GENERALIZED SPIN BASES FOR QUANTUM CHEMISTRY AND QUANTUM INFORMATION

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Dedicated to Professor Rudolf Zahradník on the occasion of his 80th birthday.

Symmetry-adapted bases in quantum chemistry and bases adapted to quantum information share a common characteristics: both of them are constructed from subspaces of the representation space of the group $SO(3)$ or its double group (i.e., spinor group) $SU(2)$. We exploit this fact for generating spin bases of relevance for quantum systems with cyclic symmetry and equally well for quantum information and quantum computation. Our approach is based on the use of generalized Pauli matrices arising from a polar decomposition of $SU(2)$. This approach leads to a complete solution for the construction of mutually unbiased bases in the case where the dimension d of the considered Hilbert subspace is a prime number. We also give the starting point for studying the case where d is the power of a prime number. A connection of this work to the unitary group $U(d)$ and the Pauli group is briefly underlined.

Keywords: Symmetry-adapted functions; Unitary bases; Generalized Pauli matrices; Unitary groups; Pauli group; Quantum chemistry; Quantum information.

The notion of symmetry-adapted functions (or vectors) in physical chemistry and solid state physics goes back to the fifties[1]. The use of bases consisting of such functions allows to simplify the calculation of matrix elements of operators and to factorize the secular equation. Symmetry adaptation generally requires two types of groups: the symmetry group for the hamiltonian (often a finite group when dealing with molecules) and a chain of classification groups for the operators and state vectors (often continuous groups like unitary groups[2–4] and finite groups[5–9]). The interest in symmetry-adapted bases (atomic orbitals, molecular orbitals, spin waves, etc.) is well known in quantum chemistry. In particular, the spherical har-

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monics (e.g., in atomic spectroscopy) and cubic, tetragonal or trigonal harmonics (e.g., in crystal-field theory and ligand-field theory[10]) are quite familiar to the practitioner in theoretical chemistry and chemical physics.

The symmetry-adapted functions generally span bases for finite-dimensional Hilbert spaces associated with reducible or irreducible representations of a symmetry group. In the case of low dimensions, such spaces are especially useful in the emerging fields of quantum information and quantum computation (quantum state tomography and quantum cryptography), two fields at the crossing of informatics, mathematics and quantum physics. In fact, a Hilbert space of finite dimension d can describe a system of qudits (qubits correspond to $d = 2$, qudits to d arbitrary). Qudits can be realized from many physical systems. We undersee that qudits could be also produced from chemical systems.

It is the object of this paper to construct bases which play an important role for quantum systems with cyclic symmetry and for quantum measurements and quantum information theory.

The organisation of this paper is as follows. Section 1 is devoted to an alternative to the $\{j^2,j_z\}$ quantization scheme of angular momentum. In Section 2, this scheme is worked out for generating bases in a form adapted to physical and chemical cyclic systems as well as to quantum information. Section 3 deals with some examples in low dimensions. Finally, in Section 4 we develop a systematic construction of generalized Pauli matrices which are at the origin of generalized spin bases. In the closing remarks, we mention the interest of this work in the special unitary group and the Pauli group.

Throughout the present work, we use the Dirac notation familiar in quantum chemistry. As usual, $A^\dagger$ stands for the hermitian conjugate of the operator A. In addition, $[A,B]_-$ and $[A,B]_+$ denote the commutator and the anticommutator of A and B. Finally, i is the pure imaginary.

1. AN ALTERNATIVE TO THE $\{j^2,j_z\}$ SCHEME

Let us consider a generalized angular momentum. We note j^2 its square and j_z its z-component. The common eigenvectors of j^2 and j_z are denoted as $|j,m\rangle$. We know that[11]

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

in a system of units where the rationalized Planck constant is equal to 1.

For a fixed value of the quantum number j (with $2j \in \mathbb{N}$), we note $\varepsilon(2j + 1)$ the $(2j + 1)$-dimensional Hilbert space spanned by the basis

$$b_s = \{|j,m\rangle: m = j, j - 1, ..., -j\}. \quad (2)$$

The basis b_s is adapted to spherical symmetry (adapted to the group $SO(3)$ if j is an integer or the group $SU(2)$ if j is a half of an odd integer). We take the basis b_s in an orthonormal form, i.e., the scalar product $\langle j,m|j,m'\rangle$ satisfies

$$\langle j,m|j,m'\rangle = \delta_{m,m'} \quad (3)$$

for any value of m and m'.

In the applications to quantum chemistry, the generalized angular momentum can be an angular momentum, a spin angular momentum, a total (spin + orbital) angular momentum, etc. The vectors $|j,m\rangle$ can have several realizations. For instance, in the spectroscopy of $4f^N$ lanthanide ions, we have state vectors of type $|J,M\rangle \equiv |4f^N\tau SLJM\rangle$ in the Russell–Saunders coupling (here $j = J$ and $m = M$). This constitutes one of many possible realizations of the vectors $|j,m\rangle$.

Besides the basis b_s, another interesting basis can be obtained as follows. Let us consider the operator

$$v_{ra} = e^{i2\pi jr}|j,-j\rangle\langle j,j| + \sum_{m=-j}^{j-1} q^{(j-m)a}|j,m+1\rangle\langle j,m| \quad (4)$$

where we use the notation of Dirac for projectors. In Eq. (*4*), we have

$$r \in \mathbb{R}, \quad a = 0, 1, ..., 2j, \quad q = \exp\left(\frac{2\pi i}{2j+1}\right). \quad (5)$$

The operator v_{ra} is an extension of the operator U_r defined in a previous work[12] ($U_r = v_{r0}$). From Eq. (*4*), we can check that the action of v_{ra} on the state $|j,m\rangle$ is given by

$$v_{ra}|j,m\rangle = (1-\delta_{m,j})q^{(j-m)a}|j,m+1\rangle + \delta_{m,j}e^{i2\pi jr}|j,-j\rangle . \quad (6)$$

Furthermore, the matrix V_{ra} of the operator v_{ra} on the basis b_s reads

$$V_{ra} = \begin{pmatrix} 0 & q^a & 0 & \cdots & 0 \\ 0 & 0 & q^{2a} & \cdots & 0 \\ \vdots & \vdots & \vdots & \cdots & \vdots \\ 0 & 0 & 0 & \cdots & q^{2ja} \\ \mathrm{e}^{\mathrm{i}2\pi jr} & 0 & 0 & \cdots & 0 \end{pmatrix} \tag{7}$$

where the lines and columns are labeled in the order $|j,j\rangle$, $|j,j-1\rangle$, ..., $|j,-j\rangle$. It can be shown that the operators j^2 and v_{ra} commute so that the complete set $\{j^2,v_{ra}\}$ of commuting operators constitutes an alternative to the set $\{j^2,j_z\}$.

We may ask what are the analogues of the vectors $|j,m\rangle$ in the scheme $\{j^2,v_{ra}\}$? Indeed, they are the common eigenvectors of the operators j^2 and v_{ra}. As a result, these eigenvectors are

$$|j\alpha;ra\rangle = \frac{1}{\sqrt{2j+1}} \sum_{m=-j}^{j} q^{(j+m)(j-m+1)a/2-jmr+(j+m)\alpha} |j,m\rangle \tag{8}$$

for $\alpha = 0, 1, ..., 2j$. More precisely, we have the eigenvalue equations

$$v_{ra}|j\alpha;ra\rangle = q^{j(a+r)-\alpha}|j\alpha;ra\rangle, \quad j^2|j\alpha;ra\rangle = j(j+1)|j\alpha;ra\rangle\,. \tag{9}$$

For fixed j and a ($2j \in \mathbb{N}$, $a = 0, 1, ..., 2j$), the basis

$$B_{ra} = \{|j\alpha;ra\rangle : \alpha = 0, 1, ..., 2j\} \tag{10}$$

is an orthonormal basis since

$$\langle j\alpha;ra|j\alpha';ra\rangle = \delta_{\alpha,\alpha'} \tag{11}$$

for any value of α and α'. In the particular case where $2j + 1$ is a prime integer, the overlap between the bases B_{ra} and B_{rb} is such that[13]

$$|\langle j\alpha;ra|j\beta;rb\rangle = \delta_{\alpha,\beta}\delta_{a,b} + \frac{1}{\sqrt{2j+1}}(1-\delta_{a,b}) \tag{12}$$

a property of considerable importance in quantum information. Note that Eq. (*12*) is compatible with Eq. (*11*).

2. A FORMULATION FOR *d*-DIMENSIONAL QUANTUM SYSTEMS

The parameter r is of interest for group-theoretical analyses but turns out to be of no concern here. Therefore, we will restrict ourselves in the following to the case $r = 0$. In addition, we shall adopt the notation

$$k = j - m, \quad |k\rangle = |j,m\rangle, \quad |a\alpha\rangle = |j\alpha;0a\rangle, \quad d = 2j + 1 \tag{13}$$

that is especially adapted to quantum information (the vectors $|0\rangle$, $|1\rangle$, ..., $|d - 1\rangle$ are then called qudits, the case $d = 2$ corresponding to ordinary qubits) and to cyclic chemical systems (for which $|d\rangle \equiv |0\rangle$, $|d + 1\rangle \equiv |1\rangle$, etc.).

The basis b_s becomes

$$B_d = \{|k\rangle: k = 0, 1, \ldots, d - 1\} \tag{14}$$

known as the computational basis in quantum information theory. The action of v_{0a} on the basis B_d of $\varepsilon(2j + 1)$ is described by

$$v_{0a}|k\rangle = q^{ka}|k - 1\rangle \tag{15}$$

where $k - 1$ should be understood modulo d (i.e., $|-1\rangle = |d - 1\rangle$). The vectors $|a\alpha\rangle$ of the orthonormal basis

$$B_{0a} = \{|a\alpha\rangle: \alpha = 0, 1, \ldots, d - 1\} \tag{16}$$

can be written as

$$|a\alpha\rangle = \frac{1}{\sqrt{d}} \sum_{k=0}^{d-1} q^{(d-k-1)(k+1)a/2-(k+1)\alpha}|k\rangle \tag{17}$$

where α can take the values $\alpha = 0, 1, \ldots, d - 1$. These vectors satisfy the eigenvalue equation

$$v_{0a}|a\alpha\rangle = q^{(d-1)a/2-\alpha}|a\alpha\rangle \tag{18}$$

that corresponds to a nondegenerate spectrum for the operator v_{0a}.

All relations given in Section 1 up to this point are valid for d arbitrary. In the special case where d is a prime integer, Eq. (*12*) yields

$$|\langle a\alpha|b\beta\rangle| = \delta_{\alpha,\beta}\delta_{a,b} + \frac{1}{\sqrt{d}}(1 - \delta_{a,b}) \tag{19}$$

a relation valid for any value of a, b, α and β in the set $\{0, 1, ..., d-1\}$. In quantum information, two bases B_{0a} and B_{0b} satisfying Eq. (*19*) are said to be mutually unbiased[14]. Such bases play an important role in quantum cryptography and quantum state tomography. It is well known that a complete set of $d + 1$ mutually unbiased bases can be found when d is a prime integer or the power of a prime integer.

We continue with some typical examples.

3. SOME TYPICAL EXAMPLES

The Case d = 2

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

$$V_{00} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad V_{01} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}. \tag{20}$$

We note in passing a connection (to be generalized below) with the Pauli matrices since $V_{00} = \sigma_x$ and $V_{01} = -i\sigma_y$. From Eqs (*14*), (*16*) and (*17*), the bases B_2, B_{00} and B_{01} are

$$B_2 : |0\rangle, \quad |1\rangle \tag{21}$$

$$B_{00} : |00\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle), \quad |01\rangle = \frac{1}{\sqrt{2}}(-|0\rangle + |1\rangle) \tag{22}$$

$$B_{01} : |10\rangle = \frac{1}{\sqrt{2}}(i|0\rangle + |1\rangle), \quad |11\rangle = \frac{1}{\sqrt{2}}(-i|0\rangle + |1\rangle) \tag{23}$$

which satisfy Eq. (*19*). Note that by using the spin-orbital

$$\alpha = |\frac{1}{2}, \frac{1}{2}\rangle = |0\rangle, \quad \beta = |\frac{1}{2}, -\frac{1}{2}\rangle = |1\rangle \tag{24}$$

(α for spin up and β for spin down) familiar to the quantum chemist, Eqs (*21*)–(*23*) can be rewritten as

$$B_2 : \alpha, \quad \beta \tag{25}$$

$$B_{00} : |00\rangle = \frac{1}{\sqrt{2}}(\alpha + \beta), \quad |01\rangle = -\frac{1}{\sqrt{2}}(\alpha - \beta) \tag{26}$$

$$B_{01} : |10\rangle = \mathrm{i}\frac{1}{\sqrt{2}}(\alpha - \mathrm{i}\beta), \quad |11\rangle = -\mathrm{i}\frac{1}{\sqrt{2}}(\alpha + \mathrm{i}\beta)\,. \tag{27}$$

In terms of eigenvectors of the matrices V_{0a}, we must replace the vectors $|a\alpha\rangle$ by column vectors. This leads to

$$B_2 : \alpha \to \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \beta \to \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{28}$$

$$B_{00} : |00\rangle \to \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad |01\rangle \to \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix} \tag{29}$$

$$B_{01} : |10\rangle \to \mathrm{i}\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -\mathrm{i} \end{pmatrix}, \quad |11\rangle \to -\mathrm{i}\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ \mathrm{i} \end{pmatrix}. \tag{30}$$

The Case d = 3

This case corresponds to a spin $j = 1$ or to a qutrit. Here, we have $q = \exp(2\pi\mathrm{i}/3)$ and $a, \alpha \in \{0, 1, 2\}$. The matrices of the operators v_{0a} are

$$V_{00} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}, \; V_{01} = \begin{pmatrix} 0 & q & 0 \\ 0 & 0 & q^2 \\ 1 & 0 & 0 \end{pmatrix}, \; V_{02} = \begin{pmatrix} 0 & q^2 & 0 \\ 0 & 0 & q \\ 1 & 0 & 0 \end{pmatrix}. \tag{31}$$

The bases B_3, B_{00} and B_{01}, B_{02} are

$$B_3 : |0\rangle, \quad |1\rangle, \quad |2\rangle \tag{32}$$

$$B_{00} : |00\rangle = \frac{1}{\sqrt{3}}(|0\rangle + |1\rangle + |2\rangle), \quad |01\rangle = \frac{1}{\sqrt{3}}(q^2|0\rangle + q|1\rangle + |2\rangle) \tag{33}$$

$$|02\rangle = \frac{1}{\sqrt{3}}(q|0\rangle + q^2|1\rangle + |2\rangle) \tag{34}$$

$$B_{01} : |10\rangle = \frac{1}{\sqrt{3}}(q|0\rangle + q|1\rangle + |2\rangle), \quad |11\rangle = \frac{1}{\sqrt{3}}(|0\rangle + q^2|1\rangle + |2\rangle) \tag{35}$$

$$|12\rangle = \frac{1}{\sqrt{3}}(q^2|0\rangle + |1\rangle + |2\rangle) \tag{36}$$

$$B_{02} : |20\rangle = \frac{1}{\sqrt{3}}(q^2|0\rangle + q^2|1\rangle + |2\rangle), \quad |21\rangle = \frac{1}{\sqrt{3}}(q|0\rangle + |1\rangle + |2\rangle) \tag{37}$$

$$|22\rangle = \frac{1}{\sqrt{3}}(|0\rangle + q|1\rangle + |2\rangle)\,. \tag{38}$$

They satisfy Eq. (*19*). In terms of column vectors, we have

$$B_3 : |0\rangle \to \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad |1\rangle \to \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad |2\rangle \to \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \tag{39}$$

$$B_{00} : |00\rangle \to \frac{1}{\sqrt{3}}\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}, \quad |01\rangle \to \frac{1}{\sqrt{3}}\begin{pmatrix} q^2 \\ q \\ 1 \end{pmatrix}, \quad |02\rangle \to \frac{1}{\sqrt{3}}\begin{pmatrix} q \\ q^2 \\ 1 \end{pmatrix} \tag{40}$$

$$B_{01} : |10\rangle \to \frac{1}{\sqrt{3}}\begin{pmatrix} q \\ q \\ 1 \end{pmatrix}, \quad |11\rangle \to \frac{1}{\sqrt{3}}\begin{pmatrix} 1 \\ q^2 \\ 1 \end{pmatrix}, \quad |12\rangle \to \frac{1}{\sqrt{3}}\begin{pmatrix} q^2 \\ 1 \\ 1 \end{pmatrix} \tag{41}$$

$$B_{02} : |20\rangle \to \frac{1}{\sqrt{3}}\begin{pmatrix} q^2 \\ q^2 \\ 1 \end{pmatrix}, \quad |21\rangle \to \frac{1}{\sqrt{3}}\begin{pmatrix} q \\ 1 \\ 1 \end{pmatrix}, \quad |22\rangle \to \frac{1}{\sqrt{3}}\begin{pmatrix} 1 \\ q \\ 1 \end{pmatrix}. \tag{42}$$

The Case d = 4

This case corresponds to a spin $j = 3/2$. Here, we have $q = i$ and $a, \alpha \in \{0, 1, 2, 3\}$. Equation (*17*) can be applied to this case too. However, the resulting bases B_4, B_{00}, B_{01}, B_{02} and B_{03} do not constitute a complete system of mutually unbiased bases ($d = 4$ is not a prime number). Nevertheless, it is possible to find $d + 1 = 5$ mutually unbiased bases because $d = 2^2$ is the power of a prime number. This can be achieved by replacing the space $\varepsilon(4)$ spanned by $\{|3/2,m\rangle: m = 3/2, 1/2, -1/2, -3/2\}$ by the tensor product space $\varepsilon(2) \otimes \varepsilon(2)$ spanned by the basis

$$\{\alpha \otimes \alpha, \alpha \otimes \beta, \beta \otimes \alpha, \beta \otimes \beta\} . \qquad (43)$$

The space $\varepsilon(2) \otimes \varepsilon(2)$ 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). An alternative basis for $\varepsilon(2) \otimes \varepsilon(2)$ is

$$\{\alpha \otimes \alpha, \frac{1}{2}(\alpha \otimes \beta + \beta \otimes \alpha), \beta \otimes \beta, \frac{1}{2}(\alpha \otimes \beta - \beta \otimes \alpha)\} . \qquad (44)$$

The vectors in (*44*) are well known in the treatment of spin systems. The first three vectors are symmetric under the interchange $1 \leftrightarrow 2$ and describe a total angular momentum $J = 1$ while the last one is antisymmetric and corresponds to $J = 0$. It should be observed that the basis (*44*) illustrates a connection between the special unitary group $SU(2)$ and the permutation group S_2 (a particular case of a reciprocity theorem between irreducible representation classes of SU_n and S_m).

In addition to the bases (*43*) and (*44*), it is possible to find other bases of $\varepsilon(2) \otimes \varepsilon(2)$ which are mutually unbiased. The $d = 4$ mutually unbiased bases, besides the canonical or computational basis (*43*), can be constructed from the eigenvectors

$$|ab\alpha\beta\rangle = |a\alpha\rangle \otimes |b\beta\rangle \qquad (45)$$

of the operators $w_{ab} = v_{0a} \otimes v_{0b}$ (the vectors $|a\alpha\rangle$ and $|b\beta\rangle$ refer to the two spaces $\varepsilon(2)$). As a result, we have the $d + 1 = 5$ following mutually unbiased bases where $\lambda = (1 - i)/2$ and $\mu = (1 + i)/2$.

The canonical basis:

$$\alpha \otimes \alpha, \quad \alpha \otimes \beta, \quad \beta \otimes \alpha, \quad \beta \otimes \beta \qquad (46)$$

or in column vectors

$$\begin{pmatrix}1\\0\\0\\0\end{pmatrix},\quad \begin{pmatrix}0\\1\\0\\0\end{pmatrix},\quad \begin{pmatrix}0\\0\\1\\0\end{pmatrix},\quad \begin{pmatrix}0\\0\\0\\1\end{pmatrix}. \tag{47}$$

The w_{00} basis:

$$|0000\rangle = \frac{1}{2}(\alpha\otimes\alpha+\alpha\otimes\beta+\beta\otimes\alpha+\beta\otimes\beta) \tag{48}$$

$$|0001\rangle = \frac{1}{2}(\alpha\otimes\alpha-\alpha\otimes\beta+\beta\otimes\alpha-\beta\otimes\beta) \tag{49}$$

$$|0010\rangle = \frac{1}{2}(\alpha\otimes\alpha+\alpha\otimes\beta-\beta\otimes\alpha-\beta\otimes\beta) \tag{50}$$

$$|0011\rangle = \frac{1}{2}(\alpha\otimes\alpha-\alpha\otimes\beta-\beta\otimes\alpha+\beta\otimes\beta) \tag{51}$$

or in column vectors

$$\frac{1}{2}\begin{pmatrix}1\\1\\1\\1\end{pmatrix},\quad \frac{1}{2}\begin{pmatrix}1\\-1\\1\\-1\end{pmatrix},\quad \frac{1}{2}\begin{pmatrix}1\\1\\-1\\-1\end{pmatrix},\quad \frac{1}{2}\begin{pmatrix}1\\-1\\-1\\1\end{pmatrix}. \tag{52}$$

The w_{11} basis:

$$|1100\rangle = \frac{1}{2}(\alpha\otimes\alpha+\mathrm{i}\alpha\otimes\beta+\mathrm{i}\beta\otimes\alpha-\beta\otimes\beta) \tag{53}$$

$$|1101\rangle = \frac{1}{2}(\alpha\otimes\alpha-\mathrm{i}\alpha\otimes\beta+\mathrm{i}\beta\otimes\alpha+\beta\otimes\beta) \tag{54}$$

$$|1110\rangle = \frac{1}{2}(\alpha\otimes\alpha+\mathrm{i}\alpha\otimes\beta-\mathrm{i}\beta\otimes\alpha+\beta\otimes\beta) \tag{55}$$

$$|1111\rangle = \frac{1}{2}(\alpha\otimes\alpha-\mathrm{i}\alpha\otimes\beta-\mathrm{i}\beta\otimes\alpha-\beta\otimes\beta) \tag{56}$$

or in column vectors

$$\frac{1}{2}\begin{pmatrix}1\\ \mathrm{i}\\ \mathrm{i}\\ -1\end{pmatrix},\quad \frac{1}{2}\begin{pmatrix}1\\ -\mathrm{i}\\ \mathrm{i}\\ 1\end{pmatrix},\quad \frac{1}{2}\begin{pmatrix}1\\ \mathrm{i}\\ -\mathrm{i}\\ 1\end{pmatrix},\quad \frac{1}{2}\begin{pmatrix}1\\ -\mathrm{i}\\ -\mathrm{i}\\ -1\end{pmatrix}. \tag{57}$$

The w_{01} basis:

$$\lambda|0100\rangle + \mu|0111\rangle = \frac{1}{2}(\alpha\otimes\alpha + \alpha\otimes\beta - \mathrm{i}\beta\otimes\alpha + \mathrm{i}\beta\otimes\beta) \tag{58}$$

$$\mu|0100\rangle + \lambda|0111\rangle = \frac{1}{2}(\alpha\otimes\alpha - \alpha\otimes\beta + \mathrm{i}\beta\otimes\alpha + \mathrm{i}\beta\otimes\beta) \tag{59}$$

$$\lambda|0101\rangle + \mu|0110\rangle = \frac{1}{2}(\alpha\otimes\alpha - \alpha\otimes\beta - \mathrm{i}\beta\otimes\alpha - \mathrm{i}\beta\otimes\beta) \tag{60}$$

$$\mu|0101\rangle + \lambda|0110\rangle = \frac{1}{2}(\alpha\otimes\alpha + \alpha\otimes\beta + \mathrm{i}\beta\otimes\alpha - \mathrm{i}\beta\otimes\beta) \tag{61}$$

or in column vectors

$$\frac{1}{2}\begin{pmatrix}1\\ 1\\ -\mathrm{i}\\ \mathrm{i}\end{pmatrix},\quad \frac{1}{2}\begin{pmatrix}1\\ -1\\ \mathrm{i}\\ \mathrm{i}\end{pmatrix},\quad \frac{1}{2}\begin{pmatrix}1\\ -1\\ -\mathrm{i}\\ -\mathrm{i}\end{pmatrix},\quad \frac{1}{2}\begin{pmatrix}1\\ 1\\ \mathrm{i}\\ -\mathrm{i}\end{pmatrix}. \tag{62}$$

The w_{10} basis:

$$\lambda|1000\rangle + \mu|1011\rangle = \frac{1}{2}(\alpha\otimes\alpha - \mathrm{i}\alpha\otimes\beta + \beta\otimes\alpha + \mathrm{i}\beta\otimes\beta) \tag{63}$$

$$\mu|1000\rangle + \lambda|1011\rangle = \frac{1}{2}(\alpha\otimes\alpha + \mathrm{i}\alpha\otimes\beta - \beta\otimes\alpha + \mathrm{i}\beta\otimes\beta) \tag{64}$$

$$\lambda|1001\rangle + \mu|1010\rangle = \frac{1}{2}(\alpha\otimes\alpha + \mathrm{i}\alpha\otimes\beta + \beta\otimes\alpha - \mathrm{i}\beta\otimes\beta) \tag{65}$$

$$\mu|1001\rangle + \lambda|1010\rangle = \frac{1}{2}(\alpha\otimes\alpha - \mathrm{i}\alpha\otimes\beta - \beta\otimes\alpha - \mathrm{i}\beta\otimes\beta) \tag{66}$$

or in column vectors

$$\frac{1}{2}\begin{pmatrix}1\\-\mathrm{i}\\1\\\mathrm{i}\end{pmatrix},\quad \frac{1}{2}\begin{pmatrix}1\\\mathrm{i}\\-1\\\mathrm{i}\end{pmatrix},\quad \frac{1}{2}\begin{pmatrix}1\\\mathrm{i}\\1\\-\mathrm{i}\end{pmatrix},\quad \frac{1}{2}\begin{pmatrix}1\\-\mathrm{i}\\-1\\-\mathrm{i}\end{pmatrix}. \tag{67}$$

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).

4. GENERALIZED PAULI MATRICES

From the operators v_{0a}, it is possible to define two basic operators x and z which can be used for generating generalized Pauli matrices. Let us put

$$x = v_{00}, \quad z = v_{00}^{\dagger} v_{00}. \tag{68}$$

The action of x and z on the space $\varepsilon(2j + 1)$ is given by

$$x|j,m\rangle = (1-\delta_{m,j})|j,m+1\rangle + \delta_{m,j}|j,-j\rangle \Leftrightarrow x|k\rangle = |k-1\rangle \tag{69}$$

and

$$z|j,m\rangle = q^{j-m}|j,m\rangle \Leftrightarrow z|k\rangle = q^{k}|k\rangle \tag{70}$$

where $q = \exp(2\pi\mathrm{i}/d)$ with $d = 2j + 1$. The d-dimensional matrices X and Z of x and z are

$$X = \begin{pmatrix}0&1&0&\cdots&0\\0&0&1&\cdots&0\\\vdots&\vdots&\vdots&\cdots&\vdots\\0&0&0&\cdots&1\\1&0&0&\cdots&0\end{pmatrix},\quad Z = \begin{pmatrix}1&0&0&\cdots&0\\0&q&0&\cdots&0\\0&0&q^2&\cdots&0\\\vdots&\vdots&\vdots&\cdots&\vdots\\0&0&0&\cdots&q^{d-1}\end{pmatrix}. \tag{71}$$

The operators x and z are unitary and satisfy the q-commutation relation

$$xz - qzx = 0 . \tag{72}$$

Pairs of operators satisfying a relation of type (*72*) are nowadays referred to as Weyl pairs. Thus, the operators x and z constitute a Weyl pair. Weyl pairs were introduced at the beginning of quantum mechanics[15]. They were extensively used for factorizing the secular equation in connection with a study of alternating hydrocarbons[16] and for constructing analogues of the usual Pauli matrices[14,17–19].

Let us now define the operators

$$u_{ab} = x^a z^b , \quad a, b = 0, 1, ..., d - 1 . \tag{73}$$

The d^2 operators u_{ab} are unitary and satisfy the following trace relation

$$\mathrm{Tr}_{\varepsilon(2j+1)}(u_{ab}^{\dagger} u_{a'b'}) = (2j + 1)\, \delta_{a,a'}\, \delta_{b,b'} \tag{74}$$

where the trace is taken on the d-dimensional space $\varepsilon(2j + 1)$. Additionally, the commutator $[u_{ab}, u_{a'b'}]_-$ and the anticommutator $[u_{ab}, u_{a'b'}]_+$ of u_{ab} and $u_{a'b'}$ are given by

$$[u_{ab}, u_{a'b'}]_{\mp} = (q^{-ba'} \mp q^{-ab'}) u_{a''b''} , \quad a'' = a + a', \quad b'' = b + b'. \tag{75}$$

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

Two consequences follow from Eqs (*74*) and (*75*). First, the trace relation (*74*) shows that the d^2 operators u_{ab} are pairwise orthogonal operators so that they can serve as a basis for developing any operator acting on the Hilbert space $\varepsilon(d)$. Second, the commutation relation (*75*) shows that the set $\{u_{ab}: a, b = 0, 1, ..., d - 1\}$ generates a d^2-dimensional Lie algebra. This algebra turns out to be the Lie algebra of the unitary group $U(d)$. The subset $\{u_{ab}\}: a, b = 0, 1, ..., d - 1\} \setminus \{u_{00}\}$ thus spans the Lie algebra of the special unitary group $SU(d)$.

All this is reminiscent of the group $SU(2)$, the generators of which are the well-known Pauli matrices. Therefore, the operators u_{ab} shall be referred to generalized Pauli operators and their matrices as generalized Pauli matrices. As an illustration, let us deal with the cases $d = 2$ and 3.

Example 1

In the case $j = 1/2 \Leftrightarrow d = 2$ ($\Rightarrow q = -1$), the matrices of the 4 operators u_{ab} with $a, b = 0, 1$ are

$$I = X^0 Z^0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad X = X^1 Z^0 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{76}$$

$$Z = X^0 Z^1 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad Y = X^1 Z^1 = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}. \tag{77}$$

In terms of the usual (hermitian and unitary) Pauli matrices σ_x, σ_y and σ_z, we have $X = \sigma_x$, $Y = -i\sigma_y$, $Z = \sigma_z$. The approach developed in the present paper leads to Pauli matrices in dimension 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. It should be observed that the commutation and anticommutation relations given by (*75*) with $d = 2$ correspond to the well-known commutation and anticommutation relations for the usual Pauli matrices (transcribed in the normalization $X^1Z^0 = \sigma_x$, $X^1Z^1 = -i\sigma_y$, $X_0Z^1 = \sigma_z$).

Example 2

In the case $j = 1 \Leftrightarrow d = 3$ ($\Rightarrow q = \exp(2\pi i/3)$), the matrices of the 9 operators u_{ab} with $a, b = 0, 1, 2$, viz.,

$$X^0 Z^0 = I \qquad X^1 Z^0 = X \qquad X^2 Z^0 = X^2 \qquad X^0 Z^1 = Z \qquad X^0 Z^2 = Z^2 \tag{78}$$

$$X^1 Z^1 = XZ \qquad X^2 Z^2 \qquad X^2 Z^1 = X^2 Z \qquad X^1 Z^2 = XZ^2 \tag{79}$$

are

$$I = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad X = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}, \quad X^2 = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \tag{80}$$

$$Z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & q & 0 \\ 0 & 0 & q^2 \end{pmatrix}, \quad Z^2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & q^2 & 0 \\ 0 & 0 & q \end{pmatrix}, \quad XZ = \begin{pmatrix} 0 & q & 0 \\ 0 & 0 & q^2 \\ 1 & 0 & 0 \end{pmatrix} \tag{81}$$

$$X^2Z^2 = \begin{pmatrix} 0 & 0 & q \\ 1 & 0 & 0 \\ 0 & q^2 & 0 \end{pmatrix}, \quad X^2Z = \begin{pmatrix} 0 & 0 & q^2 \\ 1 & 0 & 0 \\ 0 & q & 0 \end{pmatrix}, \quad XZ^2 = \begin{pmatrix} 0 & q^2 & 0 \\ 0 & 0 & q \\ 1 & 0 & 0 \end{pmatrix}. \tag{82}$$

These generalized Pauli matrices differ from the Gell–Mann matrices[20] used in elementary particle physics. They constitute a natural extension of the Pauli matrices in dimension $d = 3$.

5. CONCLUDING REMARKS

The various bases described in the present paper are of central importance in quantum information and quantum computation. They also play an important role for quantum (chemical and physical) systems with cyclic symmetry. By way of illustration, we would like to mention two examples.

Let us consider a ring shape molecule with N atoms (or aggregates) at the vertices of a regular polygon with N sides ($N = 6$ for the benzene molecule C_6H_6). The atoms are labelled by the integer n with $n = 0, 1, \ldots, N - 1$. Hence, the cyclic character of the ring shape molecule makes it possible to identify the atom with the number n to the one with the number $n + kN$ where $k \in \mathbb{Z}$ (the location of an atom is defined modulo N). Let $|\varphi_n\rangle$ be the atomic state vector, or atomic orbital in quantum chemistry parlance, describing a π-electron located in the neighboring of site n. From symmetry considerations, the molecular state vector, or molecular orbital, for the molecule reads[21]

$$|\kappa_s\rangle = \frac{1}{\sqrt{N}} \sum_{n=0}^{N-1} \mathrm{e}^{\mathrm{i}\, 2\pi ns/N} |\varphi_n\rangle , \tag{83}$$

with $s = 0, 1, \ldots, N - 1$. As a result, the molecular orbital $|\kappa_s\rangle$ assumes the same form, up to a global phase factor, as the state $|a\alpha\rangle$ given by Eq. (*17*) with $a = 0$ and $\alpha = s$.

A similar result can be obtained for a one-dimensional chain of N 1/2-spins (numbered with $n = 0, 1, \ldots, N - 1$) used as a modeling tool of a

ferromagnetic substance. Here again, we have a cyclic symmetry since the spins numbered $n = N$ and $n = 0$ are considered to be identical. The spin waves can then be described by state vectors[21] very similar to the ones given by Eq. (*17*) again with $a = 0$.

We close this work with two remarks of a group-theoretical nature, one concerning a continuous group, the other a finite group, connected with the operators u_{ab}.

First, as mentioned in Section 4, the set $\{u_{ab}: a, b = 0, 1, ..., d - 1\}\backslash\{u_{00}\}$ constitutes a basis for the Lie algebra $SU(d)$. Such a basis differs from the well-known Cartan basis or from the Gelfand–Tsetlin basis. In the special case $d = p$, with p prime integer, the basis $\{u_{ab}: a, b = 0, 1, ..., d - 1\}\backslash\{u_{00}\}$ can be partioned into $p + 1$ disjoint subsets, each subset containing $p - 1$ commuting operators[18,22]. In other words, it is possible to decompose the Lie algebra of $SU(p)$ into $p + 1$ Cartan subalgebras of dimension $p - 1$. It can be proved that each subalgebra is associated with a basis of $\varepsilon(p)$ and that the set of the $p + 1$ corresponding bases is a complete set of mutually unbiased bases. A similar decomposition holds for $SU(d)$ in the case where $d = p^e$, with p prime integer and e positive integer[22]. However, in this case we need to replace $\varepsilon(d)$ by $\varepsilon(p)^{\otimes e}$.

A second group-theoretical remark concerns a finite group known as the Pauli group or the finite Heisenberg–Weyl group[17,18,22–24]. The set $\{u_{ab}: a, b = 0, 1, ..., d - 1\}$ is not closed under multiplication. However, it is possible to extend the latter set in order to have a group. For this purpose, let us define the operators w_{abc} via[22]

$$w_{abc} = q^a u_{bc}, \quad a, b, c = 0, 1, \ldots, d - 1. \tag{84}$$

Then, the set $\{w_{abc}: a, b = 0, 1, ..., d - 1\}$, endowed with the multiplication of operators, is a group of order d^3. This group (the Pauli group) is of paramount importance in quantum information and quantum computation[24,25].

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