An angular momentum approach to quadratic Fourier transform, Hadamard matrices, Gauss sums, mutually unbiased bases, unitary group and Pauli group

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An angular momentum approach to quadratic Fourier transform, Hadamard matrices, Gauss sums, mutually unbiased bases, unitary group and Pauli group[1]

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Abstract
The construction of unitary operator bases in a finite-dimensional Hilbert space is reviewed through a nonstandard approach combinining angular momentum theory and representation theory of $SU(2)$. A single formula for the bases is obtained from a polar decomposition of $SU(2)$ and analysed in terms of cyclic groups, quadratic Fourier transforms, Hadamard matrices and generalized Gauss sums. Weyl pairs, generalized Pauli operators and their application to the unitary group and the Pauli group naturally arise in this approach.

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[1] Dedicated to the memory of Yurii Fedorovich Smirnov.

1 Introduction

Angular momentum theory [1] and its group-theoretical formulation in terms of the Wigner-Racah algebra of SU(2) [2, 3, 4] (see also [5] for an extension to a finite or compact group) are of central importance in subatomic, atomic, molecular and condensed matter physics. The components of any angular momentum (spin, isopin, orbital angular momentum, etc.) generate the Lie algebra of the group $SU(2)$. Therefore, $SU(2)$ and its noncompact extension $SU(1,1)$ are basic ingredients for dealing with generalized angular momenta. Chains of groups ending with $SO(3) \simeq SU(2)/\mathbb{Z}_2(+)$ or $SO(3) \subset SO(2)$ are of interest in subatomic and atomic physics. In this direction, one can mention the group $SU(3) \otimes SU(2) \otimes U(1)$ (related to the chain $U(3) \subset SU(2) \otimes U(1) \subset U(1)$) and its grand unified and/or supersymmetric extensions for describing elementary particles and their (strong and electroweak) interactions [6]. Furthermore, one know the relevance in atomic physics of the chain $U(7) \subset SO(7) \subset G_2 \subset SO(3) \subset SO(2)$ for the electronic spectroscopy of f^N ions [3]. On the other side, chains ending with $SU(2) \subset G$, where G is a finite group (or a chain involving finite groups), proved to be of considerable interest in molecular and condensed matter spectroscopy [7, 8, 9]. Recently, chains of type $SU(2) \subset G$ were also used in attempts to understand the flavor structure of quarks and leptons [10]. The groups $SU(2)$ and $SU(1,1)$, as well as their q- or qp-deformations in the sense of Hopf algebras (see for instance [11, 12], thus play a pivotal role in many areas of physical sciences.

The representation theory of $SU(2)$ is generally adressed in two different ways. The standard one amounts to diagonalise the complete set $\{j^2, j_z\}$ involving the Casimir operator j^2 and one generator j_z of $SU(2)$. Another way is to consider a set $\{j^2, v\}$, where v is an operator defined in the enveloping algebra of $SU(2)$ and invariant under a subgroup of $SU(2)$. A third way (not very well-known) consists in diagonalising a complete set $\{j^2, v_{ra}\}$, where v_{ra} stands for a two-parameter operator which commutes with j^2 and is a pseudoinvariant under a cyclic group [13].

It is the aim of this review paper to show that the third approach to the representation theory of $SU(2)$ opens a window on the apparently disconnected subjects enumerated in the title.

The plan of the paper is as follows. The minimal requirements for a $\{j^2, v_{ra}\}$ approach to $SU(2)$ (i.e., a nonstandard approach to angular momentum theory) are given in Section 2 and in two appendices. Section 3 deals with quadratic sums (in relation with quadratic discrete Fourier transforms, generalized Hadamard matrices, generalized quadratic Gauss sums and mutually unbiased bases) and Section 4 is devoted to unitary groups and Pauli groups.

The present paper is dedicated to the memory of the late Professor Yurii Fedorovich Smirnov who contributed to many domains of mathematical physics (e.g., Lie groups and Lie algebras, quantum groups, special functions) and theoretical physics (e.g., nuclear, atomic and molecular physics, crystal- and ligand-field theory).

A few words about some of the notations is in order. The bar indicates complex conjugation. The symbol $\delta_{a,b}$ stands for the Kronecker symbol of a and b. We use I and I_d to denote the identity operator and the d-dimensional unity matrix, respectively. The operator $A^\dagger$ stands for the adjoint of the operator A. We note as $[A,B]_-$ and $[A,B]_+$ the commutator and the anticommutator of the operators A and B, respectively. We use the Dirac notation $|\psi\rangle$ for a vector in an Hilbert space; furthermore, $\langle\phi|\psi\rangle$ and $|\phi\rangle\langle\psi|$ are respectively the inner product and the outer product of the vectors $|\psi\rangle$ and $|\phi\rangle$. The symbols $\oplus$ and $\ominus$ stand respectively for the addition and subtraction modulo d while $\otimes$ and $\uplus$ are used respectively for the direct product of vectors or operators and the direct sum of vector spaces. The matrices of type $E_{\lambda,\mu}$ with the matrix elements

$$(E_{\lambda,\mu})_{\lambda',\mu'} := \delta_{\lambda,\lambda'}\delta_{\mu,\mu'} \tag{1}$$

stand for generators of the Lie group $GL(d,\mathbb{C})$. For a and b coprime, we take

$$\left(\begin{matrix} a \\ b \end{matrix}\right)_L := \begin{cases} +1 \text{ if } a = k^2 \bmod(b) \\ \\ -1 \text{ si } a \neq k^2 \bmod(b) \end{cases} \tag{2}$$

to denote the Legendre symbol of a and b (equal to 1 if a is a quadratic residu modulo b and -1 if a is not a quadratic residu modulo b). In addition, the integer inverse $(a\backslash b)$ of a with respect to b is given by

$$a(a\backslash b) = 1 \bmod(b). \tag{3}$$

Finally, the q-deformed number $[n]_q$ and the q-deformed factorial $[n]_q!$, with $n \in \mathbb{N}$, are defined by

$$[n]_q := \frac{1-q^n}{1-q} \tag{4}$$

and

$$[n]_q! := [1]_q\,[2]_q \ldots [n]_q \qquad [0]_q! := 1 \tag{5}$$

where q is taken is this paper as a primitive root of unity.

2 A nonstandard approach to $su(2)$

In some previous works [13], we developed a nonstandard approach to the Lie algebra $su(2)$ and studied the corresponding Wigner-Racah algebra of the group $SU(2)$. This nonstandard approach is based on a polar decomposition of $su(2)$, based in turn on a troncated oscillator algebra (see Appendices A and B). It yields nonstandard bases for the irreducible representations of $SU(2)$ and new Clebsch-Gordan coefficients for the angular momentum theory. Basically, the approach amounts to replace the set $\{j^2, j_z\}$, familiar in quantum mechanics, by a set $\{j^2, v_{ra}\}$ (j^2 and j_z are the Casimir operator and the Cartan generator of $su(2)$, respectively).

The operator v_{ra} acts on the $(2j+1)$-dimensional subspace $\mathcal{E}(2j+1)$, associated with the angular momentum j, of the representation space of $SU(2)$. We define it here by

$$v_{ra} := e^{i2\pi jr}|j,-j\rangle\langle j,j| + \sum_{m=-j}^{j-1} q^{(j-m)a}|j,m+1\rangle\langle j,m| \tag{6}$$

where

$$q := \exp\left(\frac{2\pi i}{2j+1}\right) \qquad 2j \in \mathbb{N} \qquad r \in \mathbb{R} \qquad a \in \mathbb{Z}_{2j+1} \tag{7}$$

and, for fixed j, the vectors $|j,m\rangle$ (with $m = j, j-1, \ldots, -j$) satisfy the eigenvalue equations

$$j^2|j,m\rangle = j(j+1)|j,m\rangle \qquad j_z|j,m\rangle = m|j,m\rangle \tag{8}$$

familiar in angular momentum theory. The vectors $|j,m\rangle$ span the Hilbert space $\mathcal{E}(2j+1) \sim \mathbb{C}^{2j+1}$ and are taken in an orthonormalized form with

$$\langle j,m|j,m'\rangle = \delta_{m,m'}. \tag{9}$$

Obviously, the operator v_{ra} is unitary and commutes with j^2. The spectrum of the set $\{j^2, v_{ra}\}$ is described by

Result 1. *For fixed j, r and a, the $2j+1$ vectors*

$$|j\alpha;ra\rangle := \frac{1}{\sqrt{2j+1}} \sum_{m=-j}^{j} q^{(j+m)(j-m+1)a/2 - jmr + (j+m)\alpha}|j,m\rangle \tag{10}$$

with $\alpha = 0, 1, \ldots, 2j$, are common eigenvectors of v_{ra} and j^2. The eigenvalues of v_{ra} and j^2 are given by

$$v_{ra}|j\alpha;ra\rangle = q^{j(a+r)-\alpha}|j\alpha;ra\rangle \quad j^2|j\alpha;ra\rangle = j(j+1)|j\alpha;ra\rangle \quad \alpha = 0,1,\ldots,2j. \tag{11}$$

The spectrum of v_{ra} is nondegenerate.

The set $\{|j\alpha; ra\rangle : \alpha = 0, 1, \ldots, 2j\}$ constitutes another orthonormal basis, besides the basis $\{|j, m\rangle : m = j, j-1, \ldots, -j\}$, of $\mathcal{E}(2j+1)$ in view of

$$\langle j\alpha; ra|j\beta; ra\rangle = \delta_{\alpha,\beta}. \tag{12}$$

Note that the value of $\langle j\alpha; ra|j\beta; sb\rangle$ is much more involved for $r \neq s$ and $a \neq b$ and needs the calculation of Gauss sums as we shall see below.

The Wigner-Racah algebra of $SU(2)$ can be developed in the $\{j^2, v_{ra}\}$ scheme. This leads to Clebsch-Gordan coefficients and (3 – $j\alpha$)$_{ra}$ symbols with properties very different from the ones of the usual $SU(2) \subset U(1)$ Clebsch-Gordan coefficients and 3 – jm symbols corresponding to the $\{j^2, j_z\}$ scheme [13].

The nonstandard approach to angular momentum theory briefly summarized above is especially useful in quantum chemistry for problems involving cyclic symmetry. This is the case for a ring-shape molecule with $2j+1$ atoms at the vertices of a regular polygon with $2j+1$ sides or for a one-dimensional chain of $2j+1$ spins ($\frac{1}{2}$-spin each) [14]. In this connection, we observe that the vectors of type $|j\alpha; ra\rangle$ are specific symmetry-adapted vectors [15, 16]. Symmetry-adapted vectors are widely used in quantum chemistry, molecular physics and condensed matter physics as for instance in rotational spectroscopy of molecules [17] and ligand-field theory [18]. However, the vectors $|j\alpha; ra\rangle$ differ from the symmetry-adapted vectors considered in Refs. [19, 20, 21, 22] in the sense that v_{ra} is not an invariant under some finite subgroup (of crystallographic interest) of the orthogonal group $O(3)$. Indeed, v_{ra} is a pseudoinvariant [23] under the Wigner operator $P_{R(\varphi)}$ associated with the rotation $R(\varphi)$, around the quantization axis Oz, with the angle

$$\varphi := p\frac{2\pi}{2j+1} \qquad p = 0, 1, \ldots, 2j \tag{13}$$

since

$$P_{R(\varphi)} v_{ra} P^{\dagger}_{R(\varphi)} = e^{-i\varphi} v_{ra}. \tag{14}$$

More precisely, we have

Result 2. *The operator v_{ra} transforms according to an irreducible representation of the cyclic subgroup $C_{2j+1} \sim \mathbb{Z}_{2j+1}(+)$ of the special orthogonal group $SO(3)$. In terms of vectors, one has*

$$P_{R(\varphi)}|j\alpha; ra\rangle = q^{jp}|j\beta; ra\rangle \qquad \beta := \alpha \ominus p \tag{15}$$

so that the set $\{|j\alpha; ra\rangle : \alpha = 0, 1, \ldots, 2j\}$ is stable under $P_{R(\varphi)}$. The latter set spans the regular representation of C_{2j+1}.

3 Variations on quadratic sums

3.1 Quadratic discrete Fourier transform

We leave the domain of angular momentum theory and adopt the following notations

$$d := 2j + 1 \qquad k := j - m \qquad |k\rangle := |j, m\rangle. \tag{16}$$

These notations are particularly adapted to quantum information and quantum computation. In these new notations, we have

$$v_{ra} = e^{i\pi(d-1)r}|d-1\rangle\langle 0| + \sum_{k=1}^{d-1} q^{ka}|k-1\rangle\langle k|. \tag{17}$$

From now on, we assume that $d \geq 2$ and $r = 0$ (the case $d = 1$ and $r \neq 0$, although of interest in the theory of angular momentum, is not essential for what follows). In addition, we put

$$|a\alpha\rangle := |j\alpha; 0a\rangle \tag{18}$$

with a and α in the ring $\mathbb{Z}_d := \mathbb{Z}/d\mathbb{Z}$. Then, Eq. (11) gives

$$v_{0a}|a\alpha\rangle = q^{(d-1)a/2-\alpha}|a\alpha\rangle \tag{19}$$

with

$$|a\alpha\rangle = \frac{1}{\sqrt{d}} \sum_{k=0}^{d-1} q^{(k+1)(d-k-1)a/2-(k+1)\alpha}|k\rangle. \tag{20}$$

Equation (20) can be rewritten as

$$|a\alpha\rangle = \sum_{k=0}^{d-1} (F_a)_{k\alpha}\,|k\rangle \tag{21}$$

where

$$(F_a)_{k\alpha} := \frac{1}{\sqrt{d}} q^{(k+1)(d-k-1)a/2-(k+1)\alpha} \tag{22}$$

is the $k\alpha$-th matrix element of a $d \times d$ matrix F_a (the matrix F_a can be seen as the matrix associated with the character table of the cyclic group C_d pre- and post-multiplied by diagonal matrices).

Equations (21)-(22) define a quadratic quantum Fourier transform. The matrix F_a is unitary so that (21) can be inverted to give

$$|k\rangle = \sum_{\alpha=0}^{d-1} \overline{(F_a)_{k\alpha}} |a\alpha\rangle \tag{23}$$

or

$$|k\rangle = \frac{1}{\sqrt{d}} \sum_{\alpha=0}^{d-1} q^{-(k+1)(d-k-1)a/2+(k+1)\alpha} |a\alpha\rangle. \tag{24}$$

In the special case $a = 0$, we have

$$|0\alpha\rangle = q^{-\alpha} \frac{1}{\sqrt{d}} \sum_{k=0}^{d-1} e^{-\frac{2\pi i}{d}\alpha k} |k\rangle \Leftrightarrow |k\rangle = \frac{1}{\sqrt{d}} \sum_{\alpha=0}^{d-1} e^{\frac{2\pi i}{d}(k+1)\alpha} |0\alpha\rangle. \tag{25}$$

Consequently, the quadratic quantum Fourier transform reduces to the ordinary quantum Fourier transform (up to a phase factor). The corresponding matrix F_0 satisfies

$$F_0^4 = qI_d \tag{26}$$

to be compared to the well-known relation $F^4 = I_d$ for the standard quantum Fourier transform [24].

At this stage, we forsee that $d+1$ (orthonormal) bases of the space $\mathcal{E}(d)$ play an important role in the present paper: (i) the basis

$$B_d := \{|j,m\rangle : m = j, j-1, \ldots, -j\} \Leftrightarrow B_d := \{|k\rangle : k = 0, 1, \ldots, d-1\} \tag{27}$$

associated with the $\{j^2, j_z\}$ scheme, known as the spherical or canonical basis in the theory of angular momentum, and as the computational basis in quantum information and quantum computation and (ii) the d bases

$$B_a := \{|a\alpha\rangle : \alpha = 0, 1, \ldots, d-1\} \qquad a = 0, 1, \ldots, d-1 \tag{28}$$

(noted B_{0a} in Ref. [25]) associated with the $\{j^2, v_{0a}\}$ scheme.

To close this subsection, let us show how the preceding developments can be used for defining a quadratic discrete Fourier transform. We start from the formal transformation

$$x := \{x(k) \in \mathbb{C} : k = 0, 1, \ldots, d-1\} \to y := \{y(\alpha) \in \mathbb{C} : \alpha = 0, 1, \ldots, d-1\} \tag{29}$$

defined via

$$y(\alpha) := \frac{1}{\sqrt{d}} \sum_{k=0}^{d-1} q^{(k+1)(d-k-1)a/2-(k+1)\alpha} x(k) \tag{30}$$

where a can take any of the values $0, 1, \ldots, d-1$. Alternatively, for fixed a we have

$$y(\alpha) = \sum_{k=0}^{d-1} (F_a)_{k\alpha}\, x(k) \qquad \alpha = 0, 1, \ldots, d-1. \tag{31}$$

The inverse transformation $y \to x$ is described by

$$x(k) = \sum_{\alpha=0}^{d-1} \overline{(F_a)_{k\alpha}} y(\alpha) \qquad k = 0, 1, \ldots, d-1. \tag{32}$$

The bijective transformation $x \leftrightarrow y$ can be thought of as a quadratic discrete Fourier transform. The case $a = 0$ corresponds to the ordinary discrete Fourier transform (up to a phase factor). These matters lead to the following result which generalizes the Parseval-Plancherel theorem for the ordinary discrete Fourier transform.

Result 3. *The quadratic discrete Fourier transforms $x \leftrightarrow y$ and $x' \leftrightarrow y'$ associated withe same matrix matrix F_a, $a \in \mathbb{Z}_d$, satisfy the conservation rule*

$$\sum_{\alpha=0}^{d-1} \overline{y(\alpha)} y'(\alpha) = \sum_{k=0}^{d-1} \overline{x(k)} x'(k) \tag{33}$$

where the common value is independent of a.

3.2 Generalized Hadamard matrices

The modulus of each matrix element of F_a (with $a \in \mathbb{Z}_d$) is equal to $1/\sqrt{d}$. Therefore, the unitary matrix F_a turns out to be a generalized Hadamard matrix. We adopt here the following definition. A $d \times d$ generalized Hadamard matrix is a unitary matrix whose each entry has a modulus equal to $1/\sqrt{d}$ [26]. Note that the latter normalization, used in quantum information [27, 28], differs from the usual one according to which a $d \times d$ generalized Hadamard matrix H is a complex matrix such that $H^\dagger H = dI_d$ and for which the modulus of each element is 1 [29]. In this respect, the generalized Hadamard matrix H_a considered in [14] corresponds to $\sqrt{d}F_a$ up to permutations.

Example 1. By way of illustration, from (22) we get the familiar Hadamard matrices

$$F_0 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} \qquad F_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} i & -i \\ 1 & 1 \end{pmatrix} \tag{34}$$

for $d = 2$ and

$$F_0 = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & \omega^2 & \omega \\ 1 & \omega & \omega^2 \\ 1 & 1 & 1 \end{pmatrix} \; F_1 = \frac{1}{\sqrt{3}} \begin{pmatrix} \omega & 1 & \omega^2 \\ \omega & \omega^2 & 1 \\ 1 & 1 & 1 \end{pmatrix} \; F_2 = \frac{1}{\sqrt{3}} \begin{pmatrix} \omega^2 & \omega & 1 \\ \omega^2 & 1 & \omega \\ 1 & 1 & 1 \end{pmatrix} \tag{35}$$

(with $\omega := e^{i2\pi/3}$) for $d = 3$. Another example is

$$F_0 = \frac{1}{\sqrt{6}} \begin{pmatrix} 1 & \tau & \tau^2 & -1 & -\tau & -\tau^2 \\ 1 & \tau^2 & -\tau & 1 & \tau^2 & -\tau \\ 1 & -1 & 1 & -1 & 1 & -1 \\ 1 & -\tau & \tau^2 & 1 & -\tau & \tau^2 \\ 1 & -\tau^2 & -\tau & -1 & \tau^2 & \tau \\ 1 & 1 & 1 & 1 & 1 & 1 \end{pmatrix} \tag{36}$$

(with $\tau := e^{-i\pi/3}$) which readily follows from (22) for $d = 6$ and $a = 0$.

We sum up and complete this section with the following result (see also [14, 30]).

Result 4. *The matrix*

$$F_a = \frac{1}{\sqrt{d}} \sum_{k=0}^{d-1} \sum_{\alpha=0}^{d-1} q^{(k+1)(d-k-1)a/2-(k+1)\alpha} E_{k,\alpha} \tag{37}$$

associated with the quadratic quantum Fourier transform (21) is a $d \times d$ generalized Hadamard matrix. It reduces the endomorphism associated with the operator v_{0a}:

$$F_a^\dagger V_{0a} F_a = q^{(d-1)a/2} \sum_{\alpha=0}^{d-1} q^{-\alpha} E_{\alpha,\alpha} = q^{(d-1)a/2} \begin{pmatrix} 1 & 0 & \dots & 0 \\ 0 & q^{-1} & \dots & 0 \\ \vdots & \vdots & \dots & \vdots \\ 0 & 0 & \dots & q^{-(d-1)} \end{pmatrix} \tag{38}$$

where the matrix

$$V_{0a} := \sum_{k=0}^{d-1} q^{ka} E_{k\ominus 1,k} = \begin{pmatrix} 0 & q^a & 0 & \dots & 0 \\ 0 & 0 & q^{2a} & \dots & 0 \\ \vdots & \vdots & \vdots & \dots & \vdots \\ 0 & 0 & 0 & \dots & q^{(d-1)a} \\ 1 & 0 & 0 & \dots & 0 \end{pmatrix} \tag{39}$$

represents the linear operator v_{0a} on the basis B_d.

3.3 Generalized quadratic Gauss sums

The Hadamard matrices F_a and F_b ($a, b \in \mathbb{Z}_d$) are connected to the inner product $\langle a\alpha | b\beta \rangle$. In fact, we have

$$\langle a\alpha | b\beta \rangle = \left(F_a^\dagger F_b \right)_{\alpha\beta}. \tag{40}$$

A direct calculation yields

$$\langle a\alpha | b\beta \rangle = \frac{1}{d} \sum_{k=0}^{d-1} q^{k(d-k)(b-a)/2-k(\beta-\alpha)} \tag{41}$$

or

$$\langle a\alpha|b\beta\rangle = \frac{1}{d}\sum_{k=0}^{d-1} e^{i\pi\{(a-b)k^2+[d(b-a)+2(\alpha-\beta)]k\}/d}. \tag{42}$$

Hence, each matrix element of $F_a^\dagger F_b$ can be put in the form of a generalized quadratic Gauss sum $S(u,v,w)$ defined by [31]

$$S(u,v,w) := \sum_{k=0}^{|w|-1} e^{i\pi(uk^2+vk)/w} \tag{43}$$

where u, v and w are integers such that u and w are mutually prime, $uw \neq 0$ and $uw+v$ is even. In detail, we obtain

$$\langle a\alpha|b\beta\rangle = \left(F_a^\dagger F_b\right)_{\alpha\beta} = \frac{1}{d}S(u,v,w) \tag{44}$$

with the parameters

$$u = a-b \qquad v = -(a-b)d + 2(\alpha-\beta) \qquad w = d \tag{45}$$

which ensure that $uw+v$ is necessarily even.

In the particular case $d=2$ (of special interest for qubits), we directly get

$$\langle a\alpha|b\beta\rangle = \frac{1}{2}\left[1 + e^{i\pi(b-a+2\alpha-2\beta)/2}\right] \tag{46}$$

which reduces to

$$\langle a\alpha|a\beta\rangle = \delta_{\alpha,\beta} \qquad b = a, \tag{47}$$

and

$$\langle a\alpha|b\beta\rangle = \frac{1}{2}(1 \pm i) \qquad b \neq a, \tag{48}$$

where the $+$ sign corresponds to $b-a+2(\alpha-\beta) = 1, -3$ and the $-$ sign to $b-a+2(\alpha-\beta) = -1, 3$.

In the general case d arbitrary (of interest for qudits), the calculation of $S(u,v,w)$ can be achieved by using the methods described in [31] (see also [32, 33, 34, 35]). The cases of interest for what follows are (u even, v even, w odd), (u odd, v odd, w odd) and (u odd, v even, w even). This leads to

Result 5. *For $a \neq b$, d arbitrary and $u+v+w$ odd, the inner product $\langle a\alpha|b\beta\rangle$ and the $\alpha\beta$-th element of the matrix $F_a^\dagger F_b$ follow from* *case $u = a - b$ even, $v = d(b - a) + 2(\alpha - \beta)$ even, $w = d$ odd:*

$$\langle a\alpha|b\beta\rangle = \left(F_a^\dagger F_b\right)_{\alpha\beta} = \sqrt{\frac{1}{w}} \begin{pmatrix} u \\ w \end{pmatrix}_L \exp\left(-i\frac{\pi}{4}[w - 1 + \frac{u}{w}(u\backslash w)^2 v^2]\right) \tag{49}$$

case $u = a - b$ odd, $v = d(b - a) + 2(\alpha - \beta)$ odd, $w = d$ odd:

$$\langle a\alpha|b\beta\rangle = \left(F_a^\dagger F_b\right)_{\alpha\beta} = \sqrt{\frac{1}{w}} \begin{pmatrix} u \\ w \end{pmatrix}_L \exp\left(-i\frac{\pi}{4}[w - 1 + 16\frac{u}{w}(4u\backslash w)^2 v^2]\right) \tag{50}$$

case $u = a - b$ odd, $v = d(b - a) + 2(\alpha - \beta)$ even, $w = d$ even:

$$\langle a\alpha|b\beta\rangle = \left(F_a^\dagger F_b\right)_{\alpha\beta} = \sqrt{\frac{1}{w}} \begin{pmatrix} w \\ u \end{pmatrix}_L \exp\left(-i\frac{\pi}{4}u[-1 + \frac{1}{w}(u\backslash w)^2 v^2]\right) \tag{51}$$

so that the matrix $F_a^\dagger F_b$ is a Hadamard matrix for each case under consideration.

Finally, for $a = b$ and d arbitrary we recover the orthonormality property (see (12))

$$\langle a\alpha|a\beta\rangle = \delta_{\alpha,\beta} \tag{52}$$

from a direct calculation of the right-hand side of (42).

3.4 Mutually unbiased bases

Speaking generally, two d-dimensional bases $B_a = \{|a\alpha\rangle : \alpha \in \mathbb{Z}_d\}$ and $B_b = \{|b\beta\rangle : \beta \in \mathbb{Z}_d\}$ are said to be mutually unbiased if and only if

$$|\langle a\alpha|b\beta\rangle| = \delta_{a,b}\delta_{\alpha,\beta} + (1 - \delta_{a,b})\frac{1}{\sqrt{d}} \tag{53}$$

for any α and β in the ring $\mathbb{Z}_d$. It is well-known that the number of mutually unbiased bases (MUBs) in the Hilbert space $\mathbb{C}^d$ cannot be greater than $d + 1$ [36, 37, 38, 39]. In fact, the maximum number $d + 1$ is attained when d is the power of a prime number [38, 39]. Despite a considerable amount of works, the maximum number of MUBs is unknown when d is not a power of a prime. In this respect, several numerical studies strongly suggest that there are only three MUBs for $d = 6$ (see for example [27, 28, 40, 41, 42]). MUBs are closely connected with the concept of complementarity in quantum mechanics. There are of paramount importance in classical information theory (Kerdock codes and network communication protocols) [39, 43], in quantum information theory (quantum cryptography and quantum state tomography) [44] and in the solution of the Mean King problem [45, 46, 47, 48, 49, 50]. Recently, it was pointed out and confirmed that MUBs are also of central importance in the formalism of Feynman path integrals [51, 52]. Finally, it should be emphasized that the concept of MUBs also exists in infinite dimension [53]. There are numerous ways of constructing sets of MUBs. Most of them are based on discrete Fourier analysis over Galois fields and Galois rings, discrete Wigner functions, generalized Pauli matrices, mutually orthogonal Latin squares, finite geometry methods and Lie-like approaches (see Refs. [14, 25, 27, 28, 30, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 54, 55, 56, 57, 58, 59, 60, 61, 62, 63, 64] for an nonexhaustive list of references).

3.4.1 Case d prime

We have the following important result. (See also [64] for a recent alternative group-theoretical approach to the case d prime.)

Result 6. *In the case where $d = p$ is a prime number (even or odd), one has*

$$|\langle a\alpha|b\beta\rangle| = \left|\left(F_a^\dagger F_b\right)_{\alpha\beta}\right| = \frac{1}{\sqrt{p}} \qquad a \neq b \tag{54}$$

for $a, b, \alpha, \beta \in \mathbb{Z}_p$. Therefore, the $p+1$ bases $B_0, B_1, \ldots, B_p$ constitute a complete set of MUBs in $\mathbb{C}^p$.

The proof easily follows from the calculation of the modulus of $S(a-b, pb-pa+2\alpha-2\beta, p)$ from (46), (49), (50) and (51). As a consequence, the bases B_a, with $a = 0, 1, \ldots, p-1$, are p MUBs in the sense that they satisfy (53) for any a, b, α and β in the Galois field $\mathbb{F}_p$. Obviously, each of the bases B_a (with $a = 0, 1, \ldots, p-1$) is mutually unbiased with the computational basis B_p. This completes the proof. Note that Result 6 can be proved as well from the developments in [14].

As two typical examples, let us examine the cases $d = 2$ and 3.

Example 2: case $d = 2$. In this case, relevant for a spin $j = 1/2$ or for a qubit, we have $q = -1$ and $a, \alpha \in \mathbb{Z}_2$. The matrices of the operators v_{0a} are

$$V_{00} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad V_{01} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}. \tag{55}$$

By using the notation

$$\alpha := |\frac{1}{2}, \frac{1}{2}\rangle \qquad \beta := |\frac{1}{2}, -\frac{1}{2}\rangle \tag{56}$$

familiar in quantum chemistry (α is a spinorbital for spin up and β for spin down), the $d+1=3$ MUBs are

$$B_0 \quad : \quad |00\rangle = \frac{1}{\sqrt{2}}\,(\alpha+\beta) \qquad |01\rangle = -\frac{1}{\sqrt{2}}\,(\alpha-\beta) \tag{57}$$

$$B_1 \quad : \quad |10\rangle = i\frac{1}{\sqrt{2}}\,(\alpha-i\beta) \qquad |11\rangle = -i\frac{1}{\sqrt{2}}\,(\alpha+i\beta) \tag{58}$$

$$B_2 \quad : \quad |0\rangle = \alpha \qquad |1\rangle = \beta. \tag{59}$$

Example 3: case $d=3$. This case corresponds to a spin $j=1$ or to a qutrit. Here, we have $q=\exp(i2\pi/3)$ and $a,\alpha\in\mathbb{Z}_3$. The matrices of the operators v_{0a} are

$$V_{00} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} \qquad V_{01} = \begin{pmatrix} 0 & q & 0 \\ 0 & 0 & q^2 \\ 1 & 0 & 0 \end{pmatrix} \qquad V_{02} = \begin{pmatrix} 0 & q^2 & 0 \\ 0 & 0 & q \\ 1 & 0 & 0 \end{pmatrix}. \tag{60}$$

The $d+1=4$ MUBs read

$$\begin{aligned}
B_0 : \qquad & |00\rangle = \frac{1}{\sqrt{3}}\,(|0\rangle + |1\rangle + |2\rangle) \\
& |01\rangle = \frac{1}{\sqrt{3}}\,\left(q^2|0\rangle + q|1\rangle + |2\rangle\right) \\
& |02\rangle = \frac{1}{\sqrt{3}}\,\left(q|0\rangle + q^2|1\rangle + |2\rangle\right)
\end{aligned} \tag{61}$$

$$\begin{aligned}
B_1 : \qquad & |10\rangle = \frac{1}{\sqrt{3}}\,(q|0\rangle + q|1\rangle + |2\rangle) \\
& |11\rangle = \frac{1}{\sqrt{3}}\,\left(|0\rangle + q^2|1\rangle + |2\rangle\right) \\
& |12\rangle = \frac{1}{\sqrt{3}}\,\left(q^2|0\rangle + |1\rangle + |2\rangle\right)
\end{aligned} \tag{62}$$

$$\begin{aligned}
B_2 : \qquad & |20\rangle = \frac{1}{\sqrt{3}}\,\left(q^2|0\rangle + q^2|1\rangle + |2\rangle\right) \\
& |21\rangle = \frac{1}{\sqrt{3}}\,(q|0\rangle + |1\rangle + |2\rangle) \\
& |22\rangle = \frac{1}{\sqrt{3}}\,(|0\rangle + q|1\rangle + |2\rangle)
\end{aligned} \tag{63}$$

$$B_3 : \qquad |0\rangle = |1,1\rangle \qquad |1\rangle = |1,0\rangle \qquad |2\rangle = |1,-1\rangle. \tag{64}$$

It should be observed that B_0 (respectively, B_1 and B_2) can be associated with the *vector* (respectively, *projective*) irreducible representations of the group C_3.

3.4.2 Case d power of a prime

Different constructions of MUBs in the case where d is a power of a prime were achieved by numerous authors from algebraical and geometrical techniques (see for instance [38, 39, 54, 55, 56, 57, 58, 59, 60, 61, 62, 63] and references therein). We want to show here, through an example for $d = 4$, how our angular momentum approach can be useful for addressing this case.

Example 4: case $d = 4$. This case corresponds to a spin $j = 3/2$. Here, we have $q = i$ and $a, \alpha \in \mathbb{Z}_4$. Equations (20) and (28) can be applied to this case too. However, the resulting bases B_0, B_1, B_2, B_3 and B_4 do not constitute a complete system of MUBs ($d = 4$ is not a prime number). Nevertheless, it is possible to find $d+1 = 5$ MUBs because $d = 2^2$ is the power of a prime number. This can be achieved by replacing the space $\mathcal{E}(4)$ spanned by $\{|3/2, m\rangle : m = 3/2, 1/2, -1/2, -3/2\}$ by the tensor product space $\mathcal{E}(2) \otimes \mathcal{E}(2)$ spanned by the basis

$$\{\alpha \otimes \alpha, \alpha \otimes \beta, \beta \otimes \alpha, \beta \otimes \beta\}. \tag{65}$$

The space $\mathcal{E}(2) \otimes \mathcal{E}(2)$ is associated with the coupling of two spin angular momenta $j_1 = 1/2$ and $j_2 = 1/2$ or two qubits (in the vector $u \otimes v$, u and v correspond to j_1 and j_2, respectively).

In addition to the basis (65), it is possible to find other bases of $\mathcal{E}(2) \otimes \mathcal{E}(2)$ which are mutually unbiased. The $d = 4$ MUBs besides the canonical or computational basis (65) can be constructed from the eigenvectors

$$|ab\alpha\beta\rangle := |a\alpha\rangle \otimes |b\beta\rangle \tag{66}$$

of the operators

$$w_{ab} := v_{0a} \otimes v_{0b} \tag{67}$$

(the vectors $|a\alpha\rangle$ and $|b\beta\rangle$ refer to the two spaces $\mathcal{E}(2)$). As a result, we have the $d+1 = 5$ following MUBs where $\lambda = (1-i)/2$ and $\mu = i\lambda$.

The canonical basis:

$$\alpha \otimes \alpha \qquad \alpha \otimes \beta \qquad \beta \otimes \alpha \qquad \beta \otimes \beta. \tag{68}$$

The w_{00} basis:

$$|0000\rangle \ = \ \frac{1}{2}(\alpha \otimes \alpha + \alpha \otimes \beta + \beta \otimes \alpha + \beta \otimes \beta) \tag{69}$$

$$
\begin{aligned}
|0001\rangle &= \frac{1}{2}(\alpha\otimes\alpha-\alpha\otimes\beta+\beta\otimes\alpha-\beta\otimes\beta) && (70)\\
|0010\rangle &= \frac{1}{2}(\alpha\otimes\alpha+\alpha\otimes\beta-\beta\otimes\alpha-\beta\otimes\beta) && (71)\\
|0011\rangle &= \frac{1}{2}(\alpha\otimes\alpha-\alpha\otimes\beta-\beta\otimes\alpha+\beta\otimes\beta). && (72)
\end{aligned}
$$

The w_{11} basis:

$$
\begin{aligned}
|1100\rangle &= \frac{1}{2}(\alpha\otimes\alpha+i\alpha\otimes\beta+i\beta\otimes\alpha-\beta\otimes\beta) && (73)\\
|1101\rangle &= \frac{1}{2}(\alpha\otimes\alpha-i\alpha\otimes\beta+i\beta\otimes\alpha+\beta\otimes\beta) && (74)\\
|1110\rangle &= \frac{1}{2}(\alpha\otimes\alpha+i\alpha\otimes\beta-i\beta\otimes\alpha+\beta\otimes\beta) && (75)\\
|1111\rangle &= \frac{1}{2}(\alpha\otimes\alpha-i\alpha\otimes\beta-i\beta\otimes\alpha-\beta\otimes\beta). && (76)
\end{aligned}
$$

The w_{01} basis:

$$
\begin{aligned}
\lambda|0100\rangle+\mu|0111\rangle &= \frac{1}{2}(\alpha\otimes\alpha+\alpha\otimes\beta-i\beta\otimes\alpha+i\beta\otimes\beta) && (77)\\
\mu|0100\rangle+\lambda|0111\rangle &= \frac{1}{2}(\alpha\otimes\alpha-\alpha\otimes\beta+i\beta\otimes\alpha+i\beta\otimes\beta) && (78)\\
\lambda|0101\rangle+\mu|0110\rangle &= \frac{1}{2}(\alpha\otimes\alpha-\alpha\otimes\beta-i\beta\otimes\alpha-i\beta\otimes\beta) && (79)\\
\mu|0101\rangle+\lambda|0110\rangle &= \frac{1}{2}(\alpha\otimes\alpha+\alpha\otimes\beta+i\beta\otimes\alpha-i\beta\otimes\beta). && (80)
\end{aligned}
$$

The w_{10} basis:

$$
\begin{aligned}
\lambda|1000\rangle+\mu|1011\rangle &= \frac{1}{2}(\alpha\otimes\alpha-i\alpha\otimes\beta+\beta\otimes\alpha+i\beta\otimes\beta) && (81)\\
\mu|1000\rangle+\lambda|1011\rangle &= \frac{1}{2}(\alpha\otimes\alpha+i\alpha\otimes\beta-\beta\otimes\alpha+i\beta\otimes\beta) && (82)\\
\lambda|1001\rangle+\mu|1010\rangle &= \frac{1}{2}(\alpha\otimes\alpha+i\alpha\otimes\beta+\beta\otimes\alpha-i\beta\otimes\beta) && (83)\\
\mu|1001\rangle+\lambda|1010\rangle &= \frac{1}{2}(\alpha\otimes\alpha-i\alpha\otimes\beta-\beta\otimes\alpha-i\beta\otimes\beta). && (84)
\end{aligned}
$$

It is to be noted that the vectors of the w_{00} and w_{11} bases are not intricated (i.e., each vector is the direct product of two vectors) while the vectors of the w_{01} and w_{10} bases are intricated (i.e., each vector is not the direct product of two vectors). To be more precise, the degree of intrication of the state vectors for the bases w_{00}, w_{11}, w_{01} and w_{10} can be determined in the following way. In arbitrary dimension d, let

$$
|\Phi\rangle = \sum_{k=0}^{d-1}\sum_{l=0}^{d-1} a_{kl}|k\rangle\otimes|l\rangle \qquad (85)
$$

be a double qudit state vector. Then, it can be shown that the determinant of the $d \times d$ matrix $A = (a_{kl})$ satisfies

$$0 \leq |\det A| \leq \frac{1}{\sqrt{d^d}} \tag{86}$$

as proved in the Albouy thesis [65, 66]. The case $\det A = 0$ corresponds to the absence of intrication while the case

$$|\det A| = \frac{1}{\sqrt{d^d}} \tag{87}$$

corresponds to a maximal intrication. As an illustration, we obtain that all the state vectors for w_{00} and w_{11} are not intricated and that all the state vectors for w_{01} and w_{10} are maximally intricated.

3.4.3 Case d arbitrary

In the special case where $u = 1$, the generalized Gauss sum $S(1, -d + 2\alpha - 2\beta, d)$ can be easily calculated for d arbitrary by means of the reciprocity theorem [31]

$$S(u, v, w) = \sqrt{\left|\frac{w}{u}\right|} e^{i\pi[\mathrm{sgn}(uw) - v^2/(uw)]/4} S(-w, -v, u). \tag{88}$$

This leads to the following particular result.

Result 7. *For d arbitrary and $b = a \ominus 1$, one has*

$$\langle a\alpha | a_{-1}\beta \rangle = \frac{1}{\sqrt{d}} e^{i\pi[1-(d-2\alpha+2\beta)^2/d]/4} \Rightarrow |\langle a\alpha | a_{-1}\beta \rangle| = \frac{1}{\sqrt{d}} \qquad a_{-1} = a \ominus 1. \tag{89}$$

Therefore, the three bases $B_{a \ominus 1}$, B_a and B_d are mutually unbiased in $\mathbb{C}^d$.

This result is in agreement with a well-known result proved in many papers from quite distinct ways (see for instance [41]). We thus recover, from an approach based on generalized Gauss sums, that for d arbitrary the minimum number of MUBs is 3.

Another special case, viz., $u = 2$ ($\Rightarrow d \geq 3$), is worth of value. The application of the reciprocity theorem gives here

Result 8. *For $d \geq 3$ and $b = a \ominus 2$, one has*

$$\begin{aligned} \langle a\alpha | a_{-2}\beta \rangle &= \frac{1}{\sqrt{d}} \frac{1}{\sqrt{2}} e^{i\pi[1-2(\alpha-\beta)^2/d]/4} [1 + e^{i\pi(-d+2\alpha-2\beta)/2}] \\ &\Rightarrow \quad |\langle a\alpha | a_{-2}\beta \rangle| = \sqrt{\frac{2}{d}} \left| \cos\left[\frac{\pi}{4}(d - 2\alpha + 2\beta)\right] \right| \qquad a_{-2} = a \ominus 2. \end{aligned} \tag{90}$$

Therefore, the bases $B_{a\ominus 2}$ and B_a cannot be mutually unbiased in $\mathbb{C}^d$ for d even with $d \geq 4$. In marked contrast, the bases $B_{a\ominus 2}$ and B_a are unbiased for d odd with $d \geq 3$ (d prime or not prime).

Going back to the Hadamard matrices, let us remark that, for d arbitrary, if B_a and B_b are two MUBs associated with the Hadamard matrices F_a and F_b (respectively), then $F_a^\dagger F_b$ is a Hadamard matrix too. However, for d arbitrary, if F_a and F_b are two Hadamard matrices associated with the bases B_a and B_b (respectively), the product $F_a^\dagger F_b$ is not in general a Hadamard matrix.

4 Unitary group and generalized Pauli group

4.1 Weyl pairs

We continue with the general case where d is arbitrary. The operator v_{0a} can be expressed as

$$v_{0a} = \sum_{k=0}^{d-1} q^{ka} |k \ominus 1\rangle\langle k| \Leftrightarrow v_{0a} = \sum_{m=-j}^{j} q^{(j-m)a} |j, m \oplus 1\rangle\langle j, m| \tag{91}$$

so that

$$v_{0a}|k\rangle = q^{ka}|k \ominus 1\rangle \Leftrightarrow v_{0a}|j, m\rangle = q^{(j-m)a}|j, m \oplus 1\rangle \tag{92}$$

where $q = \exp(2\pi i/d)$. The operators x (the flip or shift operator) and z (the clock operator), used in quantum information and quantum computation (see for instance [67, 68]), can be derived from the generic operator v_{0a} as follows

$$x := v_{00} \qquad z := (v_{00})^\dagger v_{01}. \tag{93}$$

Therefore, we get

$$x = \sum_{k=0}^{d-1} |k \ominus 1\rangle\langle k| = |d-1\rangle\langle 0| + |0\rangle\langle 1| + \ldots + |d-2\rangle\langle d-1| \tag{94}$$

and

$$z = \sum_{k=0}^{d-1} q^k |k\rangle\langle k| = |0\rangle\langle 0| + q|1\rangle\langle 1| + \ldots + q^{d-1}|d-1\rangle\langle d-1|. \tag{95}$$

The action of x and z on the basis B_d of $\mathcal{E}(d)$ is given by the ladder relation

$$x|k\rangle = |k \ominus 1\rangle \Leftrightarrow x|j, m\rangle = (1 - \delta_{m,j})\,|j, m+1\rangle + \delta_{m,j}|j, -j\rangle \tag{96}$$

and the phase relation

$$z|k\rangle = q^k|k\rangle \Leftrightarrow z|j,m\rangle = q^{j-m}|j,m\rangle. \tag{97}$$

Alternatively, the action of x and z on any basis B_a ($a = 0, 1, \ldots, d-1$) of $\mathcal{E}(d)$ reads

$$x|a\alpha\rangle = q^{(d-1)a/2-\alpha}|a\alpha_a\rangle \qquad \alpha_a = \alpha \oplus a \qquad \Rightarrow \qquad x|0\alpha\rangle = q^{-\alpha}|0\alpha\rangle \tag{98}$$

and

$$z|a\alpha\rangle = q^{-1}|a\alpha_{-1}\rangle \qquad \alpha_{-1} = \alpha \ominus 1. \tag{99}$$

Equations (96) and (97), on one side, and Eqs. (98) and (99), on the other side, show that the flip or clock character for x and z is basis-dependent. The relationship between x and z can be understood via the following

Result 9. *The unitary operators x and z are cyclic and q-commute:*

$$x^d = z^d = I \qquad xz - qzx = 0. \tag{100}$$

They are connected by

$$x = f^\dagger z f \Leftrightarrow z = f x f^\dagger \tag{101}$$

where the Fourier operator

$$f := \frac{1}{\sqrt{d}} \sum_{k=0}^{d-1} \sum_{k'=0}^{d-1} q^{-kk'} |k\rangle\langle k'| \tag{102}$$

is unitary and satisfies

$$f^4 = 1. \tag{103}$$

The operators x and z are isospectral operators with the common spectrum $\{1, q, \ldots, q^{d-1}\}$.

A direct proof of Result 9 can be obtained by switching to the matrices

$$X = \sum_{k=0}^{d-1} E_{k\ominus 1,k} = \begin{pmatrix} 0 & 1 & 0 & \ldots & 0 \\ 0 & 0 & 1 & \ldots & 0 \\ \vdots & \vdots & \vdots & \ldots & \vdots \\ 0 & 0 & 0 & \ldots & 1 \\ 1 & 0 & 0 & \ldots & 0 \end{pmatrix} \tag{104}$$

$$Z = \sum_{k=0}^{d-1} q^k E_{k,k} = \begin{pmatrix} 1 & 0 & 0 & \dots & 0 \\ 0 & q & 0 & \dots & 0 \\ 0 & 0 & q^2 & \dots & 0 \\ \vdots & \vdots & \vdots & \dots & \vdots \\ 0 & 0 & 0 & \dots & q^{d-1} \end{pmatrix} \tag{105}$$

of the operators x and z, in the basis B_d (cf. (97) and (98)). Let F be the matrix of the linear operator f in the basis B_d. The reduction by means of F of the endomorphism associated with the matrix X yields the matrix Z. In other words, the diagonalization of X can be achieved with the help of the matrix F via $Z = FXF^\dagger$. Note that the matrix F is connected to F_0 by

$$F = (F_0 S)^\dagger \qquad S := \sum_{\beta=0}^{d-1} q^\beta E_{\beta, d-\beta} \tag{106}$$

where S acts as a pseudopermutation.

In view of (100), the pair (x, z) is called a Weyl pair. Weyl pairs were originally introduced in finite quantum mechanics [69] and used for the construction of unitary bases in finite-dimensional Hilbert spaces [70]. It should be noted that matrices of type X and Z were introduced long time ago by Sylvester [71] in order to solve the matrix equation $PX = XQ$; in addition, such matrices were used by Morris [72] to define generalized Clifford algebras in connection with quaternion algebras and division rings. Besides the Weyl pair (x, z), other pairs can be formed with the operators v_{0a} and z. Indeed, any operator v_{0a} ($a \in \mathbb{Z}_d$) can be generated from x and z since

$$v_{0a} = xz^a. \tag{107}$$

Thus, Eq. (100) can be generalized as

$$e^{-i\pi(d-1)a}(v_{0a})^d = z^d = I \qquad v_{0a}z - qzv_{0a} = 0. \tag{108}$$

Therefore, the pair (v_{0a}, z) is a Weyl pair for $(d-1)a$ even.

4.2 Generalized Pauli matrices

For $d = 2$ the q-commutation relation of x and z reduces to an anticommutation relation. In fact, Eq. (100) with $d = 2$ can be particularized to the relations

$$x^2 = z^2 = I \qquad xz + zx = 0 \tag{109}$$

which are reminiscent of relations satisfied by the Pauli matrices. Hence, we understand that the matrices X and Z for d arbitrary can be used as an integrity basis for producing generalized Pauli matrices [37, 38, 39, 54, 55, 57, 58, 59, 60, 73, 74, 75, 76, 77, 78, 79, 80, 81, 82]. Let us develop this point.

For d arbitrary, we define the operators

$$u_{ab} = x^a z^b \qquad a, b \in \mathbb{Z}_d. \tag{110}$$

The operators u_{ab} shall be referred as generalized Pauli operators and their matrices as generalized Pauli matrices. They satisfy the ladder-phase relation

$$u_{ab}|k\rangle = q^{kb}|k \ominus a\rangle \Leftrightarrow u_{ab}|j, m\rangle = q^{(j-m)b}|j, m \oplus a\rangle \tag{111}$$

from which we can derive the following result.

Result 10. *The d^2 operators u_{ab}, with $a, b \in \mathbb{Z}_d$, are unitary and obey the multiplication rule*

$$u_{ab}u_{a'b'} = q^{-ba'} u_{a''b''} \qquad a'' := a \oplus a' \qquad b'' := b \oplus b'. \tag{112}$$

Therefore, the commutator and the anticommutator of u_{ab} and $u_{a'b'}$ are given by

$$[u_{ab}, u_{a'b'}]_{\pm} = \left(q^{-ba'} \pm q^{-ab'}\right) u_{a''b''} \qquad a'' := a \oplus a' \qquad b'' := b \oplus b'. \tag{113}$$

Furthermore, they are orthogonal with respect to the Hilbert-Schmidt inner product

$$\mathrm{Tr}_{\mathcal{E}(d)} \left[(u_{ab})^{\dagger} u_{a'b'}\right] = d\, \delta_{a,a'}\ \delta_{b,b'} \tag{114}$$

where the trace is taken on the d-dimensional space $\mathcal{E}(d)$.

As a corollary of Result 10, we have

$$[u_{ab}, u_{a'b'}]_{-} = 0 \Leftrightarrow ab' \ominus ba' = 0 \tag{115}$$

and

$$[u_{ab}, u_{a'b'}]_{+} = 0 \Leftrightarrow ab' \ominus ba' = \frac{1}{2}d. \tag{116}$$

This yields two consequences. First, Eq. (116) shows that all anticommutators $[u_{ab}, u_{a'b'}]_{+}$ are different from 0 if d is an odd integer. Second, from Eq. (115) we have the important result that, for d arbitrary, each of the three disjoint sets

$$e_{0\bullet} := \{u_{0a} = z^a : a = 1, 2, \ldots, d-1\} \tag{117}$$

$$e_{\bullet\bullet} := \{u_{aa} = x^a z^a : a = 1, 2, \ldots, d-1\} \tag{118}$$

$$e_{\bullet 0} := \{u_{a0} = x^a : a = 1, 2, \ldots, d-1\} \tag{119}$$

consist of $d-1$ mutually commuting operators. The three sets $e_{0\bullet}$, $e_{\bullet\bullet}$ and $e_{\bullet 0}$ are associated with three MUBs. This is in agreement with the fact that the bases B_0, B_1 and B_d are three MUBs for d arbitrary ($v_{00} = x \in e_{\bullet 0}$, $v_{01} = xz \in e_{\bullet\bullet}$ and $z \in e_{0\bullet}$ are associated with B_0, B_1 and B_d, respectively).

By way of illustration, let us give the matrices in the basis B_d of the operators u_{ab} for $d = 2$, 3 and 4.

Example 5: case $d = 2$. For $d = 2 \Leftrightarrow j = 1/2$ ($\Rightarrow q = -1$), the matrices in the two sets

$$E_0 := \{I_2 = X^0 Z^0, X = X^1 Z^0 \equiv V_{00}\} \tag{120}$$

$$E_1 := \{Z = X^0 Z^1, Y = X^1 Z^1 \equiv V_{01}\} \tag{121}$$

corresponding to the four operators u_{ab} are

$$I_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \qquad Y = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}. \tag{122}$$

In terms of the usual (Hermitian and unitary) Pauli matrices σ_x, σ_y and σ_z, we have

$$X = \sigma_x \qquad Y = -i\sigma_y \qquad Z = \sigma_z. \tag{123}$$

The matrices X, Y and Z are thus identical to the Pauli matrices up to a phase factor for Y. This phase factor is the price one has to pay in order to get a systematic generalization of Pauli matrices in arbitrary dimension.

Example 6: case $d = 3$. For $d = 3 \Leftrightarrow j = 1$ ($\Rightarrow q = \exp(i2\pi/3)$), the matrices in the three sets

$$E_0 := \{X^0 Z^0, X^1 Z^0 \equiv V_{00}, X^2 Z^0\} \tag{124}$$

$$E_1 := \{X^0 Z^1, X^1 Z^1 \equiv V_{01}, X^2 Z^1\} \tag{125}$$

$$E_2 := \{X^0 Z^2, X^1 Z^2 \equiv V_{02}, X^2 Z^2\} \tag{126}$$

corresponding to the nine operators u_{ab} are

$$I_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad X = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} \qquad X^2 = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \tag{127}$$

$$Z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & q & 0 \\ 0 & 0 & q^2 \end{pmatrix} \qquad XZ = \begin{pmatrix} 0 & q & 0 \\ 0 & 0 & q^2 \\ 1 & 0 & 0 \end{pmatrix} \qquad X^2 Z = \begin{pmatrix} 0 & 0 & q^2 \\ 1 & 0 & 0 \\ 0 & q & 0 \end{pmatrix} \tag{128}$$

$$Z^2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & q^2 & 0 \\ 0 & 0 & q \end{pmatrix} \qquad XZ^2 = \begin{pmatrix} 0 & q^2 & 0 \\ 0 & 0 & q \\ 1 & 0 & 0 \end{pmatrix} \qquad X^2Z^2 = \begin{pmatrix} 0 & 0 & q \\ 1 & 0 & 0 \\ 0 & q^2 & 0 \end{pmatrix}. \tag{129}$$

These generalized Pauli matrices differ from the Gell-Mann matrices and Okubo matrices used for $SU(3)$ in particle physics with three flavors of quarks [83, 84, 85]. They constitute a natural extension based on Weyl pairs of the Pauli matrices in dimension $d = 3$.

Example 7: case $d = 4$. For $d = 4 \Leftrightarrow j = 3/2$ ($\Rightarrow q = i$), the matrices in the four sets

$$E_0 \ := \ \{X^0Z^0, X^1Z^0 \equiv V_{00}, X^2Z^0, X^3Z^0\} \tag{130}$$
$$E_1 \ := \ \{X^0Z^1, X^1Z^1 \equiv V_{01}, X^2Z^1, X^3Z^1\} \tag{131}$$
$$E_2 \ := \ \{X^0Z^2, X^1Z^2 \equiv V_{02}, X^2Z^2, X^3Z^2\} \tag{132}$$
$$E_3 \ := \ \{X^0Z^3, X^1Z^3 \equiv V_{03}, X^2Z^3, X^3Z^3\} \tag{133}$$

corresponding to the 16 operators u_{ab} are

$$I_4 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \qquad X = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \end{pmatrix} \tag{134}$$

$$X^2 = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} \qquad X^3 = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix} \tag{135}$$

$$Z = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & i & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 1 & 0 & 0 & -i \end{pmatrix} \qquad XZ = \begin{pmatrix} 0 & i & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -i \\ 1 & 0 & 0 & 0 \end{pmatrix} \tag{136}$$

$$X^2Z = \begin{pmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -i \\ 1 & 0 & 0 & 0 \\ 0 & i & 1 & 0 \end{pmatrix} \qquad X^3Z = \begin{pmatrix} 0 & 0 & 0 & -i \\ 1 & 0 & 0 & 0 \\ 0 & i & 0 & 0 \\ 0 & 0 & -1 & 0 \end{pmatrix} \tag{137}$$

$$Z^2 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \qquad XZ^2 = \begin{pmatrix} 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \end{pmatrix} \tag{138}$$

$$X^2Z^2 = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix} \qquad X^3Z^2 = \begin{pmatrix} 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix} \tag{139}$$

$$Z^3 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -i & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & i \end{pmatrix} \qquad XZ^3 = \begin{pmatrix} 0 & -i & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & i \\ 1 & 0 & 0 & 0 \end{pmatrix} \tag{140}$$

$$X^2Z^3 = \begin{pmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & i \\ 1 & 0 & 0 & 0 \\ 0 & -i & 0 & 0 \end{pmatrix} \qquad X^3Z^3 = \begin{pmatrix} 0 & 0 & 0 & i \\ 1 & 0 & 0 & 0 \\ 0 & -i & 0 & 0 \\ 0 & 0 & -1 & 0 \end{pmatrix}. \tag{141}$$

These generalized Pauli matrices are linear combinations of the generators of the chain $SU(4) \supset SU(3) \supset SU(2)$ in particle physics with four flavors of quarks [86, 87, 88].

For d arbitrary, the generalized Pauli matrices arising from (110) are different from the generalized Gell-Mann λ matrices introduced in [89]. The generalized λ matrices are Hermitian and adapted to the chain of groups $SU(d) \supset SU(d-1) \supset \ldots \supset SU(2)$ while the matrices X^aZ^b are unitary and closely connected to cyclic symmetry. Indeed, for d arbitrary, each of the d sets

$$E_b := \{X^aZ^b : a = 0, 1, \ldots, d-1\} \qquad b = 0, 1, \ldots, d-1 \tag{142}$$

is associated with an irreducible representation of the cyclic group C_d. More precisely, the one-dimensional irreducible representation of C_d associated with E_b is obtained by listing the nonzero matrix elements of any matrix of E_b, column by column from left to right. In this way, we obtain the d irreducible representations of C_d. This relationship between d-dimensional Pauli matrices and irreducible representations of C_d are clearly emphasized by the examples given above for $d = 2$, 3 and 4.

4.3 Pauli basis for the unitary group

Two consequences follow from (114). (i) The Hilbert-Schmidt relation (114) in the Hilbert space $\mathbb{C}^{d^2}$ shows that the d^2 operators u_{ab} are pairwise orthogonal operators. Thus, they can serve as a basis for developing any operator acting on $\mathcal{E}(d)$. (ii) The commutator in (113) defines the Lie bracket of a d^2-dimensional Lie algebra generated by the set $\{u_{ab} : a, b = 0, 1, \ldots, d-1\}$. This algebra can be identified to the Lie algebra $u(d)$ of the unitary group $U(d)$. The subset $\{u_{ab} : a, b = 0, 1, \ldots, d-1\} \setminus \{u_{00}\}$ then spans the Lie algebra $su(d)$ of the special unitary group $SU(d)$. In other words, the Weyl pair (X, Z), consisting of the generalized Pauli matrices X and Z in dimension d, form an integrity basis for $u(d)$. More specifically, the two following results hold.

Result 11. *The set $\{X^a Z^b : a, b = 0, 1, \ldots, d-1\}$ forms a basis for the Lie algebra $u(d)$ of the unitary group $U(d)$. The Lie brackets of $u(d)$ in such a basis (denoted as the Pauli basis) are*

$$[X^a Z^b, X^e Z^f]_- = \sum_{i=0}^{d-1} \sum_{j=0}^{d-1} (ab, ef; ij) X^i Z^j \tag{143}$$

with the structure constants

$$(ab, ef; ij) = \delta(i, a \oplus e)\delta(j, b \oplus f) \left(q^{-be} - q^{-af}\right) \tag{144}$$

where $a, b, e, f, i, j \in \mathbb{Z}_d$. The structure constants $(ab, ef; ij)$ with $i = a \oplus e$ and $j = b \oplus f$ are cyclotomic polynomials associated with d. They vanish for $af \ominus be = 0$.

Result 12. *For $d = p$, with p a prime integer, the Lie algebra $su(p)$ of the special unitary group $SU(p)$ can be decomposed into a direct sum of $p+1$ abelian subalgebras of dimension $p-1$, i.e.*

$$su(p) \simeq v_0 \uplus v_1 \uplus \ldots \uplus v_p \tag{145}$$

where each of the $p+1$ subalgebras $v_0, v_1, \ldots, v_p$ is a Cartan subalgebra generated by a set of $p-1$ commuting matrices. The various sets are

$$\begin{aligned}
\mathcal{V}_0 &:= \{X^0Z^1, X^0Z^2, X^0Z^3, \ldots, X^0Z^{p-2}, X^0Z^{p-1}\} && (146)\\
\mathcal{V}_1 &:= \{X^1Z^0, X^2Z^0, X^3Z^0, \ldots, X^{p-2}Z^0, X^{p-1}Z^0\} && (147)\\
\mathcal{V}_2 &:= \{X^1Z^1, X^2Z^2, X^3Z^3, \ldots, X^{p-2}Z^{p-2}, X^{p-1}Z^{p-1}\} && (148)\\
\mathcal{V}_3 &:= \{X^1Z^2, X^2Z^4, X^3Z^6, \ldots, X^{p-2}Z^{p-4}, X^{p-1}Z^{p-2}\} && (149)\\
&\vdots && (150)\\
\mathcal{V}_{p-1} &:= \{X^1Z^{p-2}, X^2Z^{p-4}, X^3Z^{p-6}, \ldots, X^{p-2}Z^4, X^{p-1}Z^2\} && (151)\\
\mathcal{V}_p &:= \{X^1Z^{p-1}, X^2Z^{p-2}, X^3Z^{p-3}, \ldots, X^{p-2}Z^2, X^{p-1}Z^1\} && (152)
\end{aligned}$$

for $v_0, v_1, \ldots, v_p$, respectively.

Example 8: $p = 7 \Leftrightarrow j = 3$. Equations (146)-(152) give

$$\begin{aligned}
\mathcal{V}_0 &= \{(01), (02), (03), (04), (05), (06)\} && (153)\\
\mathcal{V}_1 &= \{(10), (20), (30), (40), (50), (60)\} && (154)\\
\mathcal{V}_2 &= \{(11), (22), (33), (44), (55), (66)\} && (155)\\
\mathcal{V}_3 &= \{(12), (24), (36), (41), (53), (65)\} && (156)\\
\mathcal{V}_4 &= \{(13), (26), (32), (45), (51), (64)\} && (157)\\
\mathcal{V}_5 &= \{(14), (21), (35), (42), (56), (63)\} && (158)\\
\mathcal{V}_6 &= \{(15), (23), (31), (46), (54), (62)\} && (159)\\
\mathcal{V}_7 &= \{(16), (25), (34), (43), (52), (61)\} && (160)
\end{aligned}$$

where (ab) is used as an abbreviation of $X^a Z^b$.

Result 12 can be extended to the case where $d = p^e$ with p a prime integer and e a positive integer: there exists a decomposition of $su(p^e)$ into $p^e + 1$ abelian subalgebras of dimension $p^e - 1$. In order to make this point clear, we start with a counterexample.

Counterexample: $d = 4 \Leftrightarrow j = 3/2$ ($\Rightarrow a, b = 0, 1, 2, 3$). In this case, Result 11 is valid but Result 12 does not apply. Indeed, the 16 unitary operators u_{ab} corresponding to

$$ab = 01, 02, 03, 10, 20, 30, 11, 22, 33, 12, 13, 21, 23, 31, 32, 00 \qquad (161)$$

are linearly independent and span the Lie algebra of $U(4)$ but they give only three disjoint sets, viz., $\{(01), (02), (03)\}$, $\{(10), (20), (30)\}$ and $\{(11), (22), (33)\}$, containing each 3 commuting operators, where here again (ab) stands for $X^a Z^b$. However, it is not possible to partition the set (161) in order to get a decomposition similar to (145). Nevertheless, it is possible to find another basis of $u(4)$ which can be partitioned in a way yielding a decompostion similar to (145). This can be achieved by working with tensorial products of the matrices $X^a Z^b$ corresponding to $p = 2$. In this respect, let us consider the product $u_{a_1 b_1} \otimes u_{a_2 b_2}$, where $u_{a_i b_i}$ with $i = 1, 2$ are Pauli operators for $p = 2$. Then, by using the abbreviation $(a_1 b_1 a_2 b_2)$ for $u_{a_1 b_1} \otimes u_{a_2 b_2}$ or $X^{a_1} Z^{b_1} \otimes X^{a_2} Z^{b_2}$, it can be checked that the five disjoint sets

$$\begin{aligned}
&\{(1011), (1101), (0110)\} && (162)\\
&\{(1110), (1001), (0111)\} && (163)\\
&\{(1010), (1000), (0010)\} && (164)\\
&\{(1111), (1100), (0011)\} && (165)\\
&\{(0101), (0100), (0001)\} && (166)
\end{aligned}$$

consist each of 3 commuting unitary operators and that the Lie algebra $su(4)$ is spanned by the union of the 5 sets. It is to be emphasized that the 15 operators (162)-(166) are underlaid by the geometry of the generalized quadrangle of order 2 [90]. In this geometry, the five sets given by (162)-(166) correspond to a spread of this quadrangle, i.e., to a set of 5 pairwise skew lines [90].

The considerations of the counterexample can be generalized to $d := d_1 d_2 \dots d_e$, e being an integer greater or equal to 2. Let us define

$$u_{AB} := u_{a_1 b_1} \otimes u_{a_2 b_2} \otimes \dots \otimes u_{a_e b_e} \quad A := a_1, a_2, \dots, a_e \quad B := b_1, b_2, \dots, b_e \tag{167}$$

where $u_{a_1 b_1}, u_{a_2 b_2}, \dots, u_{a_e b_e}$ are generalized Pauli operators corresponding to the dimensions $d_1, d_2, \dots, d_e$ respectively. In addition, let $q_1, q_2, \dots, q_e$ be the q-factor associated with $d_1, d_2, \dots, d_e$ respectively ($q_j := \exp(2\pi i/d_j)$). Then, Results 10, 11 and 12 can be generalized as follows.

Result 13. *The operators u_{AB} are unitary and satisfy the orthogonality relation*

$$\mathrm{Tr}_{\mathcal{E}(d_1 d_2 \dots d_e)} \left[(u_{AB})^\dagger \, u_{A'B'} \right] = d_1 d_2 \dots d_e \; \delta_{A,A'} \; \delta_{B,B'} \tag{168}$$

where

$$\delta_{A,A'} := \delta_{a_1,a'_1} \delta_{a_2,a'_2} \dots \delta_{a_e,a'_e} \qquad \delta_{B,B'} := \delta_{b_1,b'_1} \delta_{b_2,b'_2} \dots \delta_{b_e,b'_e}. \tag{169}$$

The commutator $[u_{AB}, u_{A'B'}]_-$ and the anti-commutator $[u_{AB}, u_{A'B'}]_+$ of u_{AB} and $u_{A'B'}$ are given by

$$[u_{AB}, u_{A'B'}]_{\mp} = \left(\prod_{j=1}^{e} q_j^{-b_j a'_j} \mp \prod_{j=1}^{e} q_j^{-a_j b'_j} \right) u_{A''B''} \tag{170}$$

with

$$A'' := a_1 \oplus a'_1, a_2 \oplus a'_2, \dots, a_e \oplus a'_e \qquad B'' := b_1 \oplus b'_1, b_2 \oplus b'_2, \dots, b_e \oplus b'_e. \tag{171}$$

The set $\{u_{AB} : A, B \in \mathbb{Z}_{d_1} \otimes \mathbb{Z}_{d_2} \otimes \dots \otimes \mathbb{Z}_{d_e}\}$ of the $d_1^2 d_2^2 \dots d_e^2$ unitary operators u_{AB} form a basis for the Lie algebra $u(d_1 d_2 \dots d_e)$ of the group $U(d_1 d_2 \dots d_e)$.

The operators u_{AB} may be called generalized Dirac operators since the ordinary Dirac operators correspond to specific $u_{a_1 b_1} \otimes u_{a_2 b_2}$ for $d_1 = d_2 = 2$.

In the special case where $d_1 = d_2 = \dots = d_e = p$ with p a prime integer (or equivalently $d = p^e$), we have $[u_{AB}, u_{A'B'}]_- = 0$ if and only if

$$\sum_{j=1}^{e} a_j b'_j \ominus b_j a'_j = 0 \tag{172}$$

and $[u_{AB}, u_{A'B'}]_+ = 0$ if and only if

$$\sum_{j=1}^{e} a_j b'_j \ominus b_j a'_j = \frac{1}{2} p \tag{173}$$

so that there are vanishing anti-commutators only if $p = 2$. The commutation relations given by (170)-(171) can be transcribed in terms of Lagrangian submodules [65, 91]. For $d = p^e$, there exists a decomposition of the set $\{u_{AB} : A, B \in \mathbb{Z}_p^{\otimes e}\} \setminus \{I\}$ that corresponds to a decomposition of the Lie algebra $su(p^e)$ into $p^e + 1$ abelian subalgebras of dimension $p^e - 1$ [25, 74, 92, 93, 94, 95].

4.4 Generalized Pauli group

Let us define the d^3 operators

$$w_{abc} := q^a x^b z^c = q^a u_{bc} \qquad a, b, c \in \mathbb{Z}_d. \tag{174}$$

The action of w_{abc} on the Hilbert space $\mathcal{E}(d)$ is described by

$$w_{abc}|k\rangle = q^{a+kc}|k \ominus b\rangle \Leftrightarrow w_{abc}|j, m\rangle = q^{a+(j-m)c}|j, m \oplus b\rangle. \tag{175}$$

The operators w_{abc} are unitary and satisfy

$$\mathrm{Tr}_{\mathcal{E}(d)} \left[(w_{abc})^\dagger w_{a'b'c'} \right] = q^{a'-a} \, d \, \delta_{b,b'} \, \delta_{c,c'} \tag{176}$$

which gives back (114) for $a = a' = 0$.

The product of the operators w_{abc} and $w_{a'b'c'}$ reads

$$w_{abc} w_{a'b'c'} = w_{a''b''c''} \qquad a'' = a \oplus a' \ominus cb' \qquad b'' = b \oplus b' \qquad c'' = c \oplus c'. \tag{177}$$

The set $\{w_{abc} : a, b, c \in \mathbb{Z}_d\}$ can be endowed with a group structure. In the detail, we have the following

Result 14. *The set $\{w_{abc} : a, b, c \in \mathbb{Z}_d\}$, endowed with the internal law (177), is a finite group of order d^3. This nonabelian group, noted Π_d and called generalized Pauli group in d dimensions, is nilpotent (hence solvable) with a nilpotency class equal to 2. The group Π_d is isomorphic to a subgroup of $U(d)$ for d even or $SU(d)$ for d odd. It has $d(d+1)-1$ conjugacy classes (d classes containing each 1 element and $d^2 - 1$ classes containing each d elements) and $d(d+1) - 1$ classes of irreducible representations (d^2 classes of dimension 1 and $d - 1$ classes of dimension d).*

A faithful three-dimensional representation of Π_d is provided with the application

$$\Pi_d \to GL(3, \mathbb{Z}_d) : w_{abc} \mapsto \begin{pmatrix} 1 & 0 & 0 \\ b & 1 & 0 \\ a & -c & 1 \end{pmatrix}. \tag{178}$$

This is reminiscent of the Heisenberg-Weyl group [96, 97, 98, 99, 100, 101]. Indeed, the group Π_d can be considered as a discretization $HW(\mathbb{Z}_d)$ of the Heisenberg-Weyl group $HW(\mathbb{R})$, a three-parameter Lie group. The Heisenberg-Weyl group $HW(\mathbb{R})$, also called the Heisenberg group or Weyl group, is at the root of quantum mechanics. It also plays an important role in symplectic geometry. The group Π_d was discussed by Šťovíček and Tolar [102] in connection with quantum mechanics in a discrete space-time, by Balian and Itzykson [73] in connection with finite quantum mechanics, by Patera and Zassenhaus [74] in connection with gradings of simple Lie algebras of type A_{n-1}, and by Kibler [25] in connection with Weyl pairs and the Heisenberg-Weyl group. Note that the discrete version $HW(\mathbb{Z})$ of $HW(\mathbb{R})$ was used for an analysis of the solutions of the Markoff equation [103]. Recently, the discrete version $HW[\mathbb{Z}_p \times (\mathbb{Q}_p/\mathbb{Z}_p)]$ was introduced for describing (p-adic) quantum systems with positions in $\mathbb{Z}_p$ and momenta in $\mathbb{Q}_p/\mathbb{Z}_p$ [104].

As far as $HW(\mathbb{Z}_d)$ is concerned, it is to be observed that a Lie algebra π_d can be associated with the finite group Π_d. This can be seen by considering the Frobenius algebra of Π_d (see [105] for the definition of the Lie algebra associated with an arbitray finite group). Then, the Lie brackets of π_d are

$$[w_{abc}, w_{a'b'c'}]_- = w_{\alpha\beta\gamma} - w_{\alpha'\beta'\gamma'} \tag{179}$$

with

$$\alpha = a \oplus a' \ominus cb' \quad \beta = b \oplus b' \quad \gamma = c \oplus c' \quad \alpha' = \alpha \oplus cb' \ominus bc' \quad \beta' = \beta \quad \gamma' = \gamma. \tag{180}$$

The algebra π_d, of dimension d^3, is not semisimple. It can be decomposed as the direct sum

$$\pi_d \simeq \biguplus_{1}^{d^2} u(1) \biguplus_{1}^{d-1} u(d) \tag{181}$$

which contains d^2 Lie algebras isomorphic to $u(1)$ and $d-1$ Lie algebras isomorphic to $u(d)$. The Lie algebra $u(d)$ spanned by the set $\{u_{ab} : a, b \in \mathbb{Z}_d\}$ is one of the subalgebras of π_d.

The group Π_d (noted P_d in [25]) should not be confused with the Pauli group $\mathcal{P}_n$ on n qubits spanned by n-fold tensor products of $i\sigma_0 \equiv iI_2$, σ_x and σ_z used in quantum information and quantum computation [106, 107]. The Pauli group $\mathcal{P}_n$ has 4^{n+1}

elements. It is used as an error group in quantum computing. The normaliser of $\mathcal{P}_n$ in $SU(2^n)$, known as the Clifford (or Jacobi) group Cli_n on n qubits, a group of order $2^{n^2+2n+3}\prod_{j=1}^{n}(4^j-1)$, is of great interest in the context of quantum corrector codes [41, 108, 109, 110, 111, 112, 113]. In addition to Cli_n, proper sugroups of Cli_n having $\mathcal{P}_n$ as an invariant subgroup are relevant for displaying quantum coherence [114]. The distinction bewteen $\mathcal{P}_n$ and Π_d can be clarified by the example below which shows that Π_2 is not isomorphic to $\mathcal{P}_1$. In a parallel way, it can be proved that the groups Π_4 and $\mathcal{P}_2$ (both of order 64) are distinct.

Example 9: $d = 2$. The simplest example of Π_d occurs for $d = 2$. The group Π_2 has 8 elements ($\pm I$, $\pm x$, $\pm y := \pm xz$, $\pm z$) and is isomorphic to the dihedral group D_4. It can be partitioned into 5 conjugation classes ($\{I\}, \{-I\}, \{x, -x\}, \{y, -y\}, \{z, -z\}$) and possesses 5 inequivalent irreducible representations (of dimensions 1, 1, 1, 1 and 2). The two-dimensional irreducible representation corresponds to

$$\pm I \mapsto \pm\sigma_0 \qquad \pm x \mapsto \pm\sigma_x \qquad \pm y \mapsto \mp i\sigma_y \qquad \pm z \mapsto \pm\sigma_z \tag{182}$$

in terms of the Pauli matrices σ_λ with $\lambda = 0, x, y, z$. The elements $e_1 := x$, $e_2 := y$ and $e_3 := z$ of Π_2 span the four-dimensional algebra $A(1, -1, 0) \equiv \mathbb{N}_1$, the algebra of *hyperbolic quaternions* (with $e_1^2 = -e_2^2 = e_3^2 = 1$ instead of $e_1^2 = e_2^2 = e_3^2 = -1$ as for usual quaternions). This associative and noncommutative algebra is a singular division algebra. The algebra $\mathbb{N}_1$ turns out to be a particular Cayley-Dickson algebra $A(c_1, c_2, c_3)$ [115]. Going back to Π_2, we see that not all the subgroups of Π_2 are invariant. The group Π_2 is isomorphic to the group of *hyperbolic quaternions* rather than to the group Q of *ordinary quaternions* for which all subgroups are invariant (the group Q can be realized with the help of the matrices $\pm\sigma_0$, $\pm i\sigma_x$, $\pm i\sigma_y$, $\pm i\sigma_z$). Like Q, the group Π_2 is ambivalent and simply reducible in the terminology of Wigner [2]. Indeed, Π_2 is the sole generalized Pauli group that is ambivalent.

To end up with this example, let us examine the connection between Π_2 and the 1 qubit Pauli group $\mathcal{P}_1$. The group $\mathcal{P}_1$ has 16 elements ($\pm\sigma_\lambda, \pm i\sigma_\lambda$ with $\lambda = 0, x, y, z$). Obviously, Π_2 is a subgroup of index 2 (necessarily invariant) of $\mathcal{P}_1$. The group $\mathcal{P}_1$ can be considered as a double group of Π_2 or Q in the sense that $\mathcal{P}_1$ coincides with $\Pi_2 \bigcup i\Pi_2 \equiv Q \bigcup iQ$ in terms of sets. Therefore, the group table of $\mathcal{P}_1$ easily follows from the one of Π_2 or Q. As a result, the numbers of conjugation classes and irreducible representation classes are doubled when passing from Π_2 or Q to $\mathcal{P}_1$.

5 Closing remarks

Starting from a nonstandard approach to angular momentum and its transcription in terms of representation of $SU(2)$, we derived (in an original and unified way) some results about unitary operator bases and their connection to unitary groups, Pauli groups and quadratic sums. These results (either known or formulated in a new way) shed some light on the importance of the polar decomposition of $su(2)$ and cyclic groups for the study of unitary operator bases and their relationship with unitary groups and Pauli groups. In particular, the latter decomposition and the quadratic discrete Fourier transform introduced in this work make it possible to generate in prime dimension a complete set of MUBs given by a single formula (Eq. (20)). From the point of view of the representation theory, it would be interesting to find realisation on the state vectors (20) on the sphere S^2 thus establishing a contact between the $\{j^2, v_{0a}\}$ scheme and special functions.

To close this paper, let us be mention two works dealing with *à la* Schwinger unitary operator bases in an angular momentum scheme. In Ref. [116], unitary operator bases and standard (discrete) quantum Fourier transforms in an angular momentum framework proved to be useful for spin tunneling. In addition, d-dimensional generalized Pauli matrices applied to modified Bessel functions were considered in an angular momentum approach with $j = (d-1)/2 \to \infty$ [117].

Appendix A: A polar decomposition of $su(2)$

In addition to the operator v_{ra}, a second linear operator is necessary to define a polar decomposition of $SU(2)$. Let us introduce the Hermitian operator h through

$$h := \sum_{m=-j}^{j} \sqrt{(j+m)(j-m+1)} |j,m\rangle\langle j,m|. \tag{183}$$

Then, it is a simple matter of calculation to show that the three operators

$$j_+ := hv_{ra} \qquad j_- := (v_{ra})^\dagger h \qquad j_z := \frac{1}{2}\left[h^2 - (v_{ra})^\dagger h^2 v_{ra}\right] \tag{184}$$

satisfy the ladder equations

$$j_+|j,m\rangle = q^{+(j-m+s-1/2)a}\sqrt{(j-m)(j+m+1)}|j,m+1\rangle \tag{185}$$

$$j_-|j,m\rangle = q^{-(j-m+s+1/2)a}\sqrt{(j+m)(j-m+1)}|j,m-1\rangle \tag{186}$$

and the eigenvalue equation

$$j_z|j,m\rangle = m|j,m\rangle \tag{187}$$

where $s = 1/2$. Therefore, the operators j_+, j_- and j_z satisfy the commutation relations

$$[j_z, j_+]_- = +j_+ \qquad [j_z, j_-]_- = -j_- \qquad [j_+, j_-]_- = 2j_z \tag{188}$$

and thus span the Lie algebra of $SU(2)$.

The latter result does not depend on the parameters r and a. However, the action of j_+ and j_- on $|j,m\rangle$ on the space $\mathcal{E}(2j+1)$ depends on a; the usual Condon and Shortley phase convention used in spectroscopy corresponds to $a = 0$. The writing of the ladder operators j_+ and j_- in terms of h and v_{ra} constitutes a two-parameter polar decomposition of the Lie algebra of $SU(2)$. This decomposition is an alternative to the polar decompositions obtained independently in [24, 118, 119, 120, 121].

5.1 Appendix B: A quon approach to $su(2)$

Following [122], we define a quon algebra or q-deformed oscillator algebra for q a root of unity. The three operators a_-, a_+ and N_a such that

$$a_-a_+ - qa_+a_- = I \qquad [N_a, a_\pm]_- = \pm a_\pm \qquad (a_\pm)^k = 0 \qquad N_a^\dagger = N_a \tag{189}$$

where

$$q := \exp\left(\frac{2\pi i}{k}\right) \qquad k \in \mathbb{N} \setminus \{0, 1\} \tag{190}$$

define a quon algebra or q-deformed oscillator algebra denoted as $A_q(a_-, a_+, N_a)$. The operators a_- and a_+ are referred to as quon operators. The operators a_-, a_+ and N_a are called annihilation, creation and number operators, respectively.

Let us consider two commuting quon algebras $A_q(a_-, a_+, N_a) \equiv A_q(a)$ with $a = x, y$ corresponding to the same value of the deformation parameter q. Their generators satisfy equations (189) and (190) with $a = x, y$ and $[X, Y]_- = 0$ for any X in $A_q(x)$ and any Y in $A_q(y)$. Then, let us look for Hilbertian representations of $A_q(x)$ and $A_q(y)$ on the k-dimensional Hilbert spaces $\mathcal{F}(x)$ and $\mathcal{F}(y)$ spanned by the orthonormal bases $\{|n_1) : n_1 = 0, 1, \ldots, k-1\}$ and $\{|n_2) : n_2 = 0, 1, \ldots, k-1\}$, respectively. We easily obtain the representations defined by

$$\begin{aligned} &x_+|n_1) = |n_1+1) \qquad x_+|k-1) = 0 \\ &x_-|n_1) = [n_1]_q\,|n_1-1) \qquad x_-|0) = 0 \\ &N_x|n_1) = n_1|n_1) \end{aligned} \tag{191}$$

and

$$y_+|n_2) = [n_2+1]_q\,|n_2+1) \qquad y_+|k-1) = 0$$
$$y_-|n_2) = |n_2-1) \qquad y_-|0) = 0$$
$$N_y|n_2) = n_2|n_2) \tag{192}$$

for $A_q(x)$ and $A_q(y)$, respectively.

The cornerstone of this approach is to define the two linear operators

$$h := \sqrt{N_x\,(N_y+1)} \qquad v_{ra} := s_x s_y \tag{193}$$

with

$$s_x \;:=\; q^{a(N_x+N_y)/2}x_+ + e^{i\phi_r/2}\frac{1}{[k-1]_q!}(x_-)^{k-1} \tag{194}$$

$$s_y \;:=\; y_- q^{-a(N_x-N_y)/2} + e^{i\phi_r/2}\frac{1}{[k-1]_q!}(y_+)^{k-1} \tag{195}$$

where

$$a \in \mathbb{R} \qquad \phi_r = \pi(k-1)r \qquad r \in \mathbb{R}. \tag{196}$$

The operators h and v_{ra} act on the states

$$|n_1, n_2) := |n_1) \otimes |n_2) \tag{197}$$

of the k^2-dimensional space $\mathcal{F}_k := \mathcal{F}(x) \otimes \mathcal{F}(y)$. It is immediate to show that the action of h and v_{ra} on $\mathcal{F}_k$ is given by

$$h|n_1, n_2) = \sqrt{n_1(n_2+1)}|n_1, n_2) \qquad n_i = 0, 1, 2, \cdots, k-1 \qquad i = 1, 2 \tag{198}$$

and

$$v_{ra}|n_1, n_2) = q^{an_2}|n_1+1, n_2-1) \qquad n_1 \neq k-1 \qquad n_2 \neq 0 \tag{199}$$

$$v_{ra}|k-1, n_2) = e^{i\phi_r/2}q^{-a(k-1-n_2)/2}|0, n_2-1) \qquad n_2 \neq 0 \tag{200}$$

$$v_{ra}|n_1, 0) = e^{i\phi_r/2}q^{a(k+n_1)/2}|n_1+1, k-1) \qquad n_1 \neq k-1 \tag{201}$$

$$v_{ra}|k-1, 0) = e^{i\phi_r}|0, k-1). \tag{202}$$

The operators h and v_{ra} satisfy interesting properties: the operator h is Hermitian and the operator v_{ra} is unitary.

We now adapt the trick used by Schwinger [123] in his approach to angular momentum via a coupled pair of harmonic oscillators. This can be done by introducing two new quantum numbers J and M defined by

$$J := \frac{1}{2}(n_1 + n_2) \quad M := \frac{1}{2}(n_1 - n_2) \Rightarrow |JM\rangle := |J+M, J-M) = |n_1, n_2). \tag{203}$$

Note that

$$j := \frac{1}{2}(k-1) \tag{204}$$

is an admissible value for J. Then, let us consider the k-dimensional subspace $\epsilon(j)$ of the k^2-dimensional space $\mathcal{F}(x) \otimes \mathcal{F}(y)$ spanned by the basis $\{|j,m\rangle : m = j, j-1, \ldots, -j\}$. We guess that $\epsilon(j)$ is a space of constant angular momentum j. As a matter of fact, we can check that $\epsilon(j)$ is stable under h and v_{ra}. In fact, the action of the operators h and v_{ra} on the subspace $\varepsilon(j)$ of $\mathcal{F}_k$ can be described by

$$h|j,m\rangle = \sqrt{(j+m)(j-m+1)}|j,m\rangle \tag{205}$$

and

$$v_{ra}|j,m\rangle = \delta_{m,j} e^{i2\pi jr}|j,-j\rangle + (1 - \delta_{m,j})\, q^{(j-m)a}|j,m+1\rangle \tag{206}$$

in agreement with Eq. (183) and with the master equation (6).

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