Geometric phases and Bloch-sphere constructions for SU(N) groups with a complete description of the SU(4) group

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A two-sphere ("Bloch" or "Poincare") is familiar for describing the dynamics of a spin-1/2 particle or light polarization. Analogous objects are derived for unitary groups larger than SU(2) through an iterative procedure that constructs evolution operators for higher-dimensional SU(*N*) in terms of lower-dimensional ones. We focus, in particular, on the SU(4) of two qubits which describes all possible logic gates in quantum computation and entangled states in quantum-information sciences. For a general Hamiltonian of SU(4) with 15 parameters, and for Hamiltonians of its various subgroups so that fewer parameters suffice, we derive Blochlike rotation of unit vectors analogous to the one familiar for a single spin in a magnetic field. The unitary evolution of a quantal spin pair is thereby expressed as rotations of real, many-dimensional vectors. Correspondingly, the manifolds involved are Bloch two-spheres along with higher dimensional manifolds such as a four-sphere for the SO(5) subgroup and an eight-dimensional Grassmannian manifold for the general SU(4). The latter may also be viewed as two, mutually orthogonal, real six-dimensional unit vectors moving on a five-sphere with an additional phase constraint. This geometrical picture for two spins provides the extension and generalization of the Bloch sphere that has proved invaluable for the understanding of the dynamics of a single spin.

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I. INTRODUCTION: BLOCH SPHERE AND ITS EXTENSION

In the study of the dynamics of a spin-1/2 particle, a visual metaphor that has played a powerful role is that of the "Bloch sphere" [1]. Pure states of the system are represented by the tip of a vector from the origin to the surface of such a unit sphere S^2 . In the field of nuclear magnetic resonance (NMR) [2] and elsewhere, transformations between states are then viewed as rotations of that vector, described by the Bloch equation of motion, $\vec{m} = -2\vec{B} \times \vec{m}$, for a magnetic moment in a magnetic field B. Thus various sequences of NMR manipulations can be pictured in a nice geometrical way as successive rotations of three-dimensional vectors, and this has now become central to our intuition of spin dynamics. The relevant group of unitary transformations is SU(2), a rank-one, three-parameter group that is the double covering group of the three-dimensional rotation group SO(3) [3]. The three operators of angular momentum, (J_x, J_y, J_z) , are the generators of these groups. A canonical set of parameters of SO(3) are the Euler angles. Integer values $j=0,1,\ldots$ provide various (2j+1)-dimensional representations, while for SU(2), the half-odd integers occur as well.

While the Bloch sphere S^2 is familiar, the full SU(2) has three parameters, the third being a phase at each point of the sphere. Representing this one-dimensional U(1) parameter by a line or spike, the complete picture is of a spiked sphere shown in Fig. 1 that is somewhat less familiar. Mathematicians refer to this as the "fiber bundle," SU(2)= $S^2 \times U(1)$ [4]. This latter phase is often not accessible as, for instance, when dealing with the density matrix ρ but the general state of spin-1/2 and the unitary evolution operator depend on all three parameters. The S^2 sphere is referred to as a "base manifold" and the U(1) phase as a "fiber."

Mixed states also are naturally accommodated in this geometrical picture. Their density matrices are represented by points inside the Bloch sphere so that the vector is of length less than unity. Correspondingly, $\text{Tr } \rho^2 < \text{Tr } \rho$, which constitutes a definition of a mixed state [5]. States of light polarization, also a two-valued object, map onto the same mathematics and geometry through the "Poincare" sphere [6].

It would be of interest to have analogous geometrical pictures for multiple spins, especially in today's fields of quantum computation, cryptography, and teleportation, because the fundamental elements of these subjects are built up of a few qubits [7]. Thus all logic gates for quantum computation can be built up from qubit pairs, while teleporting one qubit state requires an entangled pair held by the sender and re-

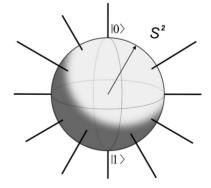


FIG. 1. The fiber bundle for SU(2), with the Bloch sphere as a base manifold, and spikes at each point representing a phase. The three parameters defining a point on the sphere and a phase value there provide the complete description of the dynamics of a spin-1/2 system.

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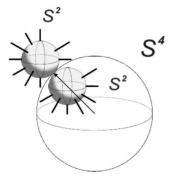


FIG. 2. Analogous to Fig. 1, for a two-qubit system that involves an so(5) subalgebra of the full SU(4). The base manifold now is a four-sphere S^4 , at each point of which is a fiber consisting of two spiked-spheres of SU(2) as in Fig. 1. See Sec. III for a full derivation and discussion.

ceiver, for a total of three qubits. With $SU(2^p)$ being the relevant group for p qubits, this calls for a similar geometrical description of higher SU(N). In this paper, we develop such a picture, through an easily accessible procedure which iteratively descends from N to N-n, with n < N, in a manner that closely follows the description of SU(2). While the number of parameters, $N^2 - 1$, is larger and, therefore, the dimensions of the geometrical objects correspondingly larger and more complex than a globelike sphere, a geometrical description still has merit. In some cases, it is also rather easily accessible; for example, in two-qubit problems that involve a subset of 10 of the full set of 15 parameters of SU(4), Fig. 2 shows a base manifold of a S^4 sphere and a "fiber" of two SU(2) spiked-spheres at each point on its surface as the analog of Fig. 1 for such problems. Rotations of a unit fivedimensional vector on S^4 , together with two single-spin SU(2) dynamics, provide a geometrical picture of two-spin dynamics. We will return in Sec. III to a full discussion and derivation of this figure, and consider the more complex manifold describing the full SU(4) in Sec. IV.

Our procedure also applies when N is odd, a situation that does not arise with qubits but elsewhere widely in physics [for example, qutrits [8], neutrino oscillations [9], the quark model, and quantum chromodynamics (QCD), etc.]. The N $\times N$ matrices of Hamiltonians and evolution operators are viewed as built up of 2×2 block matrices through this N =(N-n)+n decomposition, the block matrices then described in terms of the Pauli spinors of SU(2). Each step of this iterative reduction introduces an analog of the Bloch sphere, albeit of higher dimension and more complex structure, and constructs the effective Hamiltonians of dimension (N-n) and n for the next step. In this manner, using no more than the operations familiar from the SU(2) case, the full construction for SU(N) is achieved.

The philosophy behind such a construction may be seen as generalizing Schwinger's philosophy for representations of SU(2) or SO(3), where higher *j* representations are constructed from those of the fundamental, j=1/2 [10]. We now do the analogous step of using SU(2) as the template for solving larger SU(*N*). In particular, for the important case of SU(4) for two qubits, we give a complete description of the manifolds and phases involved and analytical expressions for them. Note again, as with light polarization and spin-1/2, that the mathematics of *N*-level systems in quantum optics, atomic and molecular physics, and elsewhere, is the same as that we describe in the language of multiple qubits. This provides an even wider context for our results.

The arrangement of this paper is as follows. Section II describes the basic iterative decomposition of the evolution operator for SU(N), mimicking the familiar procedure for spin-1/2. With N=4, and n=2, Sec. III specializes the results to SU(4), the case of two qubits, when all the manipulations involved are in terms of Pauli spinors. It also applies these results to Hamiltonians involving a restricted set of operators of the full group. An interesting one is SO(5), which can be described by a 5×5 antisymmetric matrix that is the analog of the 3×3 antisymmetric one for the magnetic field B in the Bloch equation. Section IV then considers Hamiltonians requiring the full SU(4) group for their description. Linear equations, analogous to the Bloch equation, are derived in terms of vectors \vec{m} , five- and six-dimensional vectors, respectively, for the SO(5) and full SU(4) cases. The latter also correspond to so-called "Plücker coordinates" [11] which are also presented. Appendix A deals with the generalization to non-Hermitian Hamiltonians, and Appendix B presents the isomorphism between SU(4) and the groups Spin(6) and SO(6) which we exploit.

II. ITERATIVE CONSTRUCTION OF EVOLUTION OPERATOR IN N DIMENSIONS

We wish to obtain the evolution operator $\mathbf{U}^{(N)}(t)$ for the *N*-dimensional time-dependent Hamiltonian $\mathbf{H}^{(N)}$:

$$\mathbf{H}^{(N)}(t) = \begin{pmatrix} \mathbf{H}^{(N-n)}(t) & \mathbf{V}(t) \\ \mathbf{V}^{\dagger}(t) & \mathbf{H}^{(n)}(t) \end{pmatrix}.$$
 (1)

We have blocked the Hamiltonian into (N-n)- and *n*-dimensional blocks, the diagonal blocks being square matrices while the off-diagonal **V** is $(N-n) \times n$ and **V**[†] is $n \times (N-n)$. Although our discussion is for Hermitian **H**^(N), the procedure can also apply more generally, in which case the off-diagonal blocks will not be simply related as adjoints (see Appendix A). We will also assume **H**^(N) to be traceless, again a restriction that can be easily relaxed, the time integral of the trace becoming an overall phase of **U**^(N).

To solve the evolution equation, with an overdot denoting derivative with respect to time,

$$i\dot{\mathbf{U}}^{(N)}(t) = \mathbf{H}^{(N)}(t)\mathbf{U}^{(N)}(t), \quad \mathbf{U}^{(N)}(0) = \mathbf{I},$$
 (2)

we similarly block the unitary matrix, writing it as a product of three factors, the first two further grouped as \tilde{U}_1 and the second, \tilde{U}_2 , block-diagonal in form:

$$\begin{split} \mathbf{U}^{(N)}(t) &= \widetilde{\mathbf{U}}_1 \widetilde{\mathbf{U}}_2, \quad \widetilde{\mathbf{U}}_1 = e^{\mathbf{z}(t)A_+} e^{\mathbf{w}^{\top}(t)A_-}, \\ \widetilde{\mathbf{U}}_1 &= \begin{pmatrix} \mathbf{I}^{(N-n)} & \mathbf{z}(t) \\ \mathbf{0}^{\dagger} & \mathbf{I}^{(n)} \end{pmatrix} \begin{pmatrix} \mathbf{I}^{(N-n)} & \mathbf{0} \\ \mathbf{w}^{\dagger}(t) & \mathbf{I}^{(n)} \end{pmatrix}, \end{split}$$

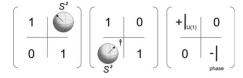


FIG. 3. Structure of the 2×2 matrix evolution operator in Eq. (3) for SU(2). The three factors involve, respectively, the Pauli spinors σ_+ , σ_- , and σ_z . A single complex number *z* provides the first two matrices, shown schematically as the Bloch sphere obtained through inverse stereographic projection. The third factor is a diagonal matrix, defined through a single number or phase, which enters with opposite signs in the two entries. The complete fiber bundle, SU(2): $S^2 \times U(1)$, in Fig. 1 may be viewed in the above factorized form. The same form of three factors can be generalized, as discussed in later sections, to any SU(*N*), with the first two factors providing the base manifold and the third the fiber.

$$\widetilde{\mathbf{U}}_{2} = \begin{pmatrix} \widetilde{\mathbf{U}}^{(N-n)}(t) & \mathbf{0} \\ \mathbf{0}^{\dagger} & \widetilde{\mathbf{U}}^{(n)}(t) \end{pmatrix},$$
(3)

where A_{\pm} are matrix generalizations of the Pauli spin step-up and step-down σ_{\pm} , and **z** and **w**[†] are rectangular matrices of complex parameters. A remark about notation: we will use the symbol tilde when the corresponding Hamiltonians may not be Hermitian or evolution operators unitary.

The above structure, with $\tilde{\mathbf{U}}_1$ having blocks of zero in the lower and upper off-diagonal blocks of its matrix factors, is crucial in our method. For the case of spin-1/2 and SU(2), the form of a product of three factors, each an exponentiation of one of the Pauli spinors, is well-known [3]. Their Cartesian form, with Euler angles in the exponents, is the familiar choice but we choose instead the triplet, $(\sigma_{\pm}, \sigma_{z})$, when the first two factors have zero off-diagonal entries. This introduces complex numbers z and w^{\dagger} in place of the Euler angles, and makes the individual factors in Eq. (3) not separately unitary although our construction ensures unitarity of the full $\mathbf{U}^{(N)}(t)$. The unitarity implies a simple relationship between w and z, so that only one is independent. In turn, this complex number z maps through an inverse stereographic transformation into the Bloch sphere, so that $\tilde{\mathbf{U}}_1$ describes the base manifold and the diagonal \mathbf{U}_2 the fiber phase. This is schematically represented in Fig. 3. The separation into base and fiber through these two factors carries over to the case of general SU(N), the matrix z describing the former. The last factor in Eq. (3) is block diagonal, with equal and opposite phase factors of $\exp(-i\mu\sigma_z)$ for a single spin-1/2. For larger SU problems, the diagonal blocks involve more than just a number but, nevertheless, this last factor is diagonal, each block being a lower-dimensional SU problem and both together providing the fiber in describing SU(N). This form in Eq. (3) proves most convenient for decomposing the evolution operator for any SU(N) into its base and fiber manifolds.

Interestingly, for non-Hermitian H when U is nonunitary, our construction still applies. The specific structure of an upper and lower triangular matrix and a diagonal one proves fruitful, giving simpler equations for \mathbf{z} and \mathbf{w}^{\dagger} , which will

have at most quadratic nonlinearity in these parameters and not more complicated trigonometric dependences as with the Euler angle decomposition [12,13]. In this nonunitary case, **z** and \mathbf{w}^{\dagger} are independent, our construction providing the requisite equations for both of them (see Appendix A); but, for the unitary case, unitarity of the full $\mathbf{U}^{(N)}(t)$ leads to relations between **z** and \mathbf{w}^{\dagger} :

$$\mathbf{z} = -\mathbf{w} \, \boldsymbol{\gamma}_2 = - \, \boldsymbol{\gamma}_1 \mathbf{w},$$
$$\boldsymbol{\gamma}_1 \equiv \widetilde{\mathbf{U}}^{(N-n)} \widetilde{\mathbf{U}}^{(N-n)\dagger} = \mathbf{I}^{(N-n)} + \mathbf{z} \mathbf{z}^{\dagger},$$
$$\boldsymbol{\gamma}_2^{-1} \equiv \widetilde{\mathbf{U}}^{(n)} \widetilde{\mathbf{U}}^{(n)\dagger} = (\mathbf{I}^{(n)} + \mathbf{z}^{\dagger} \mathbf{z})^{-1}.$$
(4)

With $\mathbf{U} = \widetilde{\mathbf{U}}_1 \widetilde{\mathbf{U}}_2$, Eq. (2) formally reduces to the evolution of $\widetilde{\mathbf{U}}_2$ alone with an effective Hamiltonian [13,14],

$$i\tilde{\mathbf{U}}_2 = \tilde{\mathbf{H}}_{\text{eff}}\tilde{\mathbf{U}}_2, \quad \tilde{\mathbf{H}}_{\text{eff}} = \tilde{\mathbf{U}}_1^{-1}\tilde{\mathbf{H}}\tilde{\mathbf{U}}_1 - i\tilde{\mathbf{U}}_1^{-1}\tilde{\mathbf{U}}_1.$$
 (5)

A key element of our construction lies in this effective Hamiltonian and corresponding evolution for the reduced problem. Since $\tilde{\mathbf{U}}_2$ and this equation are block diagonal, the off-diagonal blocks in \mathbf{H}_{eff} on the right-hand side must vanish. This condition leads to the defining equation for \mathbf{z} ,

$$i\dot{\mathbf{z}} = \mathbf{H}^{(N-n)}\mathbf{z} + \mathbf{V} - \mathbf{z}(\mathbf{V}^{\dagger}\mathbf{z} + \mathbf{H}^{(n)}).$$
(6)

For SU(2), when N=2, n=1, all the matrices above reduce to single numbers and Eq. (6) is a Riccati equation for the complex *z*. More generally, it is a matrix Riccati equation [15], and its solutions are involved in the subsequent construction. With the off-diagonal blocks of Eq. (5) accounted for, the diagonal ones defining the Hamiltonians for the (N - n) and *n* problems remain, and are given by $(\mathbf{H}^{(N-n)} - \mathbf{z}\mathbf{V}^{\dagger})$ and $(\mathbf{H}^{(n)} + \mathbf{V}^{\dagger}\mathbf{z})$, respectively. Although the overall trace is preserved in our construction and remains zero, these individual Hamiltonians are neither traceless nor Hermitian. The equations for \mathbf{z} need to be solved numerically in general but form a smaller set than the N^2 elements in the original Eq. (2).

To set up the process for iteration, the above individual Hamiltonians in (N-n)- and *n*-dimensional subspaces must be rendered Hermitian and traceless. The latter is easily achieved by subtracting $\text{Tr}(\mathbf{H}^{(N-n)}-\mathbf{z}\mathbf{V}^{\dagger})$ and $\text{Tr}(\mathbf{H}^{(n)}+\mathbf{V}^{\dagger}\mathbf{z})$ from them. These traces being equal and opposite, this translates into the introduction of a phase, the integral of the trace, in $\mathbf{U}^{(N)}$, representing a relative phase between the two subspaces.

There are alternative methods for rendering the Hamiltonians Hermitian, the most accessible one being through

$$\widetilde{\mathbf{U}}_{1}^{\dagger}\widetilde{\mathbf{U}}_{1} = \begin{pmatrix} \boldsymbol{\gamma}_{1}^{-1} & \mathbf{0} \\ \mathbf{0}^{\dagger} & \boldsymbol{\gamma}_{2} \end{pmatrix} \equiv \begin{pmatrix} \mathbf{g}_{1}\mathbf{g}_{1}^{\dagger} & \mathbf{0} \\ \mathbf{0}^{\dagger} & \mathbf{g}_{2}\mathbf{g}_{2}^{\dagger} \end{pmatrix}^{-1}.$$
 (7)

The first part of this equation is the observation that $\tilde{\mathbf{U}}_1^{\dagger}\tilde{\mathbf{U}}_1$ is block diagonal. This suggests the second part of the equation, namely, the definition of an inverse through two "Hermitian square-root" matrices \mathbf{g}_i . Together, they serve as a gauge factor to unitarize according to

$$\mathbf{U}_1 = \widetilde{\mathbf{U}}_1 \begin{pmatrix} \mathbf{g}_1 & \mathbf{0} \\ \mathbf{0}^{\dagger} & \mathbf{g}_2 \end{pmatrix}. \tag{8}$$

With that, the second factor, \tilde{U}_2 , in Eq. (3) is also unitarized,

$$\mathbf{U}_2 = \begin{pmatrix} \mathbf{g}_1^{-1} & \mathbf{0} \\ \mathbf{0}^{\dagger} & \mathbf{g}_2^{-1} \end{pmatrix} \widetilde{\mathbf{U}}_2.$$
(9)

After some algebra, the explicitly Hermitian forms of the two diagonal block Hamiltonians of dimension (N-n) and n are

$$\mathbf{H}^{(N-n)} = \frac{i}{2} \left[\frac{d}{dt} \mathbf{g}_{1}^{-1}, \mathbf{g}_{1} \right] + \frac{1}{2} [\mathbf{g}_{1}^{-1} (\mathbf{H}^{(N-n)} - \mathbf{z} \mathbf{V}^{\dagger}) \mathbf{g}_{1} + \text{H.c.}],$$
$$\mathbf{H}^{(n)} = \frac{i}{2} \left[\frac{d}{dt} \mathbf{g}_{2}^{-1}, \mathbf{g}_{2} \right] + \frac{1}{2} [\mathbf{g}_{2}^{-1} (\mathbf{H}^{(n)} + \mathbf{z}^{\dagger} \mathbf{V}) \mathbf{g}_{2} + \text{H.c.}],$$
(10)

with commutator brackets in the first term, and H.c. in the second term denoting the Hermitian conjugate of the preceding expression. Again, the trace of each Hamiltonian in Eq. (10) can be subtracted to render them traceless; as clear by inspection, this is the same trace discussed just above. These Hamiltonians in Eq. (10) can now be treated further as SU(N-n) and SU(n) problems.

The γ matrices in Eq. (4) are Hermitian with non-negative eigenvalues because of their origin from $\tilde{\mathbf{U}}_1^{\dagger} \tilde{\mathbf{U}}_1$. This permits their decomposition into **g** as shown in Eq. (7). The **g** matrices and their inverses in Eqs. (7)–(10) are square roots of them, and because any power, including fractional ones, are Hermitian term by term in a formal power-series expansion, we can choose **g** also as Hermitian. The use of identities such as

$$\mathbf{z}^{\dagger} \boldsymbol{\gamma}_{1}^{p} = \boldsymbol{\gamma}_{2}^{p} \mathbf{z}^{\dagger}, \quad \boldsymbol{\gamma}_{1}^{p} \mathbf{z} = \mathbf{z} \boldsymbol{\gamma}_{2}^{p}$$
 (11)

serves to express all **g** in terms of the linearly independent set of matrices of dimension (N-n) or *n*, whichever is smaller. With n=2, this means that all the algebra of calculating such square-root matrices and the subsequent evaluation of the effective Hamiltonian in Eq. (10) reduces to manipulation of Pauli matrices.

A count of the parameters is instructive. The original SU(N) evolution involves (N^2-1) elements and, therefore, grows quadratically with *N*. These are divided in the above construction into the 2n(N-n) elements in **z**, which for small *n* grows only linearly with *N*. The rest are contained in the elements of the SU(N-n) and SU(n) and the single phase between those two subspaces. Our construction of higher SU(N) evolution in terms of smaller ones, with the template in Eq. (3) of three factors as in SU(2), resembles the Schwinger scheme of generating higher *j* representations of SU(2) or SO(3) from the fundamental one of j=1/2 [10]. Whereas that scheme was for higher representations but of the same group, SU(2), our procedure extends in the direction of larger groups SU(N).

In mathematical language of base manifolds and fiber bundles [4], the SU(2) and its Bloch sphere are seen as the bundle $[SU(2)/U(1)] \times U(1)$, the former the two-sphere S^2

base and the latter U(1) phase the fiber. Likewise, our construction is in terms of the base manifold $\{SU(N)/[SU(N - n) \times SU(n) \times U(1)]\}$ and the fiber $[SU(N-n) \times SU(n) \times U(1)]$. For SU(2), there is a single complex *z* that defines the base manifold. The Bloch sphere of a unit threedimensional vector \vec{m} corresponding to *z* is then constructed by inverse stereographic projection from R^2 to S^2 . Similar structures of a \vec{m} associated with the larger **z** will be considered in the next sections.

III. CASE OF SU(4), WITH APPLICATION TO ITS SUBGROUPS

An important case is of N=4. Four-level systems are commonly considered in quantum optics and molecular systems and, of course, in today's quantum computation where they describe two qubits [7]. Since all logic gates can be built up from such qubit pairs, the study of the evolution operator for such N=4 problems is of current interest. As a combined description of spin and isospin, SU(4) also has central importance in the study of nuclei and particles [16]. The group also occurs in the description of unusual magnetic phases of f electron states in CeB₆ [17]. Both choices n=1,2 in the general procedure of Sec. II lead to interesting decompositions, with the latter the more natural for qubit applications. We now turn to this case.

In physics terms, a four-level Hamiltonian has three real parameters along the diagonal to fix the energy positions of the levels. (One overall element, represented by the trace, can be subsumed as an uninteresting definition of the zero energy reference level, leading also to an irrelevant overall phase in the evolution operator.) In addition, six off-diagonal couplings, which are complex, make for a total of 15 parameters to describe the full Hamiltonian. Symmetries often reduce this number so that the Hamiltonian involves only a smaller number as a closed subalgebra. For two identical qubits, there are indeed such symmetries which reduce the number of independent energies and couplings of a fourlevel system.

With N=4, n=2, all the matrices involved in the previous section can be rendered in terms of Pauli spinors and the unit 2×2 matrix. A general Hamiltonian of SU(4) has 15 independent operators and time-dependent parameters multiplying them. A standard, explicit rendering of the fifteen 4×4 matrices is given in [18,19]. **z** comprises four complex quantities, (z_4, z_i) , and the matrix Riccati equation reduces to coupled first-order equations in them with quadratic nonlinearity. Deferring this general case to the next section, we consider first the smaller sets of operators of various subgroups of SU(4).

 $su(2) \times su(2)$ subalgebra. Consider first a Hamiltonian consisting of only six of the 15 operators. Since our construction is representation independent, in a suitable representation, the six may be viewed as two independent, mutually commuting, triplets that obey su(2) algebra. Clearly, each then may be expected to have its own geometrical description in terms of a Bloch sphere and phase. In our above, general formulation, this result is realized as follows. Thus, consider two independent magnetic moments, characterized

by the standard Pauli matrices σ , in time-varying magnetic fields A(t) and B(t) which may also be independent, with Hamiltonian $H = \vec{\sigma}^{(1)} \cdot \vec{A} + \vec{\sigma}^{(2)} \cdot \vec{B}$. Using a standard set of 4 ×4 matrices [18] to cast this Hamiltonian in the form of Eq. (1), we have $\mathbf{V} = (A_x - iA_y)\mathbf{I}$ and $\mathbf{H}^{(1,2)} = \vec{\sigma} \cdot \vec{B} \pm A_z \mathbf{I}$.

The z in Eq. (3) also reduces, as with V, to a unit operator with a single complex coefficient z_4 obeying a Riccati equation in Eq. (6). The gamma matrices in Eq. (4) are also proportional to the unit operator, thus simplifying Eq. (10), the g dropping out. As a result, the Hermitian matrices in the block-diagonal effective Hamiltonian take the form of the same $\vec{\sigma} \cdot \vec{B}$ plus or minus a term proportional to a unit matrix. The first term is viewed as for a single spin with a Bloch sphere and a phase, the second represents a phase between the two 2×2 spaces. The complex z_4 can again be inverse stereographically projected into another two-sphere as in the Bloch construction. We arrive, therefore, at the same initial expectation, that a simultaneous viewing in terms of two Bloch vectors in individual two-spheres, along with their fibers, provides the geometrical picture for all such qubit-pair systems. A specific physical example occurs in the construction of optimal quantum NOT operations [20].

 $su(2) \times su(2) \times u(1)$ subalgebra: Another subalgebra, involving seven of the 15 operators, has been considered before [18,21]. It has the symmetry of $SU(2) \times SU(2) \times U(1)$. In a suitable representation, such a Hamiltonian can be cast as a diagonal form in Eq. (1) plus a term which is proportional to the unit operator in both diagonal blocks but with equal and opposite sign. Such an operator commutes with all the other six, themselves comprised of two mutually commuting triplets of 4×4 matrices [18]. With V=0, z in Eq. (6) also vanishes and we reduce trivially to the two independent SU(2) and a phase between the two spaces, together accounting for the seven parameters of this problem. An example is provided by the controlled-NOT gate constructed with two Josephson junctions [22]. Many such sets of seven operators, one of which commutes with all the remaining six, have been identified through a general procedure in footnote 11 of [21].

so(5) subalgebra. Proceeding further to other subgroups, a nontrivial example is provided by an *H* that involves ten operators satisfying an so(5) subalgebra of su(4). Again, there are many such sets of ten operators and matrices which close under commutation within the full set of 15 as noted in footnote 11 of [21]. As a physical example, a four-level system of two symmetric pairs, as naturally so with two identical qubits, has only two real parameters along the diagonal in its *H*. Selection rules often restrict the off-diagonal coupling between the levels from six to four, thus introducing four complex, or eight real, parameters. The net result of such symmetric four-level systems is a ten-parameter problem [23] and is sketched in Fig. 4.

Such *H* fall into this so(5) subalgebra. The corresponding group is the so-called spin group Spin(5) which is the double-covering group of SO(5), the group of five-dimensional rotations, much as Spin(3), isomorphic to SU(2), is the covering group of SO(3) [24]. All such Spin(5) or SO(5) will themselves have a Spin(4) or SO(4) subgroup, which in turn has the two mutually commuting SU(2) or SO(3) discussed above so that the ten matrices can be con-

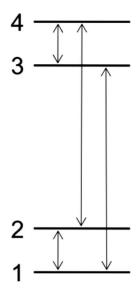


FIG. 4. A four-level system consisting of two like-pairs of energy levels, and couplings as shown. Many systems of two-qubits and elsewhere in atomic and molecular physics [23] have such a description, two real numbers providing the energy positions and four complex numbers the couplings, for a resulting so(5) subalgebra.

veniently viewed as two sets of commuting triplets plus four more which transform like a four-dimensional vector under SO(4). For completeness here in this paper, we briefly summarize results on this so(5) subalgebra that were published elsewhere [13]; see also [25].

In a convenient representation that uses Pauli matrices for two spins [18], we have $H(t) = F_{21}\sigma_z^{(2)} - F_{31}\sigma_y^{(2)} + F_{32}\sigma_x^{(2)} - F_{4i}\sigma_z^{(1)}\sigma_i^{(2)} + F_{5i}\sigma_x^{(1)}\sigma_i^{(2)} - F_{54}\sigma_y^{(1)}$, where the ten arbitrarily time-dependent coefficients $F_{\mu\nu}(t)$ form a 5×5 antisymmetric real matrix. (We will use $\mu, \nu = 1-5$ and i, j, k = 1-3 and summation over repeated indices.) Several quantum optics and multiphoton problems of four levels driven by timedependent electric fields have such a Hamiltonian. It has also been considered extensively in coherent population transfer in many molecular and solid state systems [23]. Casting this Hamiltonian in the form of Eq. (1), we have

$$\mathbf{H}^{(1,2)} = \left(\mp F_{4k} - \frac{1}{2} \epsilon_{ijk} F_{ij} \right) \sigma_k, \quad \mathbf{V} = i F_{54} \mathbf{I}^{(2)} + F_{5i} \sigma_i.$$
(12)

With the matrix Riccati equation in Eq. (6) cast in terms of Pauli spinors together with coefficients $z_{\mu}=z_4, z_i$: $\mathbf{z} = z_4 \mathbf{I}^{(2)} - i z_i \sigma_i$, it takes the form

$$\dot{z}_{\mu} = F_{5\mu}(1 - z_{\nu}^2) + 2F_{\mu\nu}z_{\nu} + 2F_{5\nu}z_{\nu}z_{\mu}.$$
 (13)

[As an alternative, **V** and **z** can also be rendered in terms of quaternions $(1, -i\sigma_i)$.] γ_1 and γ_2 in Eq. (4) become equal and proportional to a unit matrix, $(1+z_{\mu}z_{\mu})\mathbf{I}^{(2)}$. The structure of Eq. (13) admits to the four quantities *z* being real. The effective Hamiltonian in Eq. (10) in terms of these *z* becomes

$$\mathbf{H}_{\text{eff}}^{(1,2)} = \mathbf{H}^{(1,2)} - \boldsymbol{\epsilon}_{ijk} z_i F_{5j} \boldsymbol{\sigma}_k + F_{5j} z_4 \boldsymbol{\sigma}_j \pm F_{54} z_i \boldsymbol{\sigma}_i.$$
(14)

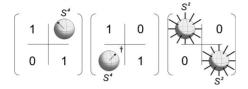


FIG. 5. Analogous to Fig. 3, schematic of the evolution operator for so(5). z, consisting of four real parameters, is inverse stereographically as per Eq. (15) rendered as a four-sphere S^4 , and the third factor has two SU(2) blocks along the diagonal. Together, these factors provide the description shown in Fig. 2.

We can now construct a five-dimensional unit vector \vec{m} out of the four z's,

$$m_{\mu} = \frac{-2z_{\mu}}{(1+z_{\nu}^2)}, \quad m_5 = \frac{(1-z_{\nu}^2)}{(1+z_{\nu}^2)}, \quad \mu,\nu = 1-4.$$
(15)

The nonlinear Eq. (6), or Eq. (13) in z, becomes of simple, linear Bloch-like form,

$$\dot{m}_{\mu} = 2F_{\mu\nu}m_{\nu}, \quad \mu, \nu = 1 - 5.$$
 (16)

As in the single spin case, this represents an inverse stereographic projection, now from the four-dimensional plane $z \in \mathbb{R}^4$ to the four-sphere S^4 . It provides a higher-dimensional polarization vector for describing such two spin problems. With z so described, the two effective SU(2) Hamiltonians in Eq. (14), when solved in turn, give the complete solution. In all, such Hamiltonians possessing Spin(5) symmetry are, therefore, described by the geometrical picture of one S^4 and two S^2 spheres along with two phases, as shown in Fig. 2 and the unitary evolution operator depicted as in Fig. 5.

su(3) subalgebra. Four-level systems with only two independent energy parameters along the Hamiltonian's diagonal and three complex off-diagonal couplings constitute a su(3) sub-algebra with eight parameters. A general three-level system, embedded into four with the fourth level completely uncoupled, constitutes a trivial example of such an su(3) sub-algebra but less trivial examples can also occur. The z now has two nonzero complex z for a total of four parameters. The description of this four-dimensional manifold, as well as the remaining SU(2) and a U(1) phase, parallel the discussion of the general SU(4) in the next section, and will be presented elsewhere [26]. Therefore we omit details except to note that setting $z_4 = -iz_1$ and $z_3 = -iz_2$ in Sec. IV reduces to such a SU(3) symmetry.

IV. GENERAL SU(4) HAMILTONIAN INVOLVING ALL FIFTEEN OPERATORS

Instead of the Hamiltonians considered in Sec. III which involve subalgebras of the full two-qubit system, consider an arbitrary 4×4 Hamiltonian with its entire complement of 15 operators and matrices. Such an *H* is obtained by adding to the previous Spin(5) Hamiltonian considered above the five additional terms, $F_{65}\sigma_z^{(1)}+F_{64}\sigma_x^{(1)}+F_{6i}\sigma_y^{(1)}\sigma_i^{(2)}$. In Fig. 4, this corresponds to the energy levels being arbitrarily positioned and the two other couplings restored. Correspondingly, Eq. (12) gets an additional term $\pm F_{65}\mathbf{I}^{(2)}$ in the diagonal $\mathbf{H}^{(1,2)}$ while in **V**, the $F_{5\mu}$ are replaced by $F_{5\mu}-iF_{6\mu}$. Thus the full SU(4) amounts to a simple modification of the previously considered Spin(5) by adding a term proportional to the unit operator to the diagonal blocks and making the four $F_{5\mu}$ complex, with $F_{6\mu}$ absorbed as their imaginary parts.

The Riccati Eq. (13), now for complex z, becomes

$$\dot{z}_{\mu} = F_{5\mu}(1 - z_{\nu}^2) - iF_{6\mu}(1 + z_{\nu}^2) + 2F_{\mu\nu}z_{\nu} + 2(F_{5\nu} + iF_{6\nu})z_{\nu}z_{\mu} - 2iF_{65}z_{\mu}, \quad \mu, \nu = 1 - 4.$$
(17)

The two gammas in Eq. (4) are given by

$$\gamma_{1,2} = (1 + z_{\mu}^2)\mathbf{I}^{(2)} + i(z_i^* z_4 - z_4^* z_i)\sigma_i \pm \frac{1}{2}i\epsilon_{ijk}(z_i z_j^* - z_j z_i^*)\sigma_k.$$
(18)

Their square-root matrices $g_{1,2}$ can also be evaluated in terms of the Pauli matrices and the two SU(2) effective Hamiltonians then constructed in explicitly traceless and Hermitian form.

Just as the very structure of Eq. (13) suggests that z_{μ} and $(1-z_{\nu}^2)$ with suitable normalization define a five-dimensional unit vector \vec{m} in Eq. (15), the occurrence of $z_{\mu}, (1-z_{\nu}^2), (1+z_{\nu}^2)$ in Eq. (17) suggests now the introduction of six quantities according to

$$m_{\mu} = \frac{-2z_{\mu}}{De^{i\phi}}, \quad m_5 = \frac{(1-z_{\nu}^2)}{De^{i\phi}}, \quad m_6 = -i\frac{(1+z_{\nu}^2)}{De^{i\phi}}, \quad (19)$$

with

Ġ

$$D \equiv (1+2|z_{\nu}|^{2}+z_{\mu}^{2}z_{\nu}^{*2})^{1/2},$$

= $-2F_{65}+iF_{5\mu}(z_{\mu}^{*}-z_{\mu})+F_{6\mu}(z_{\mu}^{*}+z_{\mu}).$ (20)

As with the so(5) case in Sec. III, with such a set of six complex quantities \vec{m} , the nonlinear Riccati equation for the four complex z_{μ} in Eq. (17) becomes a linear Bloch-like equation as before,

$$\dot{m}_{\mu} = 2F_{\mu\nu}m_{\nu}, \quad \mu, \nu = 1 - 6.$$
 (21)

Once again, the m_{μ} obey a first-order equation with an antisymmetric matrix which describes rotations. Since the 15 $F_{\mu\nu}$ are real, the real and imaginary parts of the six m_{μ} each obey such a rotational transformation. These six-dimensional rotations reflect the isomorphism between the groups SU(4) and SO(6) [more accurately, its covering group Spin(6)] and suggest a mapping between their generators (see Appendix B).

To get a geometrical picture of the manifold m, we note first the relations,

$$m_{\mu}^2 = 0, \quad |m_{\mu}|^2 = 2,$$
 (22)

which amount to three constraints. In addition, only the derivative, not the value, of ϕ is determined in Eq. (20). Thereby, the number of independent parameters in m_{μ} is eight just as in the complex z_{μ} , themselves built from **z**. The description of such an eight-dimensional manifold will be taken up in the next subsection but we note here the reduction to the previous so(5) example. This follows upon setting

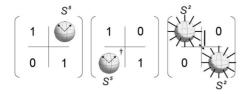


FIG. 6. Analogous to Fig. 5, schematic of the evolution operator for a SU(4) problem. Four complex parameters z are rendered as two orthogonal unit vectors on a five-sphere S^5 ; the third factor has two SU(2) blocks along the diagonal with a mutual phase between the two spaces.

 $F_{65}=0$, $F_{6\mu}=0$ which makes $\phi=0$ and $D=(1+z_{\nu}^2)$ in Eq. (20), and reduces m_{μ} and m_5 to the values in Eq. (15) whereas $m_6=-i$. This, of course, makes \vec{m} a five-dimensional unit vector and its manifold the four-sphere S^4 . The first relation in Eq. (22), of the vanishing of a square, hints at Grassmannian elements, to be discussed further below.

A. Nature of the manifold describing (z,m) for general SU(4)

Our construction of the evolution operator for (N=4, n=2) in Eq. (3) is in terms of the eight-dimensional base manifold **z** and a fiber consisting of two residual SU(2) along its diagonal blocks and a U(1) phase between them, SU(4):[SU(4)/SU(2) × SU(2) × U(1)] × [SU(2) × SU(2)

× U(1)]. To describe the former base manifold, consider first [SU(4)/SU(2)×SU(2)], which is a nine-dimensional manifold. It can also be described in terms of spin-groups as Spin(6)/Spin(4). The six complex m_{μ} in Eq. (19) with the three constraints in Eq. (22) constitute such a manifold called a Stiefel manifold St(6,2,R) $\cong \Re^9$, this name being given to manifolds consisting of *n* orthogonal vectors from an *N*-dimensional space \Re^N [27].

Geometrically, the second relation in Eq. (22) states that the real and imaginary parts of *m* are six-dimensional unit vectors while the first relation expresses their mutual orthogonality. Therefore one can view the manifold as a fivesphere S^5 with another four-sphere S^4 attached at each point on it. The absolute value of the phase parameter ϕ in Eqs. (19) and (20) being undefined, reduces such a manifold by one dimension to $[SU(4)/SU(2) \times SU(2) \times U(1)]$, which is equivalent to the reduction from the Stiefel to a Grassmannian manifold Gr(4,2,C) according to St(6,2,R) $\cong Gr(4,2,C) \times U(1)$. Such a Grassmannian manifold, which has eight dimensions, thereby describes the z in Eq. (3) or its equivalent z_{μ} in Eq. (17) or m_{μ} in Eq. (19).

A more accessible geometrical picture is to consider a single five-sphere S^5 and two six-dimensional unit vectors from the origin to the surface to represent the real and imaginary parts of m_{μ} . The two vectors are orthogonal, and one views such an orthogonally coupled pair rotating within the sphere [28]. This nine-dimensional object, combined with the zero reference of ϕ being undefined, is our eight-dimensional manifold of interest. It is sketched in Fig. 6.

B. Description in Plücker coordinates

An alternative view of these manifolds is provided in terms of what are termed Plücker coordinates, defined as a set of six complex parameters $(P_{12}, P_{13}, P_{14}, P_{23}, P_{24}, P_{34})$ formed as minors of the 2×4 submatrix of the last two columns of an arbitrary, unitary SU(4) matrix [11],

$$\mathbf{U} = \begin{pmatrix} u_{11} & u_{12} & u_{13} & u_{14} \\ u_{21} & u_{22} & u_{23} & u_{24} \\ u_{31} & u_{32} & u_{33} & u_{34} \\ u_{41} & u_{42} & u_{43} & u_{44} \end{pmatrix}.$$
 (23)

They obey the relations

$$P_{12}P_{34} - P_{13}P_{24} + P_{14}P_{23} = 0, \quad \sum |P_{ij}|^2 = 1.$$
 (24)

They are combinations of the m_{μ} according to

$$\begin{pmatrix} P_{12} \\ P_{13} \\ P_{14} \\ P_{23} \\ P_{24} \\ P_{34} \end{pmatrix} = \frac{1}{2} \begin{pmatrix} im_6 - m_5 \\ im_1 + m_2 \\ -im_3 + m_4 \\ -im_3 - m_4 \\ -im_1 + m_2 \\ im_6 + m_5 \end{pmatrix}.$$
 (25)

The linear equations for m_{μ} in Eq. (21) translate into a similar linear equation

$$i\mathbf{P} = \mathbf{H}\mathbf{P}, \quad \mathbf{P} \equiv (P_{12}, -P_{13}, P_{14}, P_{23}, P_{24}, P_{34}), \quad (26)$$

with

$$\mathbf{H}_{P} = \begin{pmatrix} H_{11,22} & H_{41} & H_{31} & -H_{42} & H_{32} & 0 \\ H_{14} & H_{11,33} & -H_{34} & -H_{12} & 0 & -H_{32} \\ H_{13} & -H_{43} & H_{11,44} & 0 & H_{12} & H_{42} \\ -H_{24} & -H_{21} & 0 & H_{22,33} & H_{34} & -H_{31} \\ H_{23} & 0 & H_{21} & H_{43} & H_{22,44} & -H_{41} \\ 0 & -H_{23} & H_{24} & -H_{13} & -H_{14} & H_{33,44} \end{pmatrix},$$
(27)

where we have adopted the notation for the diagonal entries: $H_{ii,jj}=H_{ii}+H_{jj}$.

Actually, the above equations for **P** can be arrived at directly from the evolution equation $i\dot{\mathbf{U}}=\mathbf{H}\mathbf{U}$ because the elements of **P** are quadratic in the elements of **U** in Eq. (23): $P_{ij}=i\varepsilon_{ijkl}u_k^{(3)}u_l^{(4)}$, and $i\dot{u}_k^{(3)}=H_{kj}u_j^{(3)}$. Also, **z** can be defined in terms of the two minors on the right in Eq. (23):

$$\mathbf{z} = \begin{pmatrix} u_{13} & u_{14} \\ u_{23} & u_{24} \end{pmatrix} / \begin{pmatrix} u_{33} & u_{34} \\ u_{43} & u_{44} \end{pmatrix},$$
(28)

the matrix in the denominator assumed to be nonsingular. Writing U in Eq. (23) in the form in Eq. (3), the first factor \tilde{U}_1 involving z is a map of the Grassmannian manifold $Gr(4,2,\mathbb{C})$ onto \mathbb{C}^4 , and provides a partial coordinization of that manifold. Elements of $Gr(4,2,\mathbb{C})$ are two-dimensional complex hyperplanes spanned by vectors $\mathbf{u}_3 = (u_{13}, u_{23}, u_{33}, u_{43})^T$ and $\mathbf{u}_4 = (u_{14}, u_{24}, u_{34}, u_{44})^T$. The Plücker coordinates provide a unique identification of such planes. They are an analog of the coordinization of the *n*-dimensional sphere S^n by an (n+1)-dimensional unit vector \vec{m} as in Sec. III. The matrix \mathbf{H}_P in Eq. (27) being Hermitian, $\mathbf{P}^{\dagger}\mathbf{P}$ =const =1. This can be verified by the relation between *P*'s and *m*'s in Eq. (25) which involves a unitary matrix so that $\mathbf{P}^{\dagger}\mathbf{P}$ = $\frac{1}{2}m^{\dagger}m$, and combining with Eq. (22). Further, a symplectic structure can be introduced. Defining a 6×6 matrix $\mathbf{\Omega}$ = $\delta_{i,7-j}$ with nonzero entries of 1 only along the antidiagonal, the first relation in Eq. (24) can be rendered as $\mathbf{P}^T \mathbf{\Omega} \mathbf{P}$ =0, and the matrix \mathbf{H}_P , a generator of the symplectic group Sp(6, C),

$$\mathbf{H}_{P}\mathbf{\Omega} + \mathbf{\Omega}\mathbf{H}_{P}^{T} = \mathrm{Tr}(\mathbf{H}_{P})\mathbf{\Omega} = 0.$$
(29)

Any two vectors \mathbf{P}_i , evolving according to Eq. (26), satisfy $\mathbf{P}_1^T(t)\mathbf{\Omega}\mathbf{P}_2(t)$ =const. If $\mathbf{P}_1\mathbf{\Omega}\mathbf{P}_2$ =0, then the two hyperplanes defined by \mathbf{P}_i intersect, and if $|\mathbf{P}_1\mathbf{\Omega}\mathbf{P}_2|$ =1, they do not.

Geometrically, the set $\mathbf{P}^{\dagger}\mathbf{P}=1$ is a sphere \mathbf{S}^{11} , the algebraic relation $\mathbf{P}\mathbf{\Omega}\mathbf{P}=0$ determining a nine-dimensional submanifold, an intersection between \mathbf{S}^{11} , and the affine variety of roots of the polynomial equation $\mathbf{P}\mathbf{\Omega}\mathbf{P}=0$. This manifold may be denoted \mathfrak{R}^9 . Multiplication by a phase acts as a transformation group on this manifold, that is, if $\mathbf{P} \in \mathfrak{R}^9$, then $\mathbf{P}e^{i\phi} \in \mathfrak{R}^9$. Therefore $\mathrm{Gr}(4,2,\mathbf{C})$ is a quotient space $\mathfrak{R}^9/\mathrm{U}(1)$ and has eight dimensions. The connection to $\mathrm{SU}(4)$ is, as noted before, $\mathfrak{R}^9 \cong \mathrm{SU}(4)/[\mathrm{SU}(2) \times \mathrm{SU}(2)] \cong \mathrm{Spin}(6)/\mathrm{Spin}(4)$. The stability subgroup of a vector $\mathbf{P} \in \mathfrak{R}^9$ is $\mathrm{SU}(2) \times \mathrm{SU}(2)$ while the stability subgroup of $\mathfrak{R}^9/\mathrm{U}(1)$ is $\mathrm{SU}(2) \times \mathrm{SU}(2) \times \mathrm{U}(1)$. Since $\mathrm{Spin}(6)/\mathrm{Spin}(5) \cong \mathrm{S}^5$ and $\mathrm{Spin}(5)/\mathrm{Spin}(4) \cong \mathrm{S}^4$, we can identify the fibration of \mathfrak{R}^9 with $\mathrm{S}^5 \times \mathrm{S}^4$.

V. SUMMARY

We have presented a complete analysis of the evolution operator for SU(N), setting up its construction in a hierarchical way in terms of those for smaller SU(N-n) and SU(n), with n < N and arbitrary. The evolution operator is written as a product of two $N \times N$ matrices, the second of which is block diagonal in $(N-n) \times (N-n)$ and $n \times n$ of the smaller groups. The first factor is obtained through a $(N-n) \times n$ complex matrix z obeying a matrix Riccati equation. Its solutions determine both the first factor as well as the Hermitian matrices for the subsequent N-n and n evolution problems. z is the base manifold. For SU(2), when z is a single complex number plane, its inverse stereographic projection is the familiar Bloch sphere. For larger SU(N), z is a matrix of complex numbers and the corresponding base manifold is more complicated.

This general constructive method is applied especially to a four-level system with special emphasis on two qubits. The general symmetry is of SU(4), a 15-parameter group. Our procedure expresses the evolution operator as a product of two 4×4 matrices, the second of which is block diagonal, each block an SU(2) problem. The z is also a 2×2 matrix with complex entries in general and obeys a matrix Riccati equation. Alternatively, we transform z into a sixdimensional complex vector \vec{m} , whose real and imaginary parts both separately undergo linear, six-dimensional rotational transformations. This is exactly analogous to the linear Bloch equation for real three-dimensional rotations of a vector to represent the evolution operator for a single spin in a magnetic field.

Just as a Bloch sphere describes the three-dimensional vector \vec{m} for a single spin [and, together with a phase, the complete SU(2), we also present the geometrical manifold describing z or its equivalent six-dimensional complex vector \vec{m} . Together with two residual SU(2) problems and a phase, this provides a complete description of the quantum evolution operator for SU(4). For certain subalgebras of SU(4), the manifold is an analogous higher-dimensional sphere; a four-sphere, for example, for an so(5) subalgebra as in Fig. 2. For the most general SU(4), we have an eightdimensional Grassmannian manifold. We provide a picture of it in Fig. 6 as two five-spheres with an orthogonality and phase constraint. These geometrical objects may serve for all possible four-level and two qubit systems the useful purpose that the Bloch sphere has for two-level and single qubit problems in physics.

APPENDIX A: EXTENSION TO NONUNITARY EVOLUTION FOR A NON-HERMITIAN HAMILTONIAN

The iterative method of Sec. II for the evolution operator in Eq. (2) through writing it as in Eq. (3) applies also when H in Eq. (1) is not Hermitian and, therefore, the evolution not unitary. However, \mathbf{z} and \mathbf{w} in Eq. (3) are no longer simply related as in Eq. (4) but obey independent equations, the former still in Riccati form but the latter given in terms of \mathbf{z} . Thus, instead of Eq. (1), consider

$$\widetilde{\mathbf{H}}^{(N)}(t) = \begin{pmatrix} \widetilde{\mathbf{H}}^{(N-n)}(t) & \mathbf{V}(t) \\ \mathbf{Y}^{\dagger}(t) & \widetilde{\mathbf{H}}^{(n)}(t) \end{pmatrix},$$
(A1)

where we have again indicated by tildes non-Hermiticity, and **V** and **Y** are not equal but independent.

Writing $\tilde{\mathbf{U}}^{(N)}(t)$ again as in Eq. (3), Eq. (6) now becomes

$$\begin{split} &i\dot{\mathbf{z}} = \widetilde{\mathbf{H}}^{(N-1)}\mathbf{z} - \mathbf{z}\widetilde{\mathbf{H}}^{(n)} - \mathbf{z}\mathbf{Y}^{\dagger}\mathbf{z} + \mathbf{V},\\ &i\dot{\mathbf{w}}^{\dagger} = \mathbf{w}^{\dagger}(\mathbf{z}\mathbf{Y}^{\dagger} - \widetilde{\mathbf{H}}^{(N-1)}) + (\widetilde{\mathbf{H}}^{(n)} - \mathbf{Y}^{\dagger}\mathbf{z})\mathbf{w}^{\dagger} + \mathbf{Y}^{\dagger}. \end{split}$$
(A2)

The residual problems of (N-n) and *n* dimension then become

$$i\tilde{\tilde{\mathbf{U}}}_{2} = \begin{pmatrix} \tilde{\mathbf{H}}^{(N-1)} - \mathbf{z}\mathbf{Y}^{\dagger} & \mathbf{0} \\ \mathbf{0}^{\dagger} & \tilde{\mathbf{H}}^{(n)} + \mathbf{Y}^{\dagger}\mathbf{z} \end{pmatrix} \tilde{\mathbf{U}}_{2}.$$
 (A3)

APPENDIX B: DESCRIPTION OF EVOLUTION AS SIX-DIMENSIONAL ROTATIONS

For a single spin or qubit, the rewriting of the quantum evolution operator, which is complex, as rotational transformations of a real, unit vector in three dimensions given by the Bloch equation, rests on the isomorphism of the group SU(2) to SO(3) [or its double covering Spin(3)]. A similar isomorphism between the groups SU(4) and SO(6) [or its extension Spin(6)] underlies the construction in Secs. III and IV of the complex evolution operator for two qubits in terms of rotations of a vector in six dimensions. Both groups are

described by 15 real parameters through an antisymmetric $F_{\mu\nu}, \mu, \nu=1,2,...,6$. In Secs. III and IV, explicit expressions are given for the Hamiltonian with each of these parameters multiplying one of the 15 complex generators of SU(4) in a standard representation of Pauli matrices, $\vec{\sigma}^{(1)}$

 $\otimes \mathcal{I}^{(2)}, \mathcal{I}^{(1)} \otimes \vec{\sigma}^{(2)}, \vec{\sigma}^{(1)} \otimes \vec{\sigma}^{(2)}$. An alternative rendering in terms of the 15 generators of SO(6) is useful and recorded here.

The Hamiltonian in Sec. IV, apart from a factor of $\frac{1}{2}$, can be cast in terms of a matrix array

$$\begin{pmatrix} 0 & \sigma_{z}^{(2)} & -\sigma_{y}^{(2)} & -\sigma_{z}^{(1)}\sigma_{x}^{(2)} & \sigma_{x}^{(1)}\sigma_{x}^{(2)} & \sigma_{y}^{(1)}\sigma_{x}^{(2)} \\ -\sigma_{z}^{(2)} & 0 & \sigma_{x}^{(2)} & -\sigma_{z}^{(1)}\sigma_{y}^{(2)} & \sigma_{x}^{(1)}\sigma_{y}^{(2)} & \sigma_{y}^{(1)}\sigma_{y}^{(2)} \\ \sigma_{y}^{(2)} & -\sigma_{x}^{(2)} & 0 & -\sigma_{z}^{(1)}\sigma_{z}^{(2)} & \sigma_{x}^{(1)}\sigma_{z}^{(2)} & \sigma_{y}^{(1)}\sigma_{z}^{(2)} \\ \sigma_{z}^{(1)}\sigma_{x}^{(2)} & \sigma_{z}^{(1)}\sigma_{y}^{(2)} & \sigma_{z}^{(1)}\sigma_{z}^{(2)} & 0 & -\sigma_{y}^{(1)} & \sigma_{x}^{(1)} \\ -\sigma_{x}^{(1)}\sigma_{x}^{(2)} & -\sigma_{x}^{(1)}\sigma_{z}^{(2)} & -\sigma_{x}^{(1)}\sigma_{z}^{(2)} & -\sigma_{x}^{(1)} & 0 & \sigma_{z}^{(1)} \\ -\sigma_{y}^{(1)}\sigma_{x}^{(2)} & -\sigma_{y}^{(1)}\sigma_{y}^{(2)} & -\sigma_{y}^{(1)}\sigma_{z}^{(2)} & -\sigma_{x}^{(1)} & -\sigma_{z}^{(1)} & 0 \end{pmatrix},$$
(B1)

which is explicitly antisymmetric. We thus have $H = 2F_{\mu\nu}L_{\nu\mu}$. Analogous to the familiar triplet of angular momentum generators, six-dimensional generators of SO(6) are given by $L_{\mu\nu} = -il_{\mu\nu}$, where the *l* are 15 real antisymmetric 6×6 matrices with only two nonzero entries, +1 in the $(\mu\nu)$ and -1 in the $(\nu\mu)$ position:

$$(l_{\mu\nu})_{\rho\sigma} = \delta_{\mu\rho}\delta_{\nu\sigma} - \delta_{\mu\sigma}\delta_{\nu\rho}.$$
 (B2)

Their commutators close:

$$[l_{\mu\nu}, l_{\rho\sigma}] = \delta_{\nu\rho} l_{\mu\sigma} + \delta_{\mu\sigma} l_{\nu\rho} - \delta_{\nu\sigma} l_{\mu\rho} - \delta_{\mu\rho} l_{\nu\sigma}, \qquad (B3)$$

so that $L_{\mu\nu}$ form an so(6) algebra.

The array in Eq. (B1) is also a convenient display of the generators of the various subgroups of SO(6) of lowerdimensional rotations. Either upper left or lower right corner 2×2 blocks describe the SO(2) generator of one of the qubits. Adding a third row and column gives the full triplet of SO(3) generators. To this can be added a next row and column of three nonzero entries to give the six generators of SO(4). For this purpose, any of the three remaining rows and columns can be employed, each giving an SO(4), the three added entries transforming as a vector under SO(3). This continues. Adding another row and column's four new entries, which transform as a vector under SO(4) [further subdividing into three components that transform as a vector and one as a scalar under the previous SO(3)], gives the ten SO(5) generators. The final sixth row and column adds five entries, an SO(5) vector, to give the full 15 generators of SO(6).

This hierarchical nesting of SO subgroups, together with the corresponding Clifford structure with Pauli matrices in Eq. (B1), accounts for the richness of the structures in the isomorphic groups SU(4) and SO(6), one we have exploited in Secs. III and IV. Note that the linear Bloch-like equation for \vec{m} in Eq. (21) for a general SU(4) Hamiltonian reduces to the same antisymmetric form for its subgroups such as in Eq. (16), all the way down to the standard Bloch equation for a single qubit, whose SO(3) antisymmetric F_{ij} is usually written as a vector product with a magnetic field.

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