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Variations on a theme of Heisenberg, Pauli and Weyl*

Maurice R Kibler

CNRS/IN2P3, UMR5822, Institute de Physique Nucleaire, Université Lyon 1, F-69622, Villeurbanne, France

E-mail: m.kibler@ipnl.in2p3.fr

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Abstract

The parentage between Weyl pairs, the generalized Pauli group and the unitary group is investigated in detail. We start from an abstract definition of the Heisenberg–Weyl group on the field $\mathbb{R}$ and then switch to the discrete Heisenberg–Weyl group or generalized Pauli group on a finite ring $\mathbb{Z}_d$. The main characteristics of the latter group, an abstract group of order d^3 noted P_d, are given (conjugacy classes and irreducible representation classes or equivalently Lie algebra of dimension d^3 associated with P_d). Leaving the abstract sector, a set of Weyl pairs in dimension d is derived from a polar decomposition of $SU(2)$ closely connected to angular momentum theory. Then, a realization of the generalized Pauli group P_d and the construction of generalized Pauli matrices in dimension d are revisited in terms of Weyl pairs. Finally, the Lie algebra of the unitary group $U(d)$ is obtained as a subalgebra of the Lie algebra associated with P_d. This leads to a development of the Lie algebra of $U(d)$ in a basis consisting of d^2 generalized Pauli matrices. In the case where d is a power of a prime integer, the Lie algebra of $SU(d)$ can be decomposed into $d - 1$ Cartan subalgebras.

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1. Introduction

The present paper is devoted to three major ingredients of quantum mechanics, namely the Heisenberg–Weyl group connected with Heisenberg commutation relations [1], the Pauli spin matrices [2] used in generalized angular momentum theory and the theory of unitary groups, and the pairs of Weyl [3] of relevance in finite quantum mechanics.

The Heisenberg–Weyl (or Weyl–Heisenberg or Heisenberg) group $HW(\mathbb{R})$, also called the Weyl group [4], is of central importance for the quantization process and its Lie algebra

* Dedicated to the memory of my teacher and friend Moshé Flato on the occasion of the tenth anniversary of his death.

turns out to be a basic building unit for quantum mechanics [5]. Note that the Lie algebra of $HW(\mathbb{R})$ should not be confused with the Weyl–Heisenberg algebra (or oscillator algebra spanned by the creation, annihilation and number operators) and its supersymmetric extensions W_k [6].

A discrete restriction $HW(\mathbb{Z}_d)$ of $HW(\mathbb{R})$, corresponding to the replacement of the infinite field $\mathbb{R}$ by a finite ring $\mathbb{Z}_d \equiv \mathbb{Z}/d\mathbb{Z}$, yields a group of order d^3 (d arbitrary in $\mathbb{N}\backslash\{0, 1\}$). This group was introduced by Šťovíček and Tolar [7] in connection with quantum mechanics in a discrete spacetime, by Balian and Itzykson in connection with finite quantum mechanics [8], and by Patera and Zassenhaus [9] in connection with gradings of simple Lie algebras of type A_{n-1}. The case where the ring $\mathbb{Z}_d$ is replaced by a finite (Galois) field $\mathbb{F}_q$ gave rise to several mathematical studies [10, 11]. The discrete Heisenberg–Weyl group, also known as the generalized Pauli group, plays a central role in quantum information, cf the interest of Galois fields in finite quantum mechanics [12] and, consequently, in quantum information and quantum computation. In this connection, a finite Heisenberg–Weyl group was used for a description of phase oscillations of EPR states [13].

What is the relationship between the Heisenberg–Weyl group and Weyl pairs? First of all, a definition of a Weyl pair is in order. A Weyl pair (X, Z) in d dimensions is a pair of d-dimensional unitary matrices X and Z that satisfy the q-commutation relation $XZ - qZX = 0$ and the cyclic relations $X^d = Z^d = I$ (I standing here for the unitary matrix), where q is a primitive root of unity with $q^d = 1$. The concept of a pair of Weyl, initially introduced for dealing with quantum dynamical systems in finite dimension [3], was used for the construction of unitary bases in finite-dimensional Hilbert spaces [14] and (independently) for the factorization of the secular equation corresponding to finite-dimensional eigenvalue problems [15]. In the last 20 years, the notion of Weyl pairs was used for the construction of *generalized* Pauli matrices in domains as different as graded Lie algebras and quantum information.

The *usual* Pauli matrices σ_x, σ_y and σ_z are useful for the representation theory of the Lie group $SU(2)$. Therefore, a natural extension of the Pauli matrices resulted in the 1960s from the interest of the group $SU(3)$ for the classification of elementary particles [16]. This gave rise to the Gell-Mann matrices and the Okubo matrices. Further extensions of the Pauli matrices came out of the introduction of the group $SU(4)$ for charmed particles [17] and of the group $SU(5)$ for a grand unified theory of quarks and leptons [18]. The Gell-Mann lambda matrices for $SU(3)$ and their extension to Cartan bases for $SU(d)$ undoubtedly constitute a systematic extension of the ordinary Pauli matrices. This statement is particularly justified as far as the tensor structure (involving symmetric and antisymmetric tensors) of their algebra is concerned [19]. We shall deal in this paper with another extension of the Pauli matrices in d dimensions which turns out to be of special interest in the case where d is a power of a prime integer. Indeed, generalized Pauli matrices can be constructed in a systematic way by making use of Weyl pairs. In this direction let us mention the pioneer work of Patera and Zassenhaus [9]. In the last two decades, the construction of generalized Pauli spin matrices has been extensively used in the theory of semi-simple Lie algebras, in quantum mechanics (complete state determination, reconstruction of a density matrix and discrete Wigner functions), in quantum information and quantum computation (mutually unbiased bases, unitary error bases, quantum error correction, random unitary channels, mean king's problem, positive operator valued measures and quantum entanglement), and in the study of modified Bessel functions (see for instance [8, 9, 20–32]).

From a group-theoretical point of view, the d-dimensional generalized Pauli matrices may serve to construct a generalized Pauli group in d dimensions, a group generalizing the ordinary Pauli group spanned by the ordinary Pauli matrices (see [7–12, 21, 24, 33–42]). In fact, this group is nothing but the discrete Heisenberg–Weyl group $HW(\mathbb{Z}_d)$. This generalized Pauli group has been recently the object of numerous studies partly in connection with the Clifford or Jacobi group [34, 36–38] as well as graph-theoretical and finite-geometrical analyses of the generalized Pauli operators [41, 42].

The object of this work is to further study the link between the Heisenberg–Weyl group, the Weyl pairs, the generalized Pauli matrices and the generalized Pauli group and to revisit their interest for unitary groups. We shall start with an abstract definition of the Heisenberg–Weyl group, pass to an abstract version of $HW(\mathbb{Z}_d)$ and briefly study it. Then, we shall deal with the introduction of Weyl pairs from a polar decomposition of the Lie algebra $su(2)$ and we shall use them for finding a realization of $HW(\mathbb{Z}_d)$ isomorphic to the generalized Pauli group in d dimensions. Finally, some of the generators of the Pauli group in d dimensions shall be used for constructing the Lie algebra $su(d)$ of $SU(d)$ in a basis that is especially adapted, when d is a power of a prime integer, to a decomposition of $su(d)$ into a direct sum of $d + 1$ Cartan subalgebras.

2. The Heisenberg–Weyl group

2.1. The Lie group $HW(\mathbb{R})$

We start with an abstract definition of the Heisenberg–Weyl group $HW(\mathbb{R})$. Let us consider the set of triplets,

$$S := \{(x, y, z) : x, y, z \in \mathbb{R}\}. \tag{1}$$

The set S can be equipped with the internal composition law $S \times S \to S$ defined trough

$$(x, y, z)(x', y', z') := (x + x' - zy', y + y', z + z'). \tag{2}$$

It is clear that the set S is a group with respect to the law (2). We denote $HW(\mathbb{R})$ this group and call it the Heisenberg–Weyl group (for evident reasons to be given below) on the infinite field $\mathbb{R}$. More precisely, we have the following result.

Proposition 1. *The group $HW(\mathbb{R})$ is a noncompact Lie group of order 3. This non-Abelian group is nilpotent (hence solvable) with a nilpotency class equal to 2.*

Proof. The proof is trivial. Let us simply mention that the nilpotency of $HW(\mathbb{R})$ follows by repeated use of the commutator

$$[(x', y', z'), (x, y, z)] = (zy' - yz', 0, 0) \tag{3}$$

of the elements (x', y', z') and (x, y, z) of the group $HW(\mathbb{R})$. Equation (3) shows that (x, y, z) and (x', y', z') commute if and only if $zy' - yz' = 0$. □

In the terminology of Wigner [43], the group $HW(\mathbb{R})$ is not ambivalent (ambivalent means that each conjugacy class contains its inverse elements). Indeed, since

$$(x, y, z)^{-1} = (-x - yz, -y, -z) \tag{4}$$

and

$$(x', y', z')(x, y, z)(x', y', z')^{-1} = (x + zy' - yz', y, z) \tag{5}$$

it is evident that only the class $\mathcal{C}_{(0,0,0)} = \{(0, 0, 0)\}$ of the identity element $(0, 0, 0)$ is ambivalent.

2.2. The Lie algebra of $HW(\mathbb{R})$

We may ask why to call $HW(\mathbb{R})$ the Heisenberg–Weyl group? The following result clarifies this point.

Proposition 2. *A set of infinitesimal generators of $HW(\mathbb{R})$ is*

$$\mathcal{H} = \frac{1}{\mathrm{i}}\frac{\partial}{\partial x} \qquad \mathcal{Q} = \frac{1}{\mathrm{i}}\frac{\partial}{\partial y} \qquad \mathcal{P} = \frac{1}{\mathrm{i}}\left(\frac{\partial}{\partial z} - y\frac{\partial}{\partial x}\right). \tag{6}$$

This set of generators satisfies the formal commutation relations,

$$[Q, P]_- = \mathrm{i}H \qquad [P, H]_- = 0 \qquad [H, Q]_- = 0 \tag{7}$$

with $H = \mathcal{H}$, $Q = \mathcal{Q}$ and $P = \mathcal{P}$. The Lie algebra $hw(\mathbb{R})$ of $HW(\mathbb{R})$, with the Lie brackets (7), is a three-dimensional nilpotent (hence solvable) Lie algebra with nilpotency class 2.

Proof. The proof easily follows by working in a neighbourhood of the identity $(0, 0, 0)$ of $HW(\mathbb{R})$ and by considering the series $w^1 = hw(\mathbb{R})$, $w^2 = [w^1, w^1]_-$, $w^3 = [w^1, w^2]_-, \ldots,$ where $[A, B]_-$ refers here to the set of commutators $[\alpha, \beta]_-$ with $\alpha \in A$ and $\beta \in B$. □

The connection with the Heisenberg commutation relations is clearly emphasized by (7). This constitutes a partial justification for calling $HW(\mathbb{R})$ the Heisenberg–Weyl group on $\mathbb{R}$. The Lie algebra $hw(\mathbb{R})$ was derived from a matrix group [4] and studied at length from the point of view of quantum mechanics [5]. This algebra admits infinite-dimensional representations by Hermitian matrices. In particular, we have the infinite-dimensional harmonic oscillator representation which is associated with the operator realization $H = \mathcal{H}_{ho} := \hbar 1$, $Q = \mathcal{Q}_{ho} := x$ and $P = \mathcal{P}_{ho} := \frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial x}$, where $\hbar$ is the rationalized Planck constant. On the other side, we may expect to have finite-dimensional representations of $hw(\mathbb{R})$ at the price to abandon the Hermitian character of the representation matrices.

As an example, we have the three-dimensional representation of $hw(\mathbb{R})$ defined by $H = H_3$, $Q = Q_3$ and $P = P_3$ with

$$H_3 := \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ \mathrm{i} & 0 & 0 \end{pmatrix} \qquad Q_3 := \begin{pmatrix} 0 & 0 & 0 \\ \mathrm{i} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \qquad P_3 := \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & -\mathrm{i} & 0 \end{pmatrix}. \tag{8}$$

We can look for the matrix Lie group which corresponds to the Lie algebra spanned by the set $\{H_3, Q_3, P_3\}$. This yields proposition 3.

Proposition 3. *The exponentiation*

$$M(x, y, z) := \exp[\mathrm{i}(xH_3 + yQ_3 + zP_3)] \tag{9}$$

leads to

$$M(x, y, z) = \begin{pmatrix} 1 & 0 & 0 \\ -y & 1 & 0 \\ -x - \frac{1}{2}yz & z & 1 \end{pmatrix}. \tag{10}$$

The matrices $M(x, y, z)$ satisfy the composition law

$$M(x, y, z)M(x', y', z') = M\left(x + x' + \tfrac{1}{2}zy' - \tfrac{1}{2}yz', y + y', z + z'\right) \tag{11}$$

so that the set $S' := \{M(x, y, z) : x, y, z \in \mathbb{R}\}$ endowed with the law (11) is a group isomorphic to $HW(\mathbb{R})$.

Proof. A simple expansion of (9) where H_3, Q_3 and P_3 are given by (8) yields (10). The isomorphism follows from the bijection $S \to S' : (x, y, z) \mapsto M\left(-x - \frac{1}{2}yz, -y, -z\right)$.

Note that the matrix form (10) corresponds to two other sets $\{\mathcal{H}_\pm, \mathcal{Q}_\pm, \mathcal{P}_\pm\}$ of infinitesimal generators of $HW(\mathbb{R})$, namely

$$\mathcal{H}_\pm = \pm \mathrm{i}\frac{\partial}{\partial x} \qquad \mathcal{Q}_\pm = \pm \mathrm{i}\left(\frac{\partial}{\partial y} \mp \frac{1}{2}z\frac{\partial}{\partial x}\right) \qquad \mathcal{P}_\pm = \pm \mathrm{i}\left(\frac{\partial}{\partial z} \pm \frac{1}{2}y\frac{\partial}{\partial x}\right) \tag{12}$$

which satisfies (7) with $H = \mathcal{H}_\pm$, $Q = \mathcal{Q}_\pm$ and $P = \mathcal{P}_\pm$ (cf [4, 5]). □

3. The Pauli group

3.1. The abstract Pauli group

3.1.1. The group P_d. We shall be concerned in this section with a discretization of the Heisenberg–Weyl group $HW(\mathbb{R})$. A trivial discretization of $HW(\mathbb{R})$ can be obtained by replacing the field $\mathbb{R}$ by the infinite ring $\mathbb{Z}$. This leads to an infinite-dimensional discrete group $HW(\mathbb{Z})$. A further possibility is to replace $\mathbb{R}$ by the finite ring $\mathbb{Z}_d \equiv \mathbb{Z}/d\mathbb{Z}$ where d is arbitrary in $\mathbb{N}\backslash\{0, 1\}$. (In the case where d is a prime p or a power of a prime p^e with $e \in \mathbb{N}\backslash\{0, 1\}$, the finite ring $\mathbb{Z}/d\mathbb{Z}$ can be replaced by the Galois field $\mathbb{F}_p$ or $\mathbb{F}_{p^e}$.) This yields a finite group $HW(\mathbb{Z}_d)$ which can be described by the following result.

Proposition 4. *The set*

$$S_d := \{(a, b, c) : a, b, c \in \mathbb{Z}_d\} \tag{13}$$

with the internal composition law $S_d \times S_d \to S_d$ defined through

$$(a, b, c)(a', b', c') := (a + a' - cb', b + b', c + c') \tag{14}$$

(where from now on the addition is understood modulo d) is a finite group of order d^3. This non-Abelian group $HW(\mathbb{Z}_d)$, noted P_d for short, is nilpotent (hence solvable) with a nilpotency class equal to 2.

Proof. The proof of proposition 4 is elementary. Note simply that we have the canonical decomposition

$$(a, b, c) = (a, 0, 0)(0, b, 0)(0, 0, c) \tag{15}$$

for any element (a, b, c) of P_d and that two elements (a, b, c) and (a', b', c') of P_d commute if and only if $cb' - bc' = 0 \pmod d$. □

We call the abstract group P_d the *(generalized) Pauli group* in d dimensions. At this stage, we can give the main reason for associating Heisenberg, Pauli and Weyl in the title of the present paper. As a point of fact, the discretization of the group $HW(\mathbb{R})$, a group associated with the *Heisenberg commutation relations*, via the replacement $\mathbb{R} \to \mathbb{Z}/d\mathbb{Z}$ gives rise to the group P_d, a group which can be realized in terms of *generalized Pauli matrices*, which in turn can be constructed in terms of *Weyl pairs* (see below).

3.1.2. Some subgroups of P_d. Among the subgroups of P_d, we can mention proper subgroups of order d and d^2 (there are no other proper subgroups if d is a prime integer). We simply list below the subsets of S_d, which together with the law (14), provide us with some important subgroups of P_d.

- The set $\{(a, 0, 0) : a \in \mathbb{Z}_d\}$ gives an invariant Abelian subgroup of P_d of order d isomorphic to the cyclic group $\mathbb{Z}_d$. In fact, this subgroup is the centrum $Z(P_d)$ of P_d and $P_d/Z(P_d)$ is isomorphic to $\mathbb{Z}_d \otimes \mathbb{Z}_d$.
- The set $\{(0, b, 0) : b \in \mathbb{Z}_d\}$ gives an Abelian subgroup of P_d of order d isomorphic to $\mathbb{Z}_d$.

- Similarly, the set $\{(0, 0, c) : c \in \mathbb{Z}_d\}$ gives also an Abelian subgroup of P_d of order d isomorphic to $\mathbb{Z}_d$.
- The sets $\{(a, b, 0) : a, b \in \mathbb{Z}_d\}$ and $\{(a, 0, c) : a, c \in \mathbb{Z}_d\}$ give two invariant Abelian subgroups of P_d of order d^2 isomorphic to $\mathbb{Z}_d \otimes \mathbb{Z}_d$.
- Finally, the set $\{(a, b, b) : a, b \in \mathbb{Z}_d\}$ give an invariant Abelian subgroup of P_d of order d^2.

3.1.3. Conjugacy classes of P_d. The conjugacy classes of P_d readily follow from

$$(a', b', c')(a, b, c)(a', b', c')^{-1} = (a + cb' - bc', b, c) \tag{16}$$

with addition modulo d. This can be precised by the following result.

Proposition 5. *The group P_d has $d(d + 1) - 1$ conjugacy classes: d classes containing each one element and $d^2 - 1$ classes containing each d elements.*

Proof. It can be checked that the class $\mathcal{C}_{(a,0,0)}$ of $(a, 0, 0)$ is $\mathcal{C}_{(a,0,0)} = \{(a, 0, 0)\}$; therefore, there are d classes with one element. Furthermore, the class $\mathcal{C}_{(a,b,c)}$ of (a, b, c), with the case $b = c = 0$ excluded, is $\mathcal{C}_{(a,b,c)} = \{(a', b, c) : a' \in \mathbb{Z}_d\}$; this yields $d^2 - 1$ classes with d elements. We note that the group P_d is not ambivalent in general. □

The case $d = 2$ is very special since the group P_2 of order 8 is ambivalent like the group Q of ordinary quaternions, another group of order 8. Not all the subgroups of P_2 are invariant. Therefore, the group P_2 is not isomorphic to Q (for which all subgroups are invariant). Indeed, it can be proved that P_2 is isomorphic to the group of hyperbolic quaternions associated with the Cayley–Dickson algebra $A(c_1, c_2)$ with $(c_1, c_2) \neq (-1, -1)$ defined in [44]. In this respect, the Pauli group P_2 defined in this work differs from the Pauli group in $d = 2$ dimensions considered by some authors, a group isomorphic to the group Q of ordinary quaternions. Let P_2' be this latter Pauli group. It consists of the elements $\sigma := \pm\sigma_0, \pm i\sigma_x, \pm i\sigma_y, \pm i\sigma_z$ (where σ_0 is the 2×2 unit matrix). Let us also mention that an extension of the group P_2' is used in quantum computation [45] (see also [33, 42]). This extension, say P_2'', is obtained from a doubling process: the group P_2'' consists of the elements of the set $\{\sigma, i\sigma : \sigma \in P_2'\}$. Thus, the conjugation classes and the irreducible representation classes of P_2'' trivially follow from those of P_2'.

3.1.4. Irreducible representations of P_d. The duality between conjugacy classes and classes of irreducible representations leads to the following result.

Proposition 6. *The group P_d has $d(d + 1) - 1$ classes of irreducible representations: d^2 classes of dimension 1 and $d - 1$ classes of dimension d.*

Proof. It is sufficient to apply the Burnside–Wedderburn theorem. □

As a corollary of propositions 5 and 6, the difference between the order of P_d and its number of classes (conjugacy classes or irreducible representation classes) is odd if $d = 2k$ ($k \in \mathbb{N}^*$), or a multiple of 16 if $d = 4k + 3$ ($k \in \mathbb{N}$) or a multiple of 32 if $d = 4k + 1$ ($k \in \mathbb{N}^*$). (For an arbitrary finite group of odd order, the difference is a multiple of 16.) Furthermore, the number of elements of P_d which commute with a given element (a, b, c) of P_d is d^3 or a multiple of d^2 according to whether the order of the conjugation class containing (a, b, c) is 1 or d; see [41] for a more elaborated result, in the form of a universal formula, and its interpretation in terms of the fine structure of the projective line defined over the modular ring $\mathbb{Z}_d$. Note that propositions 5 and 6 are in agreement with the results obtained [10] in the case where d is a power of a prime integer corresponding to the replacement of the ring $\mathbb{Z}_d$ by the Galois field $\mathbb{F}_d$.

3.1.5. A Lie algebra associated with P_d. We close the study of the abstract group P_d with a result devoted to the association of P_d with a Lie algebra of dimension d^3. Let us consider the group algebra (or Frobenius algebra) $F(P_d)$ of the generalized Pauli group P_d. Such an algebra is an associative algebra over the field $\mathbb{C}$. By applying the process developed by Gamba [46], we can construct from $F(P_d)$ a Lie algebra, which we shall denote as p_d, by taking

$$\langle(a, b, c), (a', b', c')\rangle := (a + a' - cb', b + b', c + c') - (a + a' - bc', b + b', c + c') \tag{17}$$

for the Lie bracket of (a, b, c) and (a', b', c'). (The right-hand side of (17) is defined in $F(P_d)$.) The set S_d constitutes a basis both for the Frobenius algebra $F(P_d)$ and the Lie algebra p_d (S_d is a Chevalley basis for p_d). As a further result, we have the following proposition.

Proposition 7. *The Lie algebra p_d of dimension d^3, associated with the finite group P_d of order d^3, is not semi-simple. It can be decomposed as the direct sum*

$$p_d = \bigoplus_{1}^{d^2} u(1) \bigoplus_{1}^{d-1} u(d), \tag{18}$$

which contains d^2 Lie algebras isomorphic to $u(1)$ and $d - 1$ Lie algebras isomorphic to $u(d)$.

Proof. The proof can be achieved by passing from the Chevalley basis of p_d, inherent to (17), to the basis generated by the idempotent (or projection) operators and nilpotent (or ladder) operators, defined in $F(P_d)$, associated with the classes of irreducible representations of P_d. Equation (18) is reminiscent of the fact that P_d has d^2 irreducible representation classes of dimension 1 and $d - 1$ irreducible representation classes of dimension d. □

3.2. A realization of the Pauli group

3.2.1. Polar decomposition of $SU(2)$. Let $\mathcal{E}(2j + 1)$, with $2j \in \mathbb{N}$, be a $(2j + 1)$-dimensional Hilbert space of constant angular momentum j. Such a space is spanned by the set $\{|j, m\rangle : m = j, j - 1, \ldots, -j\}$, where $|j, m\rangle$ is an eigenstate of the square j^2 and the z-component j_z of a generalized angular momentum [47]. The state vectors $|j, m\rangle$ are taken in an orthonormalized form, i.e., the inner product $\langle j, m|j', m'\rangle$ is equal to $\delta_{m,m'}$.

Following the approach of [48], we define the linear operator v_{ra} via

$$v_{ra}|j, m\rangle = (1 - \delta_{m,j})q^{(j-m)a}|j, m + 1\rangle + \delta_{m,j}\, \mathrm{e}^{\mathrm{i}2\pi jr}|j, -j\rangle, \tag{19}$$

where

$$r \in \mathbb{R} \qquad a \in \mathbb{R} \qquad q = \exp\left(\frac{2\pi \mathrm{i}}{2j + 1}\right). \tag{20}$$

The matrix V_{ra} of the operator v_{ra} in the spherical basis

$$b_s := \{|j, j\rangle, |j, j - 1\rangle, \ldots, |j, -j\rangle\} \tag{21}$$

reads

$$V_{ra} = \begin{pmatrix} 0 & q^a & 0 & \cdots & 0 \\ 0 & 0 & q^{2a} & \cdots & 0 \\ \vdots & \vdots & \vdots & \cdots & \vdots \\ 0 & 0 & 0 & \cdots & q^{2ja} \\ \mathrm{e}^{\mathrm{i}2\pi jr} & 0 & 0 & \cdots & 0 \end{pmatrix}. \tag{22}$$

The matrix V_{ra} constitutes a generalization of the matrix V_a introduced in [49] (see also [40]).

The shift operator v_{ra} takes its origin in the study of the Lie algebra of $SU(2)$ in a nonstandard basis with the help of two quon algebras describing q-deformed oscillators [50]. The operator v_{ra} is unitary. Furthermore, it is cyclic in the sense that

$$(v_{ra})^{2j+1} = \mathrm{e}^{\mathrm{i}2\pi j(a+r)} I, \tag{23}$$

where I is the identity. The eigenvalues and eigenvectors of v_{ra} are given by the following result.

Proposition 8. *The spectrum of the operator v_{ra} is nondegenerate. For fixed j, r and a, it follows from*

$$v_{ra}|j\alpha; ra\rangle = q^{j(a+r)-\alpha}|j\alpha; ra\rangle, \tag{24}$$

where

$$|j\alpha; ra\rangle = \frac{1}{\sqrt{2j+1}} \sum_{m=-j}^{j} q^{(j+m)(j-m+1)a/2-jmr+(j+m)\alpha}|j, m\rangle \tag{25}$$

for $\alpha = 0, 1, \ldots, 2j$.

A second linear operator is necessary to define a polar decomposition of $SU(2)$. Let us introduce the Hermitian operator h through

$$h|j, m\rangle = \sqrt{(j+m)(j-m+1)}|j, m\rangle. \tag{26}$$

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

$$j_+ = hv_{ra} \qquad j_- = v_{ra}^\dagger h \qquad j_z = \tfrac{1}{2}\left(h^2 - v_{ra}^\dagger h^2 v_{ra}\right) \tag{27}$$

satisfy the ladder equations

$$j_+|j, m\rangle = q^{+(j-m+s-1/2)a}\sqrt{(j-m)(j+m+1)}|j, m+1\rangle \tag{28}$$

$$j_-|j, m\rangle = q^{-(j-m+s+1/2)a}\sqrt{(j+m)(j-m+1)}|j, m-1\rangle \tag{29}$$

and the eigenvalue equation

$$j_z|j, m\rangle = m|j, m\rangle \tag{30}$$

where $s = 1/2$. (Note that there is one misprint in the corresponding relations of [40].) Therefore, we have the following result.

Proposition 9. *The operators j_+, j_- and j_z satisfy the commutation relations*

$$[j_z, j_+] = +j_+ \qquad [j_z, j_-] = -j_- \qquad [j_+, j_-] = 2j_z \tag{31}$$

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

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 (an *a priori* real parameter to be restricted to integer values in what follows); 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 $SU(1, 1)$ (or $SU(2)$ over the complex field). This decomposition is an alternative to the polar decompositions obtained independently in [51, 52].

3.2.2. Weyl pairs. The linear operator $x := v_{00}$ such that (cf (19))

$$x|j,m\rangle = (1 - \delta_{m,j})|j,m+1\rangle + \delta_{m,j}|j,-j\rangle \tag{32}$$

has the spectrum $(1, q, \ldots, q^{2j})$ on $\mathcal{E}(2j+1)$. Therefore, the matrix $X := V_{00}$ of x on the basis b_s is unitarily equivalent to

$$Z := \operatorname{diag}(1, q, \ldots, q^{2j}). \tag{33}$$

The linear operator z corresponding to the matrix Z can be defined by

$$z|j,m\rangle = q^{j-m}|j,m\rangle. \tag{34}$$

The two isospectral operators x (a cyclic shift operator) and z (a cyclic phase operator) are unitary and constitute a pair of Weyl (x, z) since they obey the q-commutation relation

$$xz - qzx = 0 \tag{35}$$

(or $XZ - qZX = 0$ in matrix form). These two operators are connected via

$$x = f^{\dagger}zf \Leftrightarrow z = fxf^{\dagger}, \tag{36}$$

where f is the Fourier operator such that

$$f|j,m\rangle = \frac{1}{\sqrt{2j+1}} \sum_{m'=-j}^{j} q^{-(j-m)(j-m')}|j,m'\rangle. \tag{37}$$

The operator f is unitary and satisfies

$$f^4 = 1 \tag{38}$$

(see [52] for a general treatment of Fourier operators on finite-dimensional Hilbert spaces). Let F be the matrix of the linear operator f in the basis b_s. Indeed, F is a circulant matrix. Note that the reduction 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 $Z = FXF^{\dagger}$.

We conclude that the polar decomposition of $SU(2)$ described in section 3.2.1 provides us with an alternative derivation of the Weyl pair (X, Z). Of course, other pairs of Weyl (V_{ra}, Z), corresponding to (v_{ra}, z) with the property $v_{ra}z - qzv_{ra} = 0$, can be derived by replacing v_{00} by v_{ra}. Note that $v_{ra} = v_{r0}z^a$.

3.2.3. Weyl pairs and Pauli group. Let us define the d^3 operators

$$w_{abc} := q^a x^b z^c \qquad a, b, c \in \mathbb{Z}_d. \tag{39}$$

The action of w_{abc} on the Hilbert space $\mathcal{E}(2j+1)$ is described by

$$w_{abc}|j,m\rangle = q^{a+(j-m)c}|j,m+b\rangle, \tag{40}$$

where $m + b$ is understood modulo $2j + 1$. The operators w_{abc} are unitary and satisfy

$$\operatorname{Tr}_{\mathcal{E}(2j+1)}\left(w_{abc}^{\dagger}w_{a'b'c'}\right) = q^{a'-a}d\delta_{b,b'}\delta_{c,c'} \tag{41}$$

with $d := 2j + 1$. In addition, we have the following central result.

Proposition 10. *The set $W_d := \{w_{abc} : a, b, c \in \mathbb{Z}_d\}$ endowed with the multiplication of operators is a group isomorphic to the Pauli group P_d. Thus, the group P_d is isomorphic to a subgroup of $U(d)$ for d even or $SU(d)$ for d odd.*

Proof. The proof is immediate: it is sufficient to consider the bijection $W_d \to S_d : w_{abc} \mapsto (a, b, c)$, to use repeatedly (35) or (40), and to note that the matrix of w_{abc} in the basis b_s

belongs to $U(d)$ for d even and to $SU(d)$ for d odd. As a consequence, the Lie bracket $\langle(a, b, c), (a', b', c')\rangle$, see (17), corresponds to the commutator $[w_{abc}, w_{a'b'c'}]_-$ so that the Lie algebra p_d associated with the finite group P_d corresponds to the commutation relations

$$[w_{abc}, w_{a'b'c'}]_- = w_{\alpha\beta\gamma} - w_{\alpha'\beta'\gamma'} \tag{42}$$

with $\alpha = a + a' - cb'$, $\beta = b + b'$, $\gamma = c + c'$, $\alpha' = \alpha + cb' - bc'$, $\beta' = \beta$ and $\gamma' = \gamma$. □

3.2.4. Weyl pairs and infinite-dimensional Lie algebra. We close this section by mentioning another interest of Weyl pairs (v_{ra}, z). By defining the operators

$$t_m = q^{\frac{1}{2}m_1m_2} v_{ra}^{m_1} z^{m_2} \qquad m = (m_1, m_2) \in \mathbb{N}^{*2} \tag{43}$$

we easily obtain the following result.

Proposition 11. *The commutator of the operators t_m and t_n reads*

$$[t_m, t_n]_- = 2\mathrm{i} \sin\left(\frac{\pi}{2j+1} m \wedge n\right) t_{m+n}, \tag{44}$$

where

$$m \wedge n = m_1n_2 - m_2n_1 \qquad m + n = (m_1 + n_1, m_2 + n_2). \tag{45}$$

Therefore, the linear operators t_m span an infinite-dimensional Lie algebra.

The so-obtained Lie algebra is isomorphic to the algebra introduced in [53]. The latter result parallels those derived, on the one hand, from a study of k-fermions and of the Dirac quantum phase operator through a q-deformation of the harmonic oscillator [54] and, on the other hand, from an investigation of correlation measure for finite quantum systems [55].

3.3. Mutually unbiased bases

We now briefly establish contact with quantum information. For this purpose, let us introduce the notation

$$k := j - m \qquad |k\rangle := |j, m\rangle \qquad d := 2j + 1. \tag{46}$$

Thus, the angular momentum basis $\{|j, j\rangle, |j, j-1\rangle, \ldots, |j, -j\rangle\}$ of the finite-dimensional Hilbert space $\mathcal{E}(2j + 1)$ reads $\{|0\rangle, |1\rangle, \ldots, |d-1\rangle\}$. Let us note

$$B_d := \{|k\rangle : k = 0, 1, \ldots, d-1\} \tag{47}$$

the latter orthonormal basis, known as the computational basis in quantum information and quantum computation. From now on, the real number a occurring in (25) shall be restricted to take the values $a = 0, 1, \ldots, d-1$.

From equation (25), we can write the eigenvectors $|a\alpha\rangle := |j\alpha; 0a\rangle$ of the operator v_{0a} as

$$|a\alpha\rangle = \frac{1}{\sqrt{d}} \sum_{k=0}^{d-1} q^{(d-k-1)(k+1)a/2-(k+1)\alpha} |k\rangle, \tag{48}$$

where, for fixed a ($a = 0, 1, \ldots, d-1$), the index α takes the values $0, 1, \ldots, d-1$. Note that

$$B_{0a} := \{|a\alpha\rangle : \alpha = 0, 1, \ldots, d-1\} \tag{49}$$

is another orthonormal basis of $\mathcal{E}(d)$.

Proposition 8 can be transcribed in matrix form by using the generators $E_{x,y}$ of $\mathrm{GL}(d, \mathbb{C})$ (see also [40] where a different normalization is used). The $d \times d$ matrix $E_{x,y}$ (with $x, y \in \mathbb{Z}_d$) is defined by its matrix elements

$$(E_{x,y})_{kl} = \delta_{k,x}\delta_{l,y} \qquad k, l \in \mathbb{Z}_d. \tag{50}$$

Therefore, the matrix V_{0a} of the operator v_{0a} in the computational basis B_d is

$$V_{0a} = E_{d-1,0} + \sum_{k=0}^{d-2} q^{(k+1)a} E_{k,k+1}. \tag{51}$$

The eigenvectors $\varphi(a\alpha)$ of the matrix V_{0a} are expressible in terms of the $d \times 1$ column vectors e_x (with $x \in \mathbb{Z}_d$) defined via

$$(e_x)_{k0} = \delta_{k,x} \qquad k \in \mathbb{Z}_d. \tag{52}$$

In fact, we can check that

$$\varphi(a\alpha) = \frac{1}{\sqrt{d}} \sum_{k=0}^{d-1} q^{(d-k-1)(k+1)a/2-(k+1)\alpha} e_k \tag{53}$$

satisfies the eigenvalue equation

$$V_{0a}\varphi(a\alpha) = q^{(d-1)a/2-\alpha}\varphi(a\alpha). \tag{54}$$

Furthermore, the $d \times d$ matrix

$$H_a := \sum_{\alpha=0}^{d-1}\sum_{k=0}^{d-1} q^{(d-k-1)(k+1)a/2-(k+1)\alpha} E_{k,\alpha} \tag{55}$$

reduces the endomorphism associated with V_{0a}. In other words, we have

$$H_a^{\dagger} V_{0a} H_a = q^{(d-1)a/2} d \sum_{\alpha=0}^{d-1} q^{-\alpha} E_{\alpha,\alpha}. \tag{56}$$

Note that H_a is a generalized Hadamard matrix in the sense that

$$H_a^{\dagger} H_a = dI \tag{57}$$

and the modulus of any element of H_a is unity. Observe that the Fourier matrix F can be written as

$$F = (H_0 S)^{\dagger} \qquad S := \frac{1}{\sqrt{d}} \sum_{\beta=0}^{d-1} E_{\beta,d-\beta}, \tag{58}$$

where S acts as a permutation matrix normalized by $\frac{1}{\sqrt{d}}$.

As an application of (48) or (53) to mutually unbiased bases, we have the following result (see also [40, 49]).

Proposition 12. *In the case where $d = p$ is a prime integer, the bases B_{0a} for $a = 0, 1, \ldots, p-1$ together with the computational basis B_d constitute a complete set of $p + 1$ mutually unbiased bases.*

Proof. According to the definition of mutually unbiased bases [56], we need to prove that

$$|\langle k|a\alpha\rangle| = \frac{1}{\sqrt{p}} \tag{59}$$

and

$$|\langle a\alpha|b\beta\rangle| = \delta_{\alpha,\beta}\delta_{a,b} + \frac{1}{\sqrt{p}}(1-\delta_{a,b}) \tag{60}$$

for any value of a, b, α, β and k in $\mathbb{Z}_d$. Equation (59) simply follows from (48) and equation (60) was proved in [40] by making use of generalized quadratic Gauss sums. □

The interest of (48) or (53) with $d = p$, p prime (including the case $p = 2$), is that the p^2 vectors corresponding to the p mutually unbiased bases besides the computational basis are obtainable from one single formula that is easily codable on a computer (the single formula corresponds to the diagonalization of only one matrix, namely the matrix V_{0a} where a can take the values $a = 0, 1, \ldots, p-1$). In matrix form, the p mutually unbiased bases besides the computational basis are given by the columns of the Hadamard matrices matrices H_a ($a = 0, 1, \ldots, p-1$).

Going back to d arbitrary, we can check that the bases B_{00}, B_{01} and B_d constitute a set of three mutually unbiased bases. Therefore, we recover a well-known result according to which there exists a minimum of three mutually unbiased bases when d is not a prime power.

4. Weyl pairs and unitary group

In this section, we shall focus our attention on one of the $u(d)$ subalgebras of p_d. Such a subalgebra can be constructed from a remarkable subset of $\{w_{abc} : a, b, c \in \mathbb{Z}_d\}$. This subset is made of generalized Pauli operators. It is generated by the Weyl pair (x, z) or (X, Z) in matrix form.

4.1. Generalized Pauli operators

Following the work by Patera and Zassenhaus [9], let us define the operators

$$u_{ab} := w_{0ab} = x^a z^b \qquad a, b \in \mathbb{Z}_d. \tag{61}$$

The operators u_{ab} are unitary. Note that the matrices $X^a Z^b$ of the operators u_{ab} in the basis b_s belong to the unitary group $U(d)$ for d even or to the special unitary group $SU(d)$ for d odd. The d^2 operators u_{ab} shall be referred to as generalized Pauli operators in dimension d. It should be mentioned that matrices corresponding to operators of type (61) were first introduced long-time ago by Sylvester [57] in order to solve the matrix equation $PX = XQ$; in addition, such matrices were used by Morris [58] to define generalized Clifford algebras in connection with quaternion algebras and division rings. The operators u_{ab} satisfy the two following properties which are direct consequences of (41) and (42).

Proposition 13. *The set $\{u_{ab} : a, b \in \mathbb{Z}_d\}$ is an orthogonal set with respect to the Hilbert–Schmidt inner product. More precisely,*

$$\mathrm{Tr}_{\mathcal{E}(2j+1)}\left(u_{ab}^{\dagger}u_{a'b'}\right) = d\delta_{a,a'}\delta_{b,b'}, \tag{62}$$

where the trace has to be taken on the d-dimensional space $\mathcal{E}(2j+1)$ with $d := 2j+1$.

Proposition 14. *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*

$$[u_{ab}, u_{a'b'}]_{\mp} = (q^{-ba'} \mp q^{-ab'})u_{a''b''} \qquad a'' := a + a' \qquad b'' := b + b'. \tag{63}$$

Consequently, $[u_{ab}, u_{a'b'}]_- = 0$ if and only if $ab' - ba' = 0$ (mod d) and $[u_{ab}, u_{a'b'}]_+ = 0$ if and only if $ab' - ba' = (1/2)d$ (mod d). Therefore, all anti-commutators $[u_{ab}, u_{a'b'}]_+$ are different from 0 if d is an odd integer.

The d^2 pairwise orthogonal operators u_{ab} can be used as a basis of the Hilbert space $\mathbb{C}^{d^2}$ (with the Hilbert–Schmidt scalar product) of the operators acting on the Hilbert space $\mathbb{C}^d$ (with the usual scalar product). In matrix form, they give generalized Pauli matrices in $(2j + 1) \times (2j + 1)$ dimensions, the spin angular momentum $j = 1/2$ corresponding to the ordinary Pauli matrices.

Example 1. $j = 1/2 \Rightarrow q = -1$ and $d = 2$. The matrices of the four operators u_{ab} with a, $b = 0, 1$ are

$$I = X^0Z^0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad X = X^1Z^0 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{64}$$

$$Z = X^0Z^1 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \qquad Y := X^1Z^1 = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}. \tag{65}$$

In terms of the usual (Hermitian and unitary) Pauli matrices σ_x, σ_y and σ_z, we have $X = \sigma_x$, $Y = -\mathrm{i}\sigma_y$, $Z = \sigma_z$. Note that a normalization for the Pauli matrices different from the conventional one is also used in [9]. The group-theoretical approaches developed in [9] and in the present paper lead to Pauli matrices in dimension 2×2 that differ from the usual Pauli matrices. This is the price one has to pay in order to get a systematic generalization of Pauli matrices in arbitrary dimension (see also [9, 23]). It should be observed that the commutation and anti-commutation relations given by (63) with $d = 2$ correspond to the well-known commutation and anti-commutation relations for the usual Pauli matrices (transcribed in the normalization $X^1Z^0 = \sigma_x$, $X^1Z^1 = -\mathrm{i}\sigma_y$, $X^0Z^1 = \sigma_z$).

Example 2. $j = 1 \Rightarrow q = \exp(2\pi\mathrm{i}/3)$ and $d = 3$. The matrices of the nine operators u_{ab} with $a, b = 0, 1, 2$, namely

$$X^0Z^0 = I \qquad X^1Z^0 = X \qquad X^2Z^0 = X^2 \qquad X^0Z^1 = Z \qquad X^0Z^2 = Z^2 \tag{66}$$

$$X^1Z^1 = XZ \qquad X^2Z^2 \qquad X^2Z^1 = X^2Z \qquad X^1Z^2 = XZ^2 \tag{67}$$

are

$$I = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad X = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} \qquad X^2 = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \tag{68}$$

$$Z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & q & 0 \\ 0 & 0 & q^2 \end{pmatrix} \qquad Z^2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & q^2 & 0 \\ 0 & 0 & q \end{pmatrix} \qquad XZ = \begin{pmatrix} 0 & q & 0 \\ 0 & 0 & q^2 \\ 1 & 0 & 0 \end{pmatrix} \tag{69}$$

$$X^2Z^2 = \begin{pmatrix} 0 & 0 & q \\ 1 & 0 & 0 \\ 0 & q^2 & 0 \end{pmatrix} \qquad X^2Z = \begin{pmatrix} 0 & 0 & q^2 \\ 1 & 0 & 0 \\ 0 & q & 0 \end{pmatrix} \qquad XZ^2 = \begin{pmatrix} 0 & q^2 & 0 \\ 0 & 0 & q \\ 1 & 0 & 0 \end{pmatrix}. \tag{70}$$

These matrices differ from the Gell-Mann matrices [16] used in elementary particle physics. They constitute a natural extension of the Pauli matrices in dimension 3×3 (see also [9, 23]).

4.2. The unitary group in the generalized Pauli basis

From proposition 14, it is clear that the set $\{u_{ab} : a, b = 0, 1, \ldots, d-1\}$ can be used as a set of generators of the Lie group $U(d)$. Thus the generalized Pauli matrices X and Z form an integrity basis for the Lie algebra of $U(d)$. This can be precised by the two propositions below.

Proposition 15. *The set* $\{X^a Z^b : a, b = 0, 1, \ldots, d-1\}$ *form a basis for the Lie algebra* $u(d)$ *of the unitary group* $U(d)$ *for d arbitrary. The Lie brackets of* $u(d)$ *in such a basis (that we denote as the Pauli basis) are given by*

$$[X^a Z^b, X^{a'} Z^{b'}]_- = \sum_{a''b''} (ab, a'b'; a''b'') X^{a''} Z^{b''}, \tag{71}$$

where the structure constants $(ab, a'b'; a''b'')$ *read*

$$(ab, a'b'; a''b'') = \delta(a'', a + a')\delta(b'', b + b')(q^{-ba'} - q^{-ab'}) \tag{72}$$

with $a, b, a', b' = 0, 1, \ldots, d-1$ *(mod d). The structure constants* $(ab, a'b'; a''b'')$ *with* $a'' = a + a'$ *and* $b'' = b + b'$ *are cyclotomic polynomials associated with d. They vanish for* $ab' - ba' = 0$ *(mod d).*

Proposition 16. *In the case where* $d = p$ *is 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* $p-1$*. More precisely*

$$su(p) = v_0 \oplus v_1 \oplus \cdots \oplus v_p, \tag{73}$$

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*

$$\mathcal{V}_1 := \{X^1 Z^0, X^2 Z^0, \ldots, X^{p-1} Z^0\} \tag{74}$$

$$\mathcal{V}_2 := \{X^1 Z^1, X^2 Z^2, \ldots, X^{p-1} Z^{p-1}\} \tag{75}$$

$$\mathcal{V}_3 := \{X^1 Z^2, X^2 Z^4, \ldots, X^{p-1} Z^{p-2}\} \tag{76}$$

$$\vdots \tag{77}$$

$$\mathcal{V}_{p-1} := \{X^1 Z^{p-2}, X^2 Z^{p-4}, \ldots, X^{p-1} Z^2\} \tag{78}$$

$$\mathcal{V}_p := \{X^1 Z^{p-1}, X^2 Z^{p-2}, \ldots, X^{p-1} Z^1\} \tag{79}$$

and

$$\mathcal{V}_0 := \{X^0 Z^1, X^0 Z^2, \ldots, X^0 Z^{p-1}\} \tag{80}$$

for $v_1, v_2, \ldots, v_p$ *and* v_0*, respectively.*

Proof. The proof of proposition 15 is straightforward: it follows from (62) and (63). For proposition 16, we need to pass from $u(p)$ to its subalgebra $su(p)$. A basis for the Lie algebra $su(p)$ of $SU(p)$ is provided with the set $\{X^a Z^b : a, b = 0, 1, \ldots, p-1\} \backslash \{X^0 Z^0\}$. Then, in order to prove proposition 16, it suffices to verify that the $p+1$ sets (or classes) $\mathcal{V}_0, \mathcal{V}_1, \cdots, \mathcal{V}_{p-1}$, and $\mathcal{Z}$ constitute a partition of $\{X^a Z^b : a, b = 0, 1, \ldots, p-1\} \backslash \{X^0 Z^0\}$ and that the $p-1$ operators in each set commute one with each other. Proposition 16 takes its origin in a remark [48] according to which the rank of $su(p)$ is $p-1$ so that the case of $p+1$ sets containing $p-1$ commuting operators occurs as a limiting case. The decomposition (73), also valid for $sl(p, \mathbb{C})$, was first derived in [9] in connection with the determination of finest gradings of Lie algebras of type A_{p-1}. It is little known that a decomposition of type (73) was conjectured almost three decades ago [59] for the more general case where p is replaced by a prime power (see also [60]). □

Example 3. For the purpose of clarifying the production process of the sets $\mathcal{V}_i$ (for $i = 0, 1, \ldots, p$), let us consider the case $p = 7 \Leftrightarrow j = 3$). Equations (74)–(80) give

$$\mathcal{V}_0 = \{(01), (02), (03), (04), (05), (06)\} \tag{81}$$

$$\mathcal{V}_1 = \{(10), (20), (30), (40), (50), (60)\} \tag{82}$$

$$\mathcal{V}_2 = \{(11), (22), (33), (44), (55), (66)\} \tag{83}$$

$$\mathcal{V}_3 = \{(12), (24), (36), (41), (53), (65)\} \tag{84}$$

$$\mathcal{V}_4 = \{(13), (26), (32), (45), (51), (64)\} \tag{85}$$

$$\mathcal{V}_5 = \{(14), (21), (35), (42), (56), (63)\} \tag{86}$$

$$\mathcal{V}_6 = \{(15), (23), (31), (46), (54), (62)\} \tag{87}$$

$$\mathcal{V}_7 = \{(16), (25), (34), (43), (52), (61)\}, \tag{88}$$

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

At this stage, it should be stressed that decompositions of type (73)–(80) are especially useful for the construction of mutually unbiased bases [40, 56]. Along this vein, the common eigenvectors of each of the $p+1$ subalgebras $v_0, v_1, \ldots, v_p$ give rise to $p+1$ mutually unbiased bases. Unfortunately, finding a general formula for the Lie brackets of each pair of the Cartan subalgebras is a difficult problem for which we have no answer.

Counter example 1. For $d = 4 \Leftrightarrow j = 3/2$ ($\Rightarrow a, b = 0, 1, 2, 3$), proposition 15 is valid but proposition 16 does not apply. Indeed, the 16 unitary operators u_{ab} corresponding to

$$ab = 01, 02, 03, 10, 20, 30, 11, 22, 33, 12, 13, 21, 23, 31, 32, 00 \tag{89}$$

are linearly independent and span the Lie algebra of $U(4)$ but they give only three disjoint sets, namely $\{(01), (02), (03)\}$, $\{(10), (20), (30)\}$ and $\{(11), (22), (33)\}$, containing each three commuting operators, where here again (ab) stands for $X^a Z^b$. However, it is not possible to partition the set (89) in order to get a decomposition similar to (73). Nevertheless, it is possible to find another basis of $u(4)$ which can be partitioned in a way yielding a decompostion similar to (73). 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

$$\{(1011), (1101), (0110)\} \tag{90}$$

$$\{(1001), (0111), (1110)\} \tag{91}$$

$$\{(1010), (1000), (0010)\} \tag{92}$$

$$\{(1111), (1100), (0011)\} \tag{93}$$

$$\{(0101), (0100), (0001)\} \tag{94}$$

consist each of three commuting unitary operators and that the Lie algebra $su(4)$ is spanned by the union of the five sets. It is to be emphasized that the 15 operators (90)–(94) are underlaid by the geometry of the generalized quadrangle of order 2 [30]. In this geometry, the five sets given by (90)–(94) correspond to a spread of this quadrangle, i.e., to a set of five pairwise skew lines [30].

The considerations of counter example 1 can be generalized in the case $d := d_1 d_2 \cdots d_e$, e being an integer greater or equal to 2. Let us define

$$u_{AB} := u_{a_1 b_1} \otimes u_{a_2 b_2} \otimes \cdots \otimes u_{a_e b_e} \qquad A := a_1, a_2, \ldots, a_e \qquad B := b_1, b_2, \ldots, b_e, \tag{95}$$

where $u_{a_1 b_1}, u_{a_2 b_2}, \ldots, u_{a_e b_e}$ are generalized Pauli operators corresponding to the dimensions $d_1, d_2, \ldots, d_e$ respectively. (The operators u_{AB} are elements of the group $P_{d_1} \otimes P_{d_2} \otimes \cdots \otimes P_{d_e}$. We follow [9] by calling the operators u_{AB} generalized Dirac operators since the ordinary Dirac operators correspond to $P_2 \otimes P_2$.) In addition, let $q_1, q_2, \ldots, q_e$ be the q-factor associated with $d_1, d_2, \ldots, d_e$ respectively ($q_j := \exp(2\pi \mathrm{i}/d_j)$). Then, propositions 13–15 can be generalized as follows.

Proposition 17. *The operators u_{AB} are unitary and satisfy the orthogonality relation*

$$\mathrm{Tr}_{\mathcal{E}(d_1 d_2 \cdots d_e)}\left(u_{AB}^{\dagger} u_{A'B'}\right) = d_1 d_2 \cdots d_e \delta_{A,A'} \delta_{B,B'}, \tag{96}$$

where

$$\delta_{A,A'} := \delta_{a_1,a_1'} \delta_{a_2,a_2'} \cdots \delta_{a_e,a_e'} \qquad \delta_{B,B'} := \delta_{b_1,b_1'} \delta_{b_2,b_2'} \cdots \delta_{b_e,b_e'}. \tag{97}$$

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

$$[u_{AB}, u_{A'B'}]_{\mp} = \left(\prod_{j=1}^{e} q_j^{-b_j a_j'} \mp \prod_{j=1}^{e} q_j^{-a_j b_j'} \right) u_{A''B''} \tag{98}$$

with

$$A'' := a_1 + a_1', a_2 + a_2', \ldots, a_e + a_e' \qquad B'' := b_1 + b_1', b_2 + b_2', \ldots, b_e + b_e'. \tag{99}$$

The set $\left\{u_{AB} : A, B \in \mathbb{Z}_{d_1} \otimes \mathbb{Z}_{d_2} \otimes \cdots \otimes \mathbb{Z}_{d_e}\right\}$ of the $d_1^2 d_2^2 \cdots d_e^2$ unitary operators u_{AB} form a basis for the Lie algebra $u(d_1 d_2 \cdots d_e)$ of the group $U(d_1 d_2 \cdots d_e)$. In the special case where $d_1 = d_2 = \cdots = d_e = p$ with p a prime integer (or equivalently $d = p^e$), we have $[u_{AB}, u_{A'B'}]_- = 0$ if and only if

$$\sum_{j=1}^{e} a_j b_j' - b_j a_j' = 0 \pmod p \tag{100}$$

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

$$\sum_{j=1}^{e} a_j b_j' - b_j a_j' = \frac{1}{2} p \pmod p \tag{101}$$

so that there are vanishing anti-commutators only if $p = 2$. For $d = p^e$, there exists a decomposition of the set $\left\{u_{AB} : A, B \in \mathbb{Z}_p^{\otimes e}\right\} \setminus \{I\}$ that corresponds to a decomposition of the Lie algebra $su(p^e)$ into $p^e + 1$ Abelian subalgebras of dimension $p^e - 1$.

Proof. The proof of (96)–(101) is based on repeated application of proposition 13. For $d = p^e$, we know from [24, 25, 33] that the set $\left\{u_{AB} : A, B \in \mathbb{Z}_p^{\otimes e}\right\} \setminus \{I\}$ (consisting of $p^{2e} - 1$ unitary operators that are pairwise orthogonal), which provides a basis for $su(p^e)$, can be partitioned into $p^e + 1$ disjoint classes containing each $p^e - 1$ commuting operators. Therefore, there exists a decompostion of $su(p^e)$ into a direct sum of $p^e + 1$ subalgebras of dimension $p^e - 1$. (There is a one-to-one correspondence between the $p^e + 1$ subalgebras and the $p^e + 1$ mutually unbiased bases in $\mathbb{C}^{p^e}$.) □

5. Closing remarks

Starting from an abstract definition of the Heisenberg–Weyl group, combined with a polar decompostion of $SU(2)$ arising from angular momentum theory, we have analysed in a detailed way the interelationship between Weyl pairs, generalized Pauli operators and the generalized Pauli group. The interest of these developments for the unitary group $U(d)$, d arbitrary, have been underlined with a special emphasis for a decomposition of $su(d)$ when d is the power of a prime. We would like to close with two remarks.

In arbitrary dimension d, the number of mutually unbiased bases in $\mathbb{C}^d$ is less or equal to $d + 1$ [24, 56]. Proposition 17 suggests the following remark. To prove that the number of mutually unbiased bases in $\mathbb{C}^d$ is $d + 1$ for d arbitrary amounts to prove that it is possible to find a decomposition of the Lie algebra $su(d)$ into the direct sum of $d+1$ Abelian subalgebras of dimension $d - 1$. Therefore, if such a decomposition cannot be found, it would result that the number of mutually unbiased bases in $\mathbb{C}^d$ is less than $d + 1$ when d is not a prime power (cf conjectures 5.4 and 5.5 by Boykin *et al* [60]).

The Pauli group or discrete Heisenberg–Weyl group $P_d \equiv HW(\mathbb{Z}_d)$ plays an important role in deriving mutually unbiased bases in finite-dimensional Hilbert spaces. We know that the concept of mutually unbiased bases also exists in infinite dimension [61]. In this connection, the infinite or ordinary Heisenberg–Weyl group $HW(\mathbb{R})$ might be of interest for constructing mutually unbiased bases in infinite-dimensional Hilbert spaces.

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