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Finite-level systems, Hermitian operators, isometries and a novel parametrization of Stiefel and Grassmann manifolds

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Abstract

In this paper, we provide an explicit parametrization of arbitrary n-dimensional Hermitian operators on the Hilbert space $\mathbb{C}^n$, operators that may be considered either as Hamiltonians or density matrices for finite-level quantum systems, the description of which gives a complete solution to the over parametrization problem. It is shown that all the spectral multiplicities are encoded in a flag unitary matrix obtained as an ordered product of special unitary matrices, each one generated by a complex $n-k$-dimensional unit vector, $k = 0, 1, \ldots, n-2$. As a byproduct, an alternative and simple parametrization of Stiefel and Grassmann manifolds is obtained.

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1. Introduction

There is considerable interest in a simple description of density matrices that have a wide variety of applications, particularly in quantum information theory, and many efforts have been devoted in describing them. However the problem of over-parametrization is still open [16], for an arbitrary n. We solve this problem by providing an explicit parametrization of eigenvalues as well as of the unitary matrices that diagonalize arbitrary finite-dimensional Hermitian operators. Naturally, such a description is closely related to the description of various homogeneous manifolds, as mentioned in the title. On the other hand, the Stiefel or Grassmann manifolds arise in many problems from different other domains such as encryption, coherent states, geometric phases, signal processing, geometric integration on homogeneous manifolds, numerical linear algebra algorithms and many others. In such problems, the states of interest are, in general, elements of some homogeneous space

$$X \cong G/K \tag{1.1}$$

where G is a Lie group and K is a closed subgroup of G. Further, in problems arising in engineering, physics, quantum information theory, one needs a concrete realization of these manifolds in a form able to be stored in a computer and that could be used for doing symbolic and numerical calculations. Although, the geometrical description of Grassmann and Stiefel manifolds is available in many books, see for example [7, 8], the available parametrizations of the above manifolds are not the most convenient in some concrete applications, e.g. [4, 10, 15].

Another aim of the paper is to obtain a satisfactory description of Hermitian operators that appear in the study of finite-level systems. By satisfactory, we mean as complete as possible description of equivalence classes of Hermitian operators, i.e., a full and complete parametrization of these operators.

Such a construction addresses an old fundamental question in the theory of measurement [9, 14], namely if it is possible to measure experimentally the 'variables' corresponding to an arbitrary Hermitian operator. Thus, the first question to be solved is finding the 'variables' entering a Hermitian operator. After that, the answer is simple: there does exist an experimental embodiment for every Hermitian operator in finite-dimensional Hilbert space; see [11] for details concerning its realization.

Formally, the states of an n-level quantum system are described by density matrices ρ that are positive, Hermitian operators whose trace is normalized to unity

$$\rho = \{\rho \geqslant 0, \rho = \rho^*, \mathrm{Tr}\,\rho = 1\} \tag{1.2}$$

where * denotes adjoint, i.e., the complex conjugated transpose. If we denote by $D = (\lambda_1, \ldots, \lambda_n)$, the diagonal matrix of ρ eigenvalues, elementary facts from the spectral theory of self-adjoint operators tell us that there exists a unitary operator $U \in U(n)$ generated by the eigenvectors of ρ such that

$$\rho = UDU^* \tag{1.3}$$

with $\sum_1^n \lambda_i = 1$. In particular in the physics literature, U, entering equation (1.3), is considered an element of $SU(n-1)$, that evidently leads to an over-parametrization. Thus when we have to do some symbolical, or even numerical calculations, as in [16] or [12], we have to be more careful. We shall see later that such a U is a matrix realization of the flag manifold

$$X \cong U(n)/U(1)^n \tag{1.4}$$

where $U(1)^n$ denotes the torus subgroup of $U(n)$. By obtaining a full and explicit parametrization of X, we obtain, via formula (1.3), a parametrization of all finite-dimensional Hermitian operators whose spectra are simple. In fact the parameters entering H are within the topological product $\mathbb{R}^n \times \mathrm{Fl}(n)$, where $\mathrm{Fl}(n)$ denotes the flag manifold. As concerns $U(n)$, its parametrization is given by $T^n \times \mathrm{Fl}(n)$, where T^n is the n-dimensional torus. By consequence, the parametrizations of unitary and Hermitian operators are given by different topological sets.

In modern quantum information theory the Stokes–Poincaré–Bloch form [5] of the density matrix is usually used. In this approach, ρ is written as

$$\rho = \frac{I_n}{n} + \frac{1}{2}\sum_{i=1}^{n^2-1} v_i \Lambda_i$$

where $v \in \mathbb{R}^{n^2-1}$ is a real vector and Λ_i is a Hermitian base of $SU(n)$ normalized as $\mathrm{Tr}\,\Lambda_i\Lambda_j = 2\delta_{ij}$. The weak point of that representation is that one cannot easily satisfy the positivity constraint on the spectrum of ρ. Until now only the property $\rho^2 \leqslant 1$ has been used, that leads to the condition $\|v\| \leqslant \sqrt{\frac{2(n-1)}{n}}$ on the norm of the vector v. Only for $n = 2$ is this condition necessary and sufficient for positivity. Recently [1], it was shown that the positivity property can be expressed by the constraints Tr $\rho^k \leqslant 1$, for $k = 2, \ldots, n-1$, which led to complicated relations that the components v_i have to satisfy. Even so, the introduction of ρ in the standard form (1.3) can be done only for $n = 2, 3, 4$ since only then the eigenvalue equation can be solved by known formulae. To give a flavour of what we will do let us consider the case $n = 2$ in the Bloch representation, i.e.,

$$\rho = \frac{I_2}{2} + \frac{1}{2}\sum_1^3 v_1\sigma_i = \frac{1}{2}\begin{pmatrix} 1+v_3 & v_1 - \mathrm{i}v_2 \\ v_1 + \mathrm{i}v_2 & 1 - v_3 \end{pmatrix} \tag{1.5}$$

where σ_i are the Pauli matrices. Its eigenvalues and unnormalized eigenvectors provided by *Mathematica* are

$$\lambda_{1,2} = \frac{1}{2}\big(1 \pm \sqrt{v_1^2 + v_2^2 + v_3^2}\big), \qquad u_{1,2} = \left(\frac{v_3 \pm \sqrt{v_1^2 + v_2^2 + v_3^2}}{v_1 + i v_2}, 1\right). \tag{1.6}$$

Thus, apparently both the eigenvalues and eigenvectors depend on all parameters entering v and there is no way to disentangle them, although in this simplest case it is clear that the eigenvalues depend in fact on a single parameter, the norm of v. By making in (1.5) the change of variable

$$v_3 = \cos 2\varphi \cos 2\alpha \qquad v_2 = \cos 2\varphi \sin 2\alpha \sin 2\beta \qquad v_1 = \cos 2\varphi \sin 2\alpha \cos 2\beta \tag{1.7}$$

we find the eigenvalues $\lambda_1 = \cos^2\varphi$, $\lambda_2 = \sin^2\varphi$, and the matrix of orthonormal eigenvectors

$$M_2 = \begin{pmatrix} \cos\alpha & \sin\alpha \\ \sin\alpha\, \mathrm{e}^{\mathrm{i}\beta} & -\cos\alpha\, \mathrm{e}^{\mathrm{i}\beta} \end{pmatrix} \in \mathrm{Fl}(2) \tag{1.8}$$

and ρ in (1.5) is written as

$$\rho = M_2 \begin{pmatrix} \cos^2\varphi & 0 \\ 0 & \sin^2\varphi \end{pmatrix} M_2^*. \tag{1.9}$$

In the paper, we provide explicit parametrizations of the form (1.9) treating by a unified method the spectral types of Hermitian operators, by properly taking into account their spectral multiplicities. The problem is closely related to the description of isometries between the Hilbert spaces $\mathbb{C}^k$ and $\mathbb{C}^n$, $1 \leqslant k \leqslant n$. The isometries are operators generated by $n \times k$ or $k \times n$ matrices whose columns, and respectively rows, are orthogonal and preserve the vector norms, and in the following we show that there is a close relationship between these isometries and different matrix realizations of the coset spaces generated as in (1.1). The necessity of working with matrices that have orthogonal column vectors, or row vectors, became evident in recent years; see, e.g. [4, 6].

The mathematical background necessary for obtaining such results are elementary facts from the spectral theory of self-adjoint operators and the theory of contraction operators, and a trivial lemma that we state here for the case of the n-dimensional unitary group $G = U(n)$; for the general case see [7].

Lemma 1. *The coset relation*

$$X \cong U(n)/K \tag{1.10}$$

where $K \subset U(n)$ is a subgroup can be written as a matrix relation in the following form:

$$M_n = A_n B_K \tag{1.11}$$

where $M_n \in U(n)$ is an arbitrary $n \times n$ unitary matrix, $A_n \in U(n)$ is a unitary matrix parametrized by a point of the coset X and $B_K \in K$ is an arbitrary element of the subgroup K viewed as an element embedded in $U(n)$.

Using it we obtain new parametrizations of flag, Stiefel and Grassmann manifolds. The paper contains our results concerning the factorization of unitary matrices [3] in terms of n complex vectors $v_i \in S^{2i-1}$, $i = 1, \ldots, n$, where S^k is the k-dimensional sphere in $\mathbb{C}^n$. We denote by $M(n,k)$ the set of all $n \times k$ complex matrices over $\mathbb{C}^n$, and the main mathematical result of the paper is

Main Theorem. *Let $\Im \in M(n,k)$ be an $n \times k$ complex matrix that generates an isometry, i.e., $\Im : \mathbb{C}^k \to \mathbb{C}^n$, $\Im^*\Im = I_k$. Then, the matrix representation of the coset generated by the point $\Im$ is realized in terms of a unitary matrix $A(n,k)$ that diagonalizes the projection D_{T^*}, where D_{T^*} is the defect operator associated with the isometry $\Im$, under the form*

$$I_n - D_{T^*} = A(n,k)\begin{pmatrix} I_k & 0 \\ 0 & 0_{n-k}\end{pmatrix} A(n,k)^* = \sum_{i=1}^{k} c_i \cdot c_i^* = \Im\Im^* \tag{1.12}$$

where c_i, $i = 1, \ldots, k$, are the (orthogonal) column vectors of $\Im$.

All the results discussed in this work are obtained by providing the explicit form of the corresponding objects under study, and are a direct consequence of the above theorem.

The organization of paper is as follows. In section 2, we show the close relationship between the isometries $\Im \in M(n,k)$ and matrix realizations of the coset spaces. In section 3, we reformulate our results [3] in a more convenient form for the present applications, and we find the generic parametrization of n-dimensional Hermitian operators. In section 4, we obtain our matrix parametrizations of Stiefel and Grassmann manifolds.

2. Isometries

In this section, we show how the isometries $\Im \in M(n,k)$ can be used for the parametrization of various interesting manifolds. The main idea is that the isometries generated by k rows, or columns of an arbitrary $n \times n$ matrix, $1 \leqslant k \leqslant n$, allow us to define projection operators whose spectral decomposition provides the necessary tool in finding matrix representations of various interesting manifolds. For what follows, we need a few elementary notions from contraction operator theory.

An operator T mapping the Hilbert space $\mathcal{H}$ to the Hilbert space $\mathcal{H}'$ is a contraction if for any $v \in \mathcal{H}$, $\|Tv\|_{\mathcal{H}'} \leqslant \|v\|_{\mathcal{H}}$, i.e., $\|T\| \leqslant 1$, where $\|T\|$ denotes the norm of T [13]. For any contraction we have $T^*T \leqslant I_{\mathcal{H}}$ and $TT^* \leqslant I_{\mathcal{H}'}$, where T^* denotes the adjoint, that is defined by the relation $(Tv, v') = (v, T^*v')$, $v \in \mathcal{H}$, $v' \in \mathcal{H}'$, and $(\cdot,\cdot)$ is the usual inner product in $\mathcal{H}$, or, respectively,$\mathcal{H}'$. To any contraction T, one associates two defect operators by the relations

$$D_T = (I_{\mathcal{H}} - T^*T)^{1/2}, \qquad D_{T^*} = (I_{\mathcal{H}'} - TT^*)^{1/2} \tag{2.1}$$

that are Hermitian operators in $\mathcal{H}$ and $\mathcal{H}'$, respectively. They have the property

$$TD_T = D_{T^*}T, \qquad T^*D_{T^*} = D_T T^*. \tag{2.2}$$

In the following, we will use only finite-dimensional isometries generated by $n \times k$, or $k \times n$ matrices, and for definiteness we consider the first case, i.e., T has n rows and k columns and we denote it by $\Im$. We are interested in contractions of a special form, namely the isometries between $\mathbb{C}^k$ and $\mathbb{C}^n$. They are operators $\Im : \mathbb{C}^k \to \mathbb{C}^n$ that satisfy $\Im^*\Im = I_k$, $k = 1, \ldots, n$, i.e., the columns of $\Im$ are *orthogonal* columns, and respectively, $\Im : \mathbb{C}^n \to \mathbb{C}^k$ that satisfy $\Im\Im^* = I_k$, when the k rows are *orthogonal*. With our choice, i.e. $\Im$ is an $n \times k$ matrix, we have the identification $\mathcal{H} \equiv \mathbb{C}^k$ and $\mathcal{H}' \equiv \mathbb{C}^n$.

For an isometry $\mathfrak{I}$ generated by k columns, relations (2.1) give $D_T = D_{\mathfrak{I}} = 0$. However, in the following we preserve the notation for the defect operator D_T, to be implied that it is generated by a definite contraction, and from the first relation (2.2) we deduce that

$$D_{T^*}T = TD_T = 0 = D_{T^*}\mathfrak{I} = \lambda\mathfrak{I}, \tag{2.3}$$

i.e., all columns of $\mathfrak{I}$ are in the kernel of D_{T^*}. In other words, the k column vectors are the eigenvectors that correspond to the eigenvalue $\lambda = 0$, and these eigenvectors are orthogonal. When $D_T = 0$, the other defect operator D_{T^*} is a projection, i.e. a self-adjoint operator which satisfies $D_{T^*} = D_{T^*}^2$, and we infer that rank $D_{T^*} = n - k$; thus, $I_n - D_{T^*}$ projects onto the eigenspace corresponding to the eigenvalue $\lambda = 1$. From the preceding relation we get

$$(I_n - D_{T^*})\mathfrak{I} = I_n\mathfrak{I} = \mathfrak{I} = \lambda\mathfrak{I}, \tag{2.4}$$

i.e., the k column vectors of $\mathfrak{I}$ are the orthogonal eigenvectors of $I_n - D_{T^*}$ corresponding to the k eigenvalues $\lambda = 1$, or in other words, rank $(I_n - D_{T^*}) = k$.

For us the interesting objects are the unitary matrices that diagonalize the projections D_{T^*} and $I_n - D_{T^*}$. Let $A(n, k)$ be the unitary matrix which diagonalizes the projection D_{T^*}, then

$$A(n,k)^* D_{T^*} A(n,k) = \begin{pmatrix} 0_k & 0 \\ 0 & I_{n-k} \end{pmatrix} \tag{2.5}$$

and from it we obtain a matrix representation of the projection D_{T^*} under the form

$$D_{T^*} = A(n,k) \begin{pmatrix} 0_k & 0 \\ 0 & I_{n-k} \end{pmatrix} A(n,k)^*. \tag{2.6}$$

The last relation can also be written as

$$A(n,k)^*(I_n - D_{T^*})A(n,k) = \begin{pmatrix} I_k & 0 \\ 0 & 0_{n-k} \end{pmatrix} \tag{2.7}$$

or under the form that will be used in the following:

$$I_n - D_{T^*} = A(n,k) \begin{pmatrix} I_k & 0 \\ 0 & 0_{n-k} \end{pmatrix} A(n,k)^* = \sum_{i=1}^{k} c_i \cdot c_i^* = \mathfrak{I}\mathfrak{I}^* \tag{2.8}$$

where $c_i, i = 1, \ldots, k$, are the column vectors of the isometry $\mathfrak{I}$. Equations (2.6) and (2.8) provide matrix representations for both the projections on the $n - k$-, and respectively k-dimensional, subspaces of $\mathbb{C}^n$. In our applications $A(n, k)$ will be an $n \times n$ unitary matrix generated by a *coset* as in lemma 1, coset, which at its turn, is parametrized by the *point* $\mathfrak{I}$.

The above representation does not provide a full explicit form for the matrix $A(n, k)$, its first k columns coincide with the $\mathfrak{I}$ columns. Thus, an important problem is the *completion* of the matrix $A(n, k)$ with $n-k$ columns *without introducing new parameters*, i.e., the next $n-k$ columns must be determined by the first k columns. To do this we need a parametrization of the first k columns and the most convenient one is to introduce generalized spherical coordinates. In the next section, we show that the most important case is $k = 1$, the other cases being a direct consequence of it, which leads to a factorization of unitary matrices. In the same time, we reformulate our results from [3], concerning factorization of unitary matrices, that will provide the necessary tools for obtaining matrix realizations for symmetric manifolds.

3. Factorization of unitary matrices

The idea behind such a factorization comes from the following sequence:

$$\begin{aligned} U(n) &\cong \frac{U(n)}{U(n-1)} \times \frac{U(n-1)}{U(n-2)} \times \cdots \times \frac{U(2)}{U(1)} \times U(1) \\ &\cong S^{2n-1} \times S^{2n-3} \times \cdots \times S^3 \times S^1 \end{aligned} \tag{3.1}$$

that shows that each factor can be parametrized by an arbitrary point on the corresponding complex sphere.

The matrix realization of formula (3.1), which is the main result in [3], is given by

Theorem 1. *Any element $M_n \in U(n)$ can be factored into an ordered product of n matrices of the following form:*

$$M_n = B_n^0 \cdot B_{n-1}^1 \cdots B_1^{n-1} \tag{3.2}$$

where

$$B_{n-k}^k = \begin{pmatrix} I_k & 0 \\ 0 & B_{n-k} \end{pmatrix}$$

and $B_{n-k} \in U(n-k)$ are special unitary matrices, each one generated by a single complex $(n-k)$-dimensional unit vector, $b_{n-k} \in S^{2(n-k)-1}$. For example $B_1 = \mathrm{e}^{\mathrm{i}\varphi}$, where φ is an arbitrary phase.

If $y_m \in S^{2m-1}$, $m = 1, \ldots, n$, is parametrized by

$$y_m = (\mathrm{e}^{\mathrm{i}\varphi_1}\cos\theta_1, \mathrm{e}^{\mathrm{i}\varphi_2}\sin\theta_1\cos\theta_2, \ldots, \mathrm{e}^{\mathrm{i}\varphi_m}\sin\theta_1, \ldots, \sin\theta_{m-1})^t$$

where t denotes transpose, the m columns of B_m are given by

$$v_1 = y_m = \begin{pmatrix} \mathrm{e}^{\mathrm{i}\varphi_1}\cos\theta_1 \\ \mathrm{e}^{\mathrm{i}\varphi_2}\sin\theta_1\cos\theta_2 \\ \cdot \\ \cdot \\ \cdot \\ \mathrm{e}^{\mathrm{i}\varphi_m}\sin\theta_1, \ldots, \sin\theta_{m-1} \end{pmatrix}$$

and

$$v_{k+1} = \frac{\mathrm{d}}{\mathrm{d}\theta_k} v_1(\theta_1 = \cdots = \theta_{k-1} = \pi/2), \qquad k = 1, \ldots, m-1,$$

where in the above formula one calculates first the derivative and afterwards the restriction to $\pi/2$.

For our aims we need an explicit parametrization of B_{n-k}, $k = 0, \ldots, n-1$, and we choose the n generating vectors of B_n as follows:

$$\begin{aligned} y_n &= (\mathrm{e}^{\mathrm{i}\alpha_1}\cos a_1, \mathrm{e}^{\mathrm{i}\alpha_2}\sin a_1\cos a_2, \ldots, \mathrm{e}^{\mathrm{i}\alpha_n}\sin a_1, \ldots, \sin a_{n-1})^t \\ y_{n-1} &= (\mathrm{e}^{\mathrm{i}\beta_1}\cos b_1, \mathrm{e}^{\mathrm{i}\beta_2}\sin b_1\cos b_2, \ldots, \mathrm{e}^{\mathrm{i}\beta_{n-1}}\sin b_1, \ldots, \sin b_{n-2})^t \\ &\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots \\ y_2 &= (\mathrm{e}^{\mathrm{i}\psi_1}\cos z_1, \mathrm{e}^{\mathrm{i}\psi_2}\sin z_1)^t \\ y_1 &= \mathrm{e}^{\mathrm{i}\omega_1}. \end{aligned} \tag{3.3}$$

The projection operator $I_n - D_{T^*}$ entering formula (2.8) is a self-adjoint operator, and for such an operator its eigenvectors c_i are defined up to an overall phase. We choose the phases such that the first entry of each eigenvector is nonnegative. With the generating vectors of the form (3.3), the parametrization of the matrix (3.2), given by theorem 1, is such that its first row entries have the form

$$\begin{aligned} &m_{11} = \mathrm{e}^{\mathrm{i}\alpha_1}\cos a_1, \qquad m_{12} = -\mathrm{e}^{\mathrm{i}(\alpha_1+\beta_1)}\cos b_1\sin a_1, \\ &m_{13} = \mathrm{e}^{\mathrm{i}(\alpha_1+\beta_1+\gamma_1)}\cos c_1\sin a_1\sin b_1, \ldots, \\ &m_{1n} = (-1)^{n-1}\mathrm{e}^{\mathrm{i}(\alpha_1+\cdots+\omega_1)}\sin a_1\cdots\sin z_1 \end{aligned} \tag{3.4}$$

and if we require that these matrix elements be nonnegative we have to take

$$\alpha_1 = 0, \qquad \beta_1 = \gamma_1 = \cdots = \omega_1 = \pi. \tag{3.5}$$

In the following, we shall use these constraints in relations (3.3), and so we remove the first phase of each of the vectors y_k and change the numbering as $\alpha_i \to \alpha_{i-1}$, $i = 2, \ldots, n$, $\beta_i \to \beta_{i-1}$, $i = 2, \ldots, n-1$, etc, and now each vector y_k is parametrized by $2(k-1)$ parameters, $k = 2, \ldots, n$, i.e., an equal number of phases and angles. In this way, the last vector is a number, $y_1 = -1$, such that B^1_{n-1} is the constant diagonal matrix with diagonal $(I_{n-1}, -1)$, and relation (3.2) has the following form:

$$\mathfrak{M}_n = B^0_n \cdot B^1_{n-1} \cdots B^{n-1}_1. \tag{3.6}$$

The last matrix is the matrix realization of the flag manifold

$$\mathrm{Fl}(n) \cong \frac{U(n)}{U(1) \times U(1) \times \cdots \times U(1)} \cong \frac{U(n)}{U(1)^n} \tag{3.7}$$

it depends on $n(n-1)$ parameters and it is the most general form of a unitary matrix that diagonalizes an n-dimensional Hermitian operator H all of whose eigenvalues are simple.

Putting together the information contained in theorem 1 and formulae (3.6) and (3.7) we have the following:

Corollary 1. *The matrix $\mathfrak{M}_n$ describes the spectral decomposition of a finite-dimensional Hermitian operator H whose eigenvalues are simple, i.e., they satisfy a relation as*

$$\lambda_1 > \lambda_2 > \cdots > \lambda_n$$

and the operator H is written in the form

$$H = \mathfrak{M}_n \Lambda \mathfrak{M}^*_n = \sum_{i=1}^{n} \lambda_i u_i u^*_i \tag{3.8}$$

where u_i, $i = 1, \ldots, n$, are the column vectors of the matrix (3.6) and Λ is the diagonal matrix of eigenvalues. If $H \geqslant 0$ and $\mathrm{Tr}\, H = h \in \mathbb{R}^*_+$, then λ_i, entering formula (3.12), could be parametrized as

$$\lambda_1 = h\cos^2\theta_1, \qquad \lambda_2 = h\sin^2\theta_1\cos^2\theta_2, \ldots, \qquad \lambda_n = h\sin^2\theta_1\cdots\sin^2\theta_{n-1} \tag{3.9}$$

where $\theta_i \in [0, \pi/2]$, $i = 1, \ldots, n-1$, are arbitrary angles. If H is a density operator, $h = 1$ in the above relation.

If H is not positive definite, let us suppose that its first p eigenvalues are positive and $n - p$ are negative. If $\mathrm{Tr}\, H = 0$ and $h = \mathrm{Tr}\, H_{\lambda_i>0} = -\mathrm{Tr}\, H_{\lambda_i<0} \in \mathbb{R}^*_+$, then a parametrization of eigenvalues is given by

$$\lambda_1 = h\cos^2\theta_1, \qquad \lambda_2 = h\sin^2\theta_1\cos^2\theta_2, \ldots, \qquad \lambda_p = h\sin^2\theta_1\cdots\sin^2\theta_{p-1}, \tag{3.10}$$

$$\lambda_{p+1} = -h\cos^2\theta_p, \ldots, \qquad \lambda_n = -h\sin^2\theta_p\cdots\sin^2\theta_{n-1}. \tag{3.11}$$

If $\mathrm{Tr}\, H = h \neq 0$, the parametrization of eigenvalues is given by

$$\lambda_1 = |h|\cosh^2\theta, \qquad \lambda_2 = |h|\cosh^2\theta\cos^2\theta_1, \ldots,$$

$$\lambda_p = |h|\cosh^2\theta\sin^2\theta_1\cdots\sin^2\theta_{p-2} \tag{3.12}$$

$$\lambda_{p+1} = -|h|\sinh^2\theta, \ldots, \qquad \lambda_n = -|h|\sinh^2\theta\sin^2\theta_{p-1}\cdots\sin^2\theta_{n-2} \tag{3.13}$$

if $h > 0$, where $\theta \in \mathbb{R}^*_+$, $\theta_i \in [0, \pi/2]$, $i = 1, \ldots, n-2$, are arbitrary angles, and by a similar formula in which one interchanges $ch^2\theta \rightleftharpoons sh^2\theta$, if $h < 0$.

In this way, corollary 1 gives a simple and explicit parametrization of all generic finite-dimensional Hermitian operators.

4. Matrix realizations of Stiefel and Grassmann manifolds

Looking at relation (3.7) we consider that the next, simpler, manifold is the Stiefel manifold that we define as the coset space

$$\mathrm{St}(k,n) \cong \frac{U(n)}{U(1)^k \times U(n-k)} \cong \frac{\mathrm{Fl}(n)}{\mathrm{Fl}(n-k)} \tag{4.1}$$

instead of the usual definition

$$\mathrm{St}(k,n) \cong \frac{U(n)}{U(n-k)}. \tag{4.2}$$

Both forms are similar, only the number of parameters entering them is different. According to lemma 1 we can write the first relation (4.1) as a matrix relation

$$M_n = A(n,k)\begin{pmatrix} I_k & 0 \\ 0 & M_{n-k}\end{pmatrix} \tag{4.3}$$

where $M_n \in U(n)$, $M_{n-k} \in U(n-k)$ and $A(n,k) \in \mathrm{Fl}(n)$ is the matrix realization of the Stiefel manifold $\mathrm{St}(k,n)$ parametrized by a point represented by an $n \times k$ complex matrix, with the first row entries being nonnegative numbers. Alternatively, we may consider that $M_n \in \mathrm{Fl}(n)$, $M_{n-k} \in \mathrm{Fl}(n-k)$. Looking at relation (2.8) we see that $A(n,k)$ is the same object in both relations (2.8) and (4.3). By consequence we deduce from (3.6) that

$$A(n,k) = B_n^0 \cdot B_{n-1}^1 \cdots B_{n-k+1}^{k-1} \tag{4.4}$$

is the matrix realization of the Stiefel manifold (4.1). Thus, the following holds:

Theorem 2. *The matrix representation of the Stiefel manifold* $\mathrm{St}(k,n)$ *as defined by (4.1) is obtained from the parametrization (3.6) by taking zero all the parameters entering* $U(n-k)$*, i.e.,* $U(n-k) = I_{n-k}$ *such that*

$$\mathfrak{A}(n,k) = B_n^0 \cdot B_{n-1}^1 \cdots B_{n-k+1}^{k-1}. \tag{4.5}$$

The matrix representation of the projection $I_n - D_{T^*}$ *writes*

$$I_n - D_{T^*} = \mathrm{St}(k,n) = c_1c_1^* + \cdots + c_kc_k^* \tag{4.6}$$

where $c_i, i = 1, \ldots, k$ *are the first* k *column vectors of (4.5). As long as the matrix (4.5) is parametrized by* $d = n^2 - k - (n-k)^2 = k(2n-k-1)$ *real parameters, we can choose any* k *column vectors of (4.5) in formula (4.6) and we can make this choice in* $\binom{n}{k}$ *modes. A similar formula can be obtained for a Stiefel manifold defined as in (4.2)*

As a consequence of the above theorem, we have the following

Corollary 2. *The matrix (4.5) describes the spectral decomposition of a finite-dimensional Hermitian operator* H *that has a degenerate eigenvalue of multiplicity* k, $\lambda_1 = \cdots = \lambda_k$*, and all the other eigenvalues are simple. In this case,* H *writes*

$$H = \mathfrak{A}(n,k)\Lambda\mathfrak{A}(n,k)^* = \lambda_1 \sum_{j=1}^{k} u_ju_j^* + \sum_{i=1}^{n-k} \lambda_{k+i}u_{i+k}u_{i+k}^* \tag{4.7}$$

where $u_i, i = 1, \ldots, n$*, are the column vectors of the matrix (4.5). If* H *is a density operator, then*

$$\lambda_1 = \cos^2\theta_1/k,\ \lambda_{k+1} = \sin^2\theta_1\cos^2\theta_2, \ldots, \qquad \lambda_n = \sin^2\theta_1\sin^2\theta_2\cdots\sin^2\theta_{n-k-1}$$

where $\theta_i \in [0, \pi/2], i = 1, \ldots, n-k-1$*, are arbitrary angles. If* H *is not positive definite, the eigenvalues are parametrized by similar formulae, as in corollary 1.*

The Grassmann manifold, $\mathrm{Gr}(k, n)$, is defined as the set of all k-dimensional subspaces of $\mathbb{C}^n$, and $\mathrm{Gr}(k, n)$ is viewed as the coset space

$$\mathrm{Gr}(k, n) \cong \frac{U(n)}{U(k) \times U(n-k)} \cong \frac{\mathrm{Fl}(n)}{\mathrm{Fl}(k) \times \mathrm{Fl}(n-k)} \tag{4.8}$$

and by consequence the real dimension of the Grassmann manifold $\mathrm{Gr}(k, n)$ equals

$$d_1 = n^2 - k^2 - (n-k)^2 = 2k(n-k). \tag{4.9}$$

As in the case of Stiefel manifolds, we want first to obtain a parametrization of $A(n, k)$ which is equivalent with finding a parametrization of Grassmannians. With that end in view we rewrite relation (4.9) into the form

$$M_n = A(n, k) \begin{pmatrix} B_k & 0 \\ 0 & I_{n-k} \end{pmatrix} \times \begin{pmatrix} I_k & 0 \\ 0 & C_{n-k} \end{pmatrix} \tag{4.10}$$

where $M_n \in U(n)$ is an arbitrary matrix from $U(n)$ and $B_k \in U(k)$ and, respectively, $C_{n-k} \in U(n-k)$.

If we look at relations (3.6) or (4.5) and consider one of them for the case $k = 1$, we observe that B_n^0 is equal to $A(n, 1)$. Thus, we obtain a matrix representation for

$$I_n - P = \mathrm{Gr}(1, n) = A(n, 1) \begin{pmatrix} 1 & 0 \\ 0 & 0_{n-1} \end{pmatrix} A(n, 1)^*, \tag{4.11}$$

i.e., the simplest Grassmannian, a result already known. The preceding relation can be written in an equivalent form as

$$\mathrm{Gr}(1, n) = v_1 \cdot v_1^* \tag{4.12}$$

where v_1 is the vector that generates B_n^0, i.e., the vector y_n from relation (3.3). Thus, $A(n, 1)$ can be obtained from (3.6) by taking all the phases and angles entering $U(n-1)$ equal to zero, i.e., $U(n-1) = I_{n-1}$.

In the following, we show that $A(n, k)$ can be obtained in a similar way. Taking into account the form of the projection operator $I_n - P$ and the dimensions d and d_1 for Stiefel and Grassmann manifolds, respectively, we infer that the Grassmann manifold is a special case of a Stiefel manifold. Our problem now is to find those constraints which lead to the correct parametrization of $A(n, k)$ for Grassmannians.

In order to view which are the constraints, let us consider the case $k = 2$. By taking into account that the first column of $A(n, 2)$ coincides with the vector v_1 that generates the matrix (4.12), we infer from (4.9) that the parametrization of the second column is given in terms of $2(n-3)$ new real parameters. This means that we have to remove an angle and a phase from the vector y_{n-1}, equation (3.3). A convenient choice is to take equal to zero the last angle and phase, i.e., $b_{n-2} = \beta_{n-2} = 0$. This choice induces the following form for the matrix B_{n-1}^1:

$$B_{n-1}^1(b_{n-2} = \beta_{n-2} = 0) = B_{n-1}^{1,1} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & B_{n-2} & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{4.13}$$

where B_{n-2} is generated as in theorem 1 by the vector

$$y'_{n-2} = (\cos b_1, \mathrm{e}^{\mathrm{i}\beta_1} \sin b_1 \cos b_2, \ldots, \mathrm{e}^{\mathrm{i}\beta_{n-3}} \sin b_1 \cdots \sin b_{n-3})^t. \tag{4.14}$$

It is easily seen that this structure preserves from $k \to k+1$ such that

$$B_{n-k}^{k,k} = \begin{pmatrix} I_k & 0 & 0 \\ 0 & B_{n-2k} & 0 \\ 0 & 0 & I_k \end{pmatrix}, \qquad k = 1, \ldots, \left[\frac{n}{2}\right] \tag{4.15}$$

where $[a]$ denotes the integer part of a, and B_{n-2k}, $k = 1, \ldots, [\frac{n}{2}]$, are generated by the vectors

$$
\begin{aligned}
w_1 &= (\cos a_1, e^{i\alpha_1} \sin a_1 \cos a_2, \ldots, e^{i\alpha_{n-1}} \sin a_1 \cdots \sin a_{n-1})^t \\
w_2 &= (\cos b_1, e^{i\beta_1} \sin b_1 \cos b_2, \ldots, e^{i\beta_{n-3}} \sin b_1 \cdots \sin b_{n-3})^t \\
&\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots \\
w_p &= (\cos l_1, e^{i\varphi_1} \sin l_1 \cos l_2, \ldots, e^{i\varphi_{n-(2p-1)}} \sin l_1 \cdots \sin l_{n-(2p-1)})^t \\
&\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots \\
w_{[n/2]} &= (\cos z_1, e^{i\omega_1} \sin z_1 \cos z_2, e^{i\omega_2} \sin z_1 \sin z_2)^t, \qquad \text{for } n \text{ odd} \\
w_{[n/2]} &= (\cos z_1, e^{i\omega_1} \sin z_1)^t, \qquad \text{for } n \text{ even.}
\end{aligned}
\tag{4.16}
$$

With the above notation the following holds:

Theorem 3. *The unitary matrix $A(n,k) \equiv \mathfrak{G}(n,k) \in \mathrm{Fl}(k, n-k; n)$ entering the matrix representation of Grassmann manifold has the form*

$$\mathfrak{G}(n,k) = B_n^0 \cdot B_{n-1}^{1,1} \cdots B_{n-k+1}^{k-1,k-1}, \qquad k = 1, \ldots, \left[\frac{n}{2}\right] \tag{4.17}$$

and the matrix representation of the projection onto the k-dimensional subspace of $\mathbb{C}^n$ is

$$I_n - D_{T^*} = \mathrm{Gr}(k,n) = \mathfrak{G}(n,k) \begin{pmatrix} I_k & 0 \\ 0 & 0 \end{pmatrix} \mathfrak{G}(n,k)^*. \tag{4.18}$$

An equivalent description is given by

$$\mathrm{Gr}(k,n) = \sum_1^k u_i \cdot u_i^* \tag{4.19}$$

where u_i, $i = 1, \ldots, k$, are the first k column vectors of matrix (4.17).

Corollary 3. *If H is a Hermitian operator that has only two eigenvalues whose multiplicities are k and $n-k$ then*

$$H = \mathfrak{G}(n,k) \Lambda \mathfrak{G}(n,k)^* = \lambda_1 \sum_{i=1}^k u_i u_i^* + \lambda_2 \sum_{i=k+1}^n u_i u_i^* \tag{4.20}$$

where u_i, $i = 1, \ldots, n$, are the column vectors of the matrix $\mathfrak{G}(n,k)$, equation (4.17). If H is a density matrix operator, then $\lambda_1 = \cos^2\theta/k$ and $\lambda_2 = \sin^2\theta/(n-k)$, where $\theta \in [0, \pi/2]$ is an arbitrary angle. When H is not positive definite and $\mathrm{Tr}\, H = h$, *the parametrization of eigenvalues is: $\lambda_1 = h\cosh^2\theta$ and $\lambda_2 = -h\sinh^2\theta$, if $\lambda_1 > |\lambda_2|$, and $\lambda_1 = |h|\sinh^2\theta$ and $\lambda_2 = -|h|\cosh^2\theta$, if $h < 0$.*

Matrix realization of other flag manifolds, as e.g.,

$$\mathrm{Fl}(k_1, k_2, \ldots, k_l, ; n) \cong \frac{\mathrm{Fl}(n)}{\mathrm{Fl}(k_1) \times \mathrm{Fl}(k_2) \times \cdots \times \mathrm{Fl}(k_l)} \tag{4.21}$$

with $\sum_i^l k_i \leqslant n$ that describe other spectral multiplicities, can be found in a similar way. Assembling together all the previous information we have

Corollary 4. *The flag matrix (3.6) encodes all the possible spectral decompositions of finite-dimensional Hermitian operators, acting on $\mathbb{C}^n$, i.e., any other particular unitary matrix $A(n,k)$ that describes a given spectral multiplicity of a Hermitian operator can be obtained from it by properly restricting the number of parameters entering (3.6).*

5. Conclusion

In this paper, we have obtained a constructive parametrization of all finite-level Hermitian operators. Further, this construction is recursive: if we have a parametrization of $\mathfrak{M}_n$, $\mathfrak{M}_{n+2}$ is obtained by embedding $\mathfrak{M}_n$ into $\mathfrak{M}_{n+2}$ and by multiplication at left by an appropriate matrix. We have shown that the unitary matrices which diagonalize the Hermitian operators are subsets of the flag unitary matrix $\mathfrak{M}_n$ whose explicit form is given by formula (3.6). When the eigenvalues are simple, the generic form of the unitary operators is $\mathfrak{M}_n$; when there is a k-fold degeneracy, the corresponding unitary matrices are in the set $\mathrm{St}(k, n)$. If there is a maximum degeneracy, i.e., only two eigenvalues, with multiplicities k and, respectively $n-k$, are distinct, the unitaries are in the Grassmannian $\mathrm{Gr}(k, n)$. Our explicit construction was done only for the n-dimensional unitary group $U(n)$, but it is evident that the same approach works in the case of any compact group. For example, taking as zero all the phases entering $U(n)$ and doing similar calculations, one gets results for $SO(n)$ and so on.

We consider that the above parametrization will be useful for doing calculation, especially for problems where one has to make an optimization over a set of parameters, e.g., for the characterization of entanglement.

Taking also into account our previous results [3], which state that any unitary matrix entering $\mathfrak{M}_n$ is an ordered product of $n-1$ diagonal phase matrices and $n(n-1)/2$ two-dimensional rotations, one can make use of the device designed by Reck *et al* [11] to give an operational meaning in the real world to any finite-level Hermitian operator. This means that all the Hermitian matrices could be experimentally implemented and, as a consequence, could be measured. Such multi-state devices will find applications in quantum information processing and quantum computation.

At the same time, we obtained a new and simple analytic representation of Stiefel and Grassmann manifolds, a representation that is essentially contained in a unitary matrix $A(n, k)$, which can easily be stored in a computer, and problems similar to those encountered in [4, 10], or [15] will be easier to solve.

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I would like to thank the anonymous referee of my paper [3] who recommended the following:

> [. . .] I recommend that the factorization theorem be stated clearly in the early part of the paper and that it be followed by a construction algorithm. [. . .]

Finding explicitly this algorithm I realized that it can be used to obtain novel matrix realizations for compact symmetric manifolds.

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