries. As the investigations presented constitute only the first steps in the exploration of the group and graph theoretical approach, numerous interesting open questions for further research remain open. These open questions include:

- Which k-regular complete multipartite graphs fulfill equation (4) for a given dimension d?
- What are their possible finite basis groups?
- Is it possible to construct maximum sets of mutually unbiased basis systems in a Hilbert space of dimension d in a systematic way by combining basis groups yielding maximum sets of mutually unbiases bases in Hilbert spaces of dimensions smaller than d?

As the referees have drawn our attention to two previous investigations [17, 18], in which complete sets of mutually unbiased bases are constructed in a graph theoretic setting, we would finally like to comment on these investigations in order to emphasize the similarities and differences to our results.

In [17] it was shown that bipartite entangled stabilizer complete unbiased bases (BES MUB) correspond to the maximum cliques of size $p^2 - 1$ in Cayley graphs whose vertices are elements of the two dimensional special linear groups over Z_p for prime p. The graphs have $p(p^2 - 1)$ vertices and the connection sets have size $|G| - p^2$ (G is the group). The maximum cliques (if they exist) for a given p produce complete sets of BES MUB in Hibert spaces of dimension $d = p^2$.

The graphs of [17] differ from ours in several important aspects. Our Cayley graphs are defined by (certain) finite subgroups of the complex unitary group $U(d)$, the vertices are $d \times d$ complex unitary matrices. As such the relation to representation theory of finite groups is apparent [19]. The incidence relation is different and the size of the connection sets S is not fixed. Moreover if d is related to the order of the group (the size of the vertex set), and the valency of the graph by equation (4), the graph contains maximum cliques of size $d + 1$ (the MUB bound). It is regular and complete multipartite. The vertices of the cliques correspond to unrestricted complete sets of MUB in Hilbert spaces of dimension d without any further restrictions of the kind $d = p^n$ (with n integer), for example.

In [18] a graph-state formalism is developed which produces complete sets of MUB in Hilbert spaces of dimension $d = p^n$ where p is a prime. The graphs underlying this construction have multiple edges and loops, the adjaceny matrices have entries in Z_p for prime p. On the contrary, our graphs are undirected and simple, i.e. there is at most a single edge between any two vertices and they have no loops. Maximum cliques are not considered in [18]. The construction depends on the existence of symmetric spread sets of size p^n over Z_p.

Appendix

A.1. The symmetric group S_3

The group multiplication table of the non-Abelian unitary group $G \coloneqq \langle M_C, M_D \rangle$ of order 6 with the generators of equation (8) is given by

$\circ$	M_C	M_D	$M_C M_D$	$(M_C M_D)^2$	$M_D M_C M_D$
E_2	M_C	M_D	$M_C M_D$	$(M_C M_D)^2$	$M_D M_C M_D$
M_C	E_2	$M_C M_D$	M_D	$M_D M_C M_D$	$(M_C M_D)^2$
M_D	$(M_C M_D)^2$	E_2	$M_D M_C M_D$	M_C	$M_C M_D$
$M_C M_D$	$M_D M_C M_D$	M_C	$(M_C M_D)^2$	E_2	M_D
$(M_C M_D)^2$	M_D	$M_D M_C M_D$	E_2	$M_C M_D$	M_C
$M_D M_C M_D$	$M_C M_D$	$(M_C M_D)^2$	M_C	M_D	E_2

This group is isomorphic to the symmetric group S_3 of three elements, say 1, 2, 3. Using the cycle notation for permutations this is apparent from the mapping onto permutations defined by

$$M_C \to (12),\ M_D \to (23),\ M_C M_D \to (123),$$
$$(M_C M_D)^2 \to (123)^2,\ M_D M_C M_D \to (13). \tag{19}$$

A.2. The quaternion group Q_8

The two dimensional irreducible representation of the quaternion group appearing in the unitary group $G \coloneqq \langle M_C, M_E \rangle$ of order 48 involves the unitary 2×2 matrices

$$I = \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix} = -\mathrm{i}\sigma_3,$$
$$J = \begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix} = -\mathrm{i}\sigma_1,$$
$$K = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} = IJ = -\mathrm{i}\sigma_2 \tag{20}$$

with the Pauli matrices $\sigma_1, \sigma_2, \sigma_3$. These matrices fulfill the characteristic algebraic relations

$$I^2 = J^2 = K^2 = -E_2 = IJK \tag{21}$$

with the equivalent relations for the Pauli matrices $\sigma_1^2 = \sigma_2^2 = \sigma_3^2 = E_2$ and $\sigma_1\sigma_2\sigma_3 = i$. In view of the commutation property $\sigma_1\sigma_2 = -\sigma_2\sigma_1$ the unit matrix E_2 and the three Pauli matrices form an irreducible two dimensional ray representation of the Klein group V_4 [19]. The quaternion group Q_8 constitutes a lifting of this ray representation of V_4 to an ordinary representation.

A.3. The dihedral group D_6

The two dimensional irreducible representation of the dihedral group appearing in the unitary group $G \coloneqq \langle M_C, M_E \rangle$ of order 48 is formed by the unitary 2×2 matrices $\{R_1, \cdots, R_6\}$ of equation (15). It is isomorphic to the symmetric group S_3. The matrices $N \coloneqq \{E_2 \equiv R_3^3, R_3, R_5 \equiv R_3^2\}$ form a cyclic normal subgroup of D_6 of order $6/2 = 3$ and $\{E_2, R_2\}$, $\{E_2, R_4\}$, $\{E_2, R_6\}$ are subgroups of $G \coloneqq \langle M_C, M_E \rangle$ of order 2. From this irreducible representation the characteristic dihedral group properties follow, such as $R_2 R_3^m R_2 = R_3^{\dagger m}$ for $m = 1, 2, 3 = 6/2$, which are also valid in an analogous way for dihedral groups of any order.

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