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A parametrization of bipartite systems based on $SU(4)$ Euler angles

Todd Tilma[1], **Mark Byrd**[2] **and E C G Sudarshan**[3]

[1] Physics Department, The Ilya Prigogine Center for Studies in Statistical Mechanics and Complex Systems, The University of Texas at Austin, Austin, TX 78712-1081, USA
[2] Maxwell Dworkin Laboratory, 33 Oxford Street, Harvard University, Cambridge, MA 02138, USA
[3] Physics Department, Center for Particle Physics, The University of Texas at Austin, Austin, TX 78712-1081, USA

E-mail: tilma@physics.utexas.edu, brd@hrl.harvard.edu and sudarshan@physics.utexas.edu

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Abstract

In this paper we give an explicit parametrization for all two-qubit density matrices. This is important for calculations involving entanglement and many other types of quantum information processing. To accomplish this we present a generalized Euler angle parametrization for $SU(4)$ and all possible two-qubit density matrices. The important group-theoretical properties of such a description are then manifest. We thus obtain the correct Haar (Hurwitz) measure and volume element for $SU(4)$ which follows from this parametrization. In addition, we study the role of this parametrization in the Peres–Horodecki criteria for separability and its corresponding usefulness in calculating entangled two-qubit states as represented through the parametrization.

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1. Introduction

In quantum mechanics the appropriate description of mixed states is by density matrices. For example, their compact notation makes them useful for describing entanglement and decoherence properties of multi-particle quantum systems. In particular, two two-state density matrices, also known as two-qubit density matrices, are important for their role in explaining quantum teleportation, dense coding, computation theorems and other issues pertinent to quantum information theory.

Although the ideas behind extending classical computation and communication theories into the quantum realm have been around for some decades now, the first reference to calling any generic two-state system a qubit comes from Schumacher [1] in 1995. By calling a two-state system a qubit, he quantified the relationship between classical and quantum information theory: a qubit can behave like a classical bit, but because of the quantum properties of superposition and entanglement, it has a much larger information storage capacity. It is this capacity to invoke quantum effects to increase information storage and processing, which gives qubits such a central role in quantum information theory.

Now, a qubit is just a state in a two-dimensional Hilbert space [2]. If $\mathbb{H} \sim \mathbb{C}^2$ in the vector space, the unit vectors

$$|\psi\rangle = a\,|0\rangle + b\,|1\rangle \tag{1}$$

with a and b being complex numbers satisfying

$$|a|^2 + |b|^2 = 1 \tag{2}$$

define, up to a phase, the pure quantum states. In the quantum information theory, the orthonormal basis $\{|0\rangle, |1\rangle\}$ is used to represent the bit states 0 (off) and 1 (on). As pointed out by Brown [3], the physical representation of these two bit states depends on the 'hardware' being discussed; the basis states may be polarization states of light, atomic or electronic spin states, or the ground and first excited states of a quantum dot.

If the qubit represents a mixed state, which is quite often the case, one should use a two-dimensional density matrix, which was introduced independently by Landau and von Neumann in the 1920s (see, for example, the discussion in [4]), for its representation. The formalism of density matrices allows one to exploit simple matrix algebra mechanisms to evaluate the expectation value of any physical quantity of the system. More recently, it has been pointed out by several people (see [2, 5–7], and references within) that the density matrix representation of quantum states is also a very natural representation to use with regard to quantum information calculations.

Following this we therefore express one qubit as

$$\rho = \tfrac{1}{2}(\mathbb{1}_2 + \boldsymbol{\sigma}\cdot\boldsymbol{n}) \tag{3}$$

i.e. as a general 2 by 2 Hermitian matrix with unit trace and the positivity condition $\mathrm{Tr}[\rho] \geqslant 0$ implying $\boldsymbol{n}\cdot\boldsymbol{n} \leqslant 1$ or $\rho^2 \leqslant \rho$. Therefore, these density matrices are the disc D^3, whose boundary $\partial D^3 = S^2 = \mathbb{C}P^1$ represents the pure states ($\rho^2 = \rho$, or $\boldsymbol{n}\cdot\boldsymbol{n} = 1$), and which can thus be characterized by the two angles $0 \leqslant \theta \leqslant \pi$ (the latitude) and $0 \leqslant \phi \leqslant 2\pi$ (the longitude) of the sphere S^2.

Now, two-state density matrices live in a 3 by 3 Hermitian-matrix space, with $\mathbb{C}P^2 = SU(3)/U(2)$ as a subspace of pure states. Much is already known about these two- and three-state density matrices, especially when one uses, for example, Euler angle parametrizations (see [6] for more information). But what is not well known is how the density matrices of larger-dimensional Hilbert spaces, and thus of multiple qubits, look under such a parametrization. This paper will make a great deal of progress in remedying this situation by giving an explicit parametrization of the density matrix of two qubits that is not redundant in the representation of the corresponding four-dimensional Hilbert space, and at the same time offers the natural (Bures) volume measure on the set of all two-qubit density matrices. This will be achieved by starting with a diagonal density matrix ρ_d, which represents our two-qubit system in some particular basis, and then performing a unitary ($U^{-1} = U^\dagger$), unimodular ($\mathrm{Det}[U] = 1$) transformation

$$\rho_d \rightarrow U\rho_d U^\dagger \tag{4}$$

for some $U \in SU(4)$, thus describing ρ in an arbitrary basis [6, 8–10]. We should point out that progress in this direction has also been made in a recent publication by Schlienz and Mahler [11].

2. Euler angle parametrization for $SU(4)$

We begin by giving the Euler angle parametrization for $SU(4)$. Define $U \in SU(4)$. Using the Gell–Mann basis for the elements of the algebra (found in appendix A), the Euler angle parametrization is then given by

$$U = e^{i\lambda_3\alpha_1} e^{i\lambda_2\alpha_2} e^{i\lambda_3\alpha_3} e^{i\lambda_5\alpha_4} e^{i\lambda_3\alpha_5} e^{i\lambda_{10}\alpha_6} e^{i\lambda_3\alpha_7} e^{i\lambda_2\alpha_8} e^{i\lambda_3\alpha_9} e^{i\lambda_5\alpha_{10}} \times e^{i\lambda_3\alpha_{11}} e^{i\lambda_2\alpha_{12}} e^{i\lambda_3\alpha_{13}} e^{i\lambda_8\alpha_{14}} e^{i\lambda_{15}\alpha_{15}}. \quad (5)$$

The derivation of this result is as follows. We begin by following the work of Biedenharn [12] and Hermann [13] in order to generate a Cartan decomposition of $SU(4)$. First, we look at the 4 by 4, Hermitian, traceless, Gell–Mann matrices λ_i. This set is linearly independent and is the lowest-dimensional faithful representation of the $SU(4)$ Lie algebra. From these matrices we can then calculate their commutation relations, and by observation of the corresponding structure constants f_{ijk} we can see the relationship in the algebra that can help generate the Cartan decomposition of $SU(4)$ (shown in detail in appendix A).

We now establish two subspaces of the $SU(4)$ group manifold, hereafter known as K and P. From these subspaces, there correspond two subsets of the Lie algebra of $SU(4)$, $L(K)$ and $L(P)$, such that for $k_1, k_2 \in L(K)$ and $p_1, p_2 \in L(P)$,

$$[k_1, k_2] \in L(K) \qquad [p_1, p_2] \in L(K) \qquad [k_1, p_2] \in L(P). \quad (6)$$

For $SU(4)$, $L(K) = \{\lambda_1, \ldots, \lambda_8, \lambda_{15}\}$ and $L(P) = \{\lambda_9, \ldots, \lambda_{14}\}$. Given that we can decompose the $SU(4)$ algebra into a semi-direct sum [14]

$$L(SU(4)) = L(K) \oplus L(P) \quad (7)$$

we therefore have a decomposition of the group,

$$U = K \cdot P. \quad (8)$$

From [15] we know that $L(K)$ contains the generators of the $SU(3)$ subalgebra of $SU(4)$, thus K will be the $U(3)$ subgroup obtained by exponentiating the subalgebra $\{\lambda_1, \ldots, \lambda_8\}$ combined with λ_{15} and thus can be written as (see [8, 9] for details)

$$K = e^{i\lambda_3\alpha} e^{i\lambda_2\beta} e^{i\lambda_3\gamma} e^{i\lambda_5\theta} e^{i\lambda_3 a} e^{i\lambda_2 b} e^{i\lambda_3 c} e^{i\lambda_8\chi} e^{i\lambda_{15}\phi}. \quad (9)$$

Now, as for P, of the six elements in $L(P)$ we chose the λ_2 analogue, λ_{10}, for $SU(4)$ and write any element of P as

$$P = K' e^{i\lambda_{10}\psi} K'' \quad (10)$$

where K' and K'' are copies of K.

Unfortunately, at this point in our derivation, we have a U with 28 elements, not the requisite 15

$$U = K K' e^{i\lambda_{10}\psi} K''. \quad (11)$$

But, if we recall that U is a product of operators in $SU(4)$, we can 'remove the redundancies', i.e. the first K' component as well as the three Cartan subalgebra elements of $SU(4)$ in the original K component, to arrive at the following product [8, 9]:

$$U = e^{i\lambda_3\alpha_1} e^{i\lambda_2\alpha_2} e^{i\lambda_3\alpha_3} e^{i\lambda_5\alpha_4} e^{i\lambda_3\alpha_5} e^{i\lambda_2\eta} e^{i\lambda_{10}\psi} e^{i\lambda_3\alpha} e^{i\lambda_2\beta} e^{i\lambda_3\gamma} e^{i\lambda_5\theta} e^{i\lambda_3 a} e^{i\lambda_2 b} e^{i\lambda_3 c} e^{i\lambda_8\chi} e^{i\lambda_{15}\phi}. \quad (12)$$

By insisting that our parametrization must truthfully reproduce known vector and tensor transformations under $SU(4)$, we can remove the last 'redundancy', $e^{i\lambda_2\eta}$, and, after rewriting the parameters, generate equation (5),

$$U = e^{i\lambda_3\alpha_1} e^{i\lambda_2\alpha_2} e^{i\lambda_3\alpha_3} e^{i\lambda_5\alpha_4} e^{i\lambda_3\alpha_5} e^{i\lambda_{10}\alpha_6} e^{i\lambda_3\alpha_7} e^{i\lambda_2\alpha_8} e^{i\lambda_3\alpha_9} e^{i\lambda_5\alpha_{10}} e^{i\lambda_3\alpha_{11}} \times e^{i\lambda_2\alpha_{12}} e^{i\lambda_3\alpha_{13}} e^{i\lambda_8\alpha_{14}} e^{i\lambda_{15}\alpha_{15}}. \quad (13)$$

For our purposes it is enough to note that this parametrization is special unitary by construction and can be shown to cover the group by modifying the ranges that follow and substituting them into the whole group matrix, or into the parametrization of the characters [16].

3. Derivation of the Haar measure and calculation of the group volume for $SU(4)$

Taking the Euler angle parametrization given by equation (5) we now wish to develop the differential volume element, also known as the Haar measure, for the group $SU(4)$. We initially proceed by extending the method used in [8, 9] for the calculation of the Haar measure for $SU(3)$; take a generic $U \in SU(4)$ and find the matrix

$$U^{-1} \cdot \mathrm{d}U = U^{-1} \frac{\partial U}{\partial \alpha_k} \mathrm{d}\alpha_k \tag{14}$$

of left invariant 1-forms, then wedge the 15 linearly independent forms together[4]. But due to the 15 independent parameters needed for $SU(4)$, this method is unfortunately quite time consuming and thus prohibitive. An easier way, initially given in [17], is to calculate the 4 by 4 matrices, $\partial U/\partial \alpha_k$ (for $k = \{1, \ldots, 15\}$), and take the determinant of the coefficient matrix generated by their subsequent expansion in terms of the Gell–Mann basis.

To begin with, we take the transpose of equation (5) to generate

$$\begin{aligned} u = U^T = {} & \mathrm{e}^{\mathrm{i}\lambda_{15}^T\alpha_{15}}\, \mathrm{e}^{\mathrm{i}\lambda_8^T\alpha_{14}}\, \mathrm{e}^{\mathrm{i}\lambda_3^T\alpha_{13}}\, \mathrm{e}^{\mathrm{i}\lambda_2^T\alpha_{12}}\, \mathrm{e}^{\mathrm{i}\lambda_3^T\alpha_{11}}\, \mathrm{e}^{\mathrm{i}\lambda_5^T\alpha_{10}}\, \mathrm{e}^{\mathrm{i}\lambda_3^T\alpha_9}\, \mathrm{e}^{\mathrm{i}\lambda_2^T\alpha_8} \\ & \times \mathrm{e}^{\mathrm{i}\lambda_3^T\alpha_7}\, \mathrm{e}^{\mathrm{i}\lambda_{10}^T\alpha_6}\, \mathrm{e}^{\mathrm{i}\lambda_3^T\alpha_5} \mathrm{e}^{\mathrm{i}\lambda_5^T\alpha_4}\, \mathrm{e}^{\mathrm{i}\lambda_3^T\alpha_3}\, \mathrm{e}^{\mathrm{i}\lambda_2^T\alpha_2}\, \mathrm{e}^{\mathrm{i}\lambda_3^T\alpha_1}. \end{aligned} \tag{15}$$

An observation of the components of our Lie algebra subset $(\lambda_2, \lambda_3, \lambda_5, \lambda_8, \lambda_{10}, \lambda_{15})$ shows that the transpose operation is equivalent to making the substitutions

$$\begin{array}{ll} \lambda_2^T \to -\lambda_2 & \lambda_3^T \to \lambda_3 \\ \lambda_5^T \to -\lambda_5 & \lambda_8^T \to \lambda_8 \\ \lambda_{10}^T \to -\lambda_{10} & \lambda_{15}^T \to \lambda_{15} \end{array} \tag{16}$$

in equation (15) generating

$$\begin{aligned} u = {} & \mathrm{e}^{\mathrm{i}\lambda_{15}\alpha_{15}}\, \mathrm{e}^{\mathrm{i}\lambda_8\alpha_{14}}\, \mathrm{e}^{\mathrm{i}\lambda_3\alpha_{13}}\, \mathrm{e}^{-\mathrm{i}\lambda_2\alpha_{12}}\, \mathrm{e}^{\mathrm{i}\lambda_3\alpha_{11}}\, \mathrm{e}^{-\mathrm{i}\lambda_5\alpha_{10}}\, \mathrm{e}^{\mathrm{i}\lambda_3\alpha_9}\, \mathrm{e}^{-\mathrm{i}\lambda_2\alpha_8} \\ & \times \mathrm{e}^{\mathrm{i}\lambda_3\alpha_7} \mathrm{e}^{-\mathrm{i}\lambda_{10}\alpha_6}\, \mathrm{e}^{\mathrm{i}\lambda_3\alpha_5}\, \mathrm{e}^{-\mathrm{i}\lambda_5\alpha_4}\, \mathrm{e}^{\mathrm{i}\lambda_3\alpha_3}\, \mathrm{e}^{-\mathrm{i}\lambda_2\alpha_2}\, \mathrm{e}^{\mathrm{i}\lambda_3\alpha_1}. \end{aligned} \tag{17}$$

Whichever form is used though, we then take the partial derivative of u with respect to each of the 15 parameters. In general, the differentiation will have the form

$$\begin{aligned} \frac{\partial u}{\partial \alpha_k} &= \mathrm{e}^{\mathrm{i}\lambda_{15}^T\alpha_{15}}\, \mathrm{e}^{\mathrm{i}\lambda_8^T\alpha_{14}}\, \mathrm{e}^{\mathrm{i}\lambda_3^T\alpha_{13}}\, \mathrm{e}^{\mathrm{i}\lambda_2^T\alpha_{12}} \cdots \mathrm{e}^{\mathrm{i}\lambda_m^T\alpha_{k+1}}\, \mathrm{i}\lambda_n^T\, \mathrm{e}^{\mathrm{i}\lambda_n^T\alpha_k}\, \mathrm{e}^{\mathrm{i}\lambda_p^T\alpha_{k-1}} \cdots \mathrm{e}^{\mathrm{i}\lambda_3^T\alpha_1} \\ &= \mathrm{e}^{\mathrm{i}\lambda_{15}^T\alpha_{15}}\, \mathrm{e}^{\mathrm{i}\lambda_8^T\alpha_{14}}\, \mathrm{e}^{\mathrm{i}\lambda_3^T\alpha_{13}}\, \mathrm{e}^{\mathrm{i}\lambda_2^T\alpha_{12}} \cdots \mathrm{e}^{\mathrm{i}\lambda_m^T\alpha_{k+1}}\, \mathrm{i}\lambda_n^T\, \mathrm{e}^{-\mathrm{i}\lambda_m^T\alpha_{k+1}} \cdots \mathrm{e}^{-\mathrm{i}\lambda_2^T\alpha_{12}} \\ &\quad \times \mathrm{e}^{-\mathrm{i}\lambda_3^T\alpha_{13}}\, \mathrm{e}^{-\mathrm{i}\lambda_8^T\alpha_{14}}\, \mathrm{e}^{-\mathrm{i}\lambda_{15}^T\alpha_{15}}\, u \end{aligned} \tag{18}$$

which, if we make the following definitions:

$$C(\alpha_k) \in \mathrm{i} * \left\{\lambda_2^T, \lambda_3^T, \lambda_5^T, \lambda_8^T, \lambda_{10}^T, \lambda_{15}^T\right\} \tag{19}$$

and

$$E^L = \mathrm{e}^{C(\alpha_{15})\alpha_{15}} \cdots \mathrm{e}^{C(\alpha_{k+1})\alpha_{k+1}} \qquad E^{-L} = \mathrm{e}^{-C(\alpha_{k+1})\alpha_{k+1}} \cdots \mathrm{e}^{-C(\alpha_{15})\alpha_{15}} \tag{20}$$

[4] Similarly, one can wedge together the 15 right invariant 1-forms which also yield the Haar measure in question. This is due to the fact that a compact simply-connected real Lie group has a bi-invariant measure, unique up to a constant factor. Such a group is usually referred to as 'unimodular' [15].

can be expressed, in a 'shorthanded' notation as

$$\frac{\partial u}{\partial \alpha_k} = E^L C(\alpha_k) E^{-L} u. \tag{21}$$

By using these equations and the Baker–Campbell–Hausdorff relation,

$$\mathrm{e}^X Y\,\mathrm{e}^{-X} = Y + [X, Y] + \tfrac{1}{2}[X, [X, Y]] + \cdots \tag{22}$$

we are able to consecutively solve equation (18) for $k = \{15, \ldots, 1\}$, giving us a set of 4 by 4 matrices which can be expanded in terms of the 15 *transposed* elements of the $SU(4)$ Lie algebra with expansion coefficients given by trigonometric functions of the group parameters α_i:

$$M_k \equiv \frac{\partial u}{\partial \alpha_k} u^{-1} = E^L C(\alpha_k) E^{-L} = \sum_{15 \geqslant j \geqslant 1} c_{kj} \lambda_j^T. \tag{23}$$

At this stage, we should illustrate the connection between the M_k and the 15 left invariant 1-forms that we could have used. To begin with we note that

$$\mathrm{d}u \cdot u^{-1} = \mathrm{d}(U^T) \cdot (U^T)^{-1} = (\mathrm{d}U)^T \cdot (U^{-1})^T = (U^{-1} \cdot \mathrm{d}U)^T. \tag{24}$$

Thus the following relationship between equations (14) and (23) holds:

$$\left(\frac{\partial u}{\partial \alpha_k}\,\mathrm{d}\alpha_k\right) u^{-1} = \sum_{15 \geqslant j \geqslant 1} c_{kj} \lambda_j^T\,\mathrm{d}\alpha_k = \left(U^{-1} \frac{\partial U}{\partial \alpha_k}\,\mathrm{d}\alpha_k\right)^T. \tag{25}$$

Therefore we can conclude

$$U^{-1} \frac{\partial U}{\partial \alpha_k}\,\mathrm{d}\alpha_k = \sum_{1 \leqslant j \leqslant 15} c_{kj} \lambda_j\,\mathrm{d}\alpha_k \tag{26}$$

for $k = \{1, \ldots, 15\}$. So even though we are calculating the *right* invariant 1-forms for u, we are really calculating the *left* invariant 1-forms for U. The important thing to note is that the c_{kj} do not change[5].

Now, the expansion coefficients c_{kj} are the elements of the determinant in question. They are found in the following manner

$$c_{kj} = \frac{-\mathrm{i}}{2} \operatorname{Tr}\left[\lambda_j^T \cdot M_k\right] \tag{27}$$

where the trace is done over all 15 *transposed* Gell–Mann matrices [18]. The index k corresponds to the specific α parameter and the j corresponds to the specific element of the algebra. Both the k and j indices run from 15 to 1. The determinant of this 15 by 15 matrix yields the differential volume element, also known as the Haar measure for the group, $\mathrm{d}V_{SU(4)}$ that, when integrated over the correct values for the ranges of the parameters and multiplied by a derivable normalization constant, yields the volume for the group.

The full 15 by 15 determinant $\mathrm{Det}[c_{kj}]$, $k, j \in \{15, \ldots, 1\}$, can be done, or one can note that the determinant can be written as

$$C_{SU(4)} = \begin{Vmatrix} c_{15,14} & c_{15,13} & \cdots & c_{15,1} & c_{15,15} \\ c_{14,14} & c_{14,13} & \cdots & c_{14,1} & c_{14,15} \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ c_{1,14} & c_{1,13} & \cdots & c_{1,1} & c_{1,15} \end{Vmatrix} \tag{28}$$

[5] The transpose operation on the Gell–Mann matrices only gives an overall sign difference to some of the matrices

$$\{\lambda_1^T, \lambda_2^T, \lambda_3^T, \lambda_4^T, \lambda_5^T, \lambda_6^T, \lambda_7^T, \lambda_8^T, \lambda_9^T, \lambda_{10}^T, \lambda_{11}^T, \lambda_{12}^T, \lambda_{13}^T, \lambda_{14}^T, \lambda_{15}^T\}$$
$$\rightarrow \{\lambda_1, -\lambda_2, \lambda_3, \lambda_4, -\lambda_5, \lambda_6, -\lambda_7, \lambda_8, \lambda_9, -\lambda_{10}, \lambda_{11}, -\lambda_{12}, \lambda_{13}, -\lambda_{14}, \lambda_{15}\}$$

but these sign changes are augmented by the inversion in the sum over k and therefore cancel out in the final construction of the determinant that we need. The transpose operation in equation (5) is done only to simplify the initial evaluation of the expansion coefficients c_{kj}.

which differs only by an overall sign from $\mathrm{Det}[c_{kj}]$ above, but which also yields a quasi-block form that generates

$$C_{SU(4)} = \begin{Vmatrix} O & D \\ A & B \end{Vmatrix} \tag{29}$$

where D corresponds to the 9 by 9 matrix whose determinant is equivalent to $\mathrm{d}V_{SU(3)} \cdot \mathrm{d}\alpha_{15}$ [8], B is a complicated 6 by 9 matrix, and O is a 9 by 6 matrix whose elements are all zero.

Now the interchange of two columns of an N by N matrix yields a change in sign of the corresponding determinant, but by moving six columns at once the sign of the determinant does not change and one may therefore generate a new matrix

$$C'_{SU(4)} = \begin{Vmatrix} c_{15,8} & c_{15,7} & \cdots & c_{15,1} & c_{15,15} & c_{15,14} & c_{15,13} & \cdots & c_{15,9} \\ c_{14,8} & c_{14,7} & \cdots & c_{14,1} & c_{14,15} & c_{14,14} & c_{14,13} & \cdots & c_{14,9} \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ c_{1,8} & c_{1,7} & \cdots & c_{1,1} & c_{1,15} & c_{1,14} & c_{1,13} & \cdots & c_{1,9} \end{Vmatrix} \tag{30}$$

which is now block diagonal

$$C'_{SU(4)} = \begin{Vmatrix} D & O \\ B & A \end{Vmatrix} \tag{31}$$

and which yields the same determinant as $C_{SU(4)}$. Thus, with this new form, the full determinant is just equal to the determinant of the diagonal blocks, one of which is already known[6]. So only the determinant of the 6 by 6 sub-matrix A which is equal to

$$A = \begin{Vmatrix} c_{6,14} & c_{6,13} & \cdots & c_{6,10} & c_{6,9} \\ c_{5,14} & c_{5,13} & \cdots & c_{5,10} & c_{5,9} \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ c_{1,14} & c_{1,13} & \cdots & c_{1,10} & c_{1,9} \end{Vmatrix} \tag{32}$$

is needed. Therefore the differential volume element for $SU(4)$ is nothing more than

$$\begin{aligned} \mathrm{d}V_{SU(4)} &= \mathrm{Det}[c_{kj}] \\ &= -\mathrm{Det}[A] * \mathrm{Det}[D]\,\mathrm{d}\alpha_{15}\ldots\mathrm{d}\alpha_1 \\ &= -\mathrm{Det}[A] * \mathrm{d}V_{SU(3)}\,\mathrm{d}\alpha_{15}\,\mathrm{d}\alpha_6\ldots\,\mathrm{d}\alpha_1 \end{aligned} \tag{33}$$

which when calculated yields the Haar measure

$$\begin{aligned} \mathrm{d}V_{SU(4)} = {} & \cos(\alpha_4)^3\cos(\alpha_6)\cos(\alpha_{10})\sin(2\alpha_2)\sin(\alpha_4)\sin(\alpha_6)^5 \\ & \times\sin(2\alpha_8)\sin(\alpha_{10})^3\sin(2\alpha_{12})\mathrm{d}\alpha_{15}\ldots\mathrm{d}\alpha_1. \end{aligned} \tag{34}$$

This is determined up to normalization (explained in detail in appendix B). Integration over the 15-parameter space gives the group volume

$$\int \underset{V}{\cdots} \int \mathrm{d}V_{SU(4)} = (192) \int \underset{V'}{\cdots} \int \mathrm{d}V_{SU(4)} \qquad V_{SU(4)} = \frac{\sqrt{2}\pi^9}{3} \tag{35}$$

which is in agreement with the volume obtained by Marinov [19].

[6] The general determinant formula for this type of block matrix is given, without proof, by Tucci in *Preprint* quant-ph/0103040.

4. Two-qubit density matrix parametrization

Using this Euler angle parametrization, any two-qubit density matrix can now be represented by following the convention derived by Boya *et al* [5]. As stated by Boya *et al*, any N-dimensional pure state can be written as a diagonal matrix with one element equal to 1 and the rest zero. Different classes of pure states have a different ordering of the zero and non-zero diagonal elements. Therefore, if one wants to write a mixture of these different pure states, one must take the following convex sum,

$$\rho_d = \sum_i a^{\mathrm{i}} \rho_i \tag{36}$$

where ρ_d is now the mixed state, ρ_i (i running from 1 to N) are the pure state matrices satisfying $\mathrm{Tr}[\rho_i \rho_j] = 2\delta_{ij}$ and a^i are constants that satisfy $\sum_i a^i = 1$ and $0 \leqslant a^i \leqslant 1$ [5]. Now a^i are just the eigenvalues of the density matrix ρ_d and can thus be parametrized by the squared components within the $(N-1)$-sphere, S^{N-1}. If we now want the most general mixed-state density matrix in some arbitrary basis, one only has to perform a unitary, unimodular transformation upon ρ_d, a transformation that will be an element of $SU(N)$. So for our two-qubit density matrix ρ we write

$$\rho = U \rho_d U^{\dagger} \tag{37}$$

where ρ_d is the diagonalized density matrix which corresponds to the eigenvalues of the 3-sphere, S^3 [5, 6, 10]

$$\rho_d = \begin{pmatrix} \sin^2(\theta_1)\sin^2(\theta_2)\sin^2(\theta_3) & 0 & 0 & 0 \\ 0 & \cos^2(\theta_1)\sin^2(\theta_2)\sin^2(\theta_3) & 0 & 0 \\ 0 & 0 & \cos^2(\theta_2)\sin^2(\theta_3) & 0 \\ 0 & 0 & 0 & \cos^2(\theta_3) \end{pmatrix} \tag{38}$$

and U, now an element of $SU(4)$, is from equation (5).

It is instructive to rewrite equation (38) as the exponentiated product of generators of the Cartan subalgebra that we are using in our parametrization of $SU(4)$; $\mathrm{e}^{\lambda_3 * a}$, $\mathrm{e}^{\lambda_8 * b}$ and $\mathrm{e}^{\lambda_{15} * c}$. Unfortunately, indeterminacies with the logarithm of the elements of ρ_d do not allow for such a rewrite, so ρ_d will be expressed in terms of the following sum:

$$\sum_{1 \leqslant j \leqslant 15} w_j \lambda_j + w_0 \mathbb{1}_4. \tag{39}$$

We begin by redefining ρ_d in the following way,

$$\rho_d = \begin{pmatrix} w^2x^2y^2 & 0 & 0 & 0 \\ 0 & (1-w^2)x^2y^2 & 0 & 0 \\ 0 & 0 & (1-x^2)y^2 & 0 \\ 0 & 0 & 0 & 1-y^2 \end{pmatrix} \tag{40}$$

where $w^2 = \sin^2(\theta_1)$, $x^2 = \sin^2(\theta_2)$ and $y^2 = \sin^2(\theta_3)$. Now we calculate the decomposition of equation (40) in terms of the elements of the full Lie algebra. This is accomplished by taking the trace of $\frac{1}{2}\rho_d \cdot \lambda_j$ over all 15 Gell–Mann matrices. Evaluation of these 15 trace operations yields the following decomposition of equation (40),

$$\rho_d = \tfrac{1}{4}\mathbb{1}_4 + \tfrac{1}{2}(-1+2w^2)x^2y^2 * \lambda_3 + \tfrac{1}{2\sqrt{3}}(-2+3x^2)y^2 * \lambda_8 + \tfrac{1}{2\sqrt{6}}(-3+4y^2) * \lambda_{15} \tag{41}$$

where the one-quarter $\mathbb{1}_4$ keeps the trace of ρ_d in this form still unity.

With equations (37) and (41) we can write ρ completely in terms of the Lie algebra subset of the parametrization. First, $U^\dagger$, the transpose of the conjugate of equation (5), is expressed as

$$U^\dagger = e^{-i\lambda_{15}\alpha_{15}}\, e^{-i\lambda_8\alpha_{14}}\, e^{-i\lambda_3\alpha_{13}}\, e^{-i\lambda_2\alpha_{12}}\, e^{-i\lambda_3\alpha_{11}}\, e^{-i\lambda_5\alpha_{10}}\, e^{-i\lambda_3\alpha_9}\, e^{-i\lambda_2\alpha_8} \times e^{-i\lambda_3\alpha_7}\, e^{-i\lambda_{10}\alpha_6}\, e^{-i\lambda_3\alpha_5}\, e^{-i\lambda_5\alpha_4}\, e^{-i\lambda_3\alpha_3}\, e^{-i\lambda_2\alpha_2}\, e^{-i\lambda_3\alpha_1}. \tag{42}$$

Thus equation (37) is equal to

$$\begin{aligned}\rho = {} & e^{i\lambda_3\alpha_1}\, e^{i\lambda_2\alpha_2}\, e^{i\lambda_3\alpha_3}\, e^{i\lambda_5\alpha_4}\, e^{i\lambda_3\alpha_5}\, e^{i\lambda_{10}\alpha_6}\, e^{i\lambda_3\alpha_7}\, e^{i\lambda_2\alpha_8} \\ & \times e^{i\lambda_3\alpha_9}\, e^{i\lambda_5\alpha_{10}}\, e^{i\lambda_3\alpha_{11}}\, e^{i\lambda_2\alpha_{12}}\, e^{i\lambda_3\alpha_{13}}\, e^{i\lambda_8\alpha_{14}}\, e^{i\lambda_{15}\alpha_{15}} \\ & \times \Big(\tfrac{1}{4}\mathbb{1}_4 + \tfrac{1}{2}(-1+2w^2)x^2y^2 * \lambda_3 \\ & + \tfrac{1}{2\sqrt{3}}(-2+3x^2)y^2 * \lambda_8 + \tfrac{1}{2\sqrt{6}}(-3+4y^2) * \lambda_{15}\Big) \\ & \times e^{-i\lambda_{15}\alpha_{15}}\, e^{-i\lambda_8\alpha_{14}}\, e^{-i\lambda_3\alpha_{13}}\, e^{-i\lambda_2\alpha_{12}}\, e^{-i\lambda_3\alpha_{11}}\, e^{-i\lambda_5\alpha_{10}}\, e^{-i\lambda_3\alpha_9}\, e^{-i\lambda_2\alpha_8} \\ & \times e^{-i\lambda_3\alpha_7}\, e^{-i\lambda_{10}\alpha_6}\, e^{-i\lambda_3\alpha_5}\, e^{-i\lambda_5\alpha_4}\, e^{-i\lambda_3\alpha_3}\, e^{-i\lambda_2\alpha_2}\, e^{-i\lambda_3\alpha_1}\end{aligned} \tag{43}$$

which, because $\mathbb{1}_4, \lambda_3, \lambda_8$ and λ_{15} all commute with each other, has the following simplification:

$$\begin{aligned}\rho &= \cdots e^{i\lambda_3\alpha_{13}}\, e^{i\lambda_8\alpha_{14}}\, e^{i\lambda_{15}\alpha_{15}} \Big(\tfrac{1}{4}\mathbb{1}_4 + \tfrac{1}{2}(-1+2w^2)x^2y^2 * \lambda_3 \\ &\quad + \tfrac{1}{2\sqrt{3}}(-2+3x^2)y^2 * \lambda_8 + \tfrac{1}{2\sqrt{6}}(-3+4y^2) * \lambda_{15}\Big)\, e^{-i\lambda_{15}\alpha_{15}}\, e^{-i\lambda_8\alpha_{14}}\, e^{-i\lambda_3\alpha_{13}} \cdots \\ &= \cdots \Big(\tfrac{1}{4}\mathbb{1}_4 + \tfrac{1}{2}(-1+2w^2)x^2y^2 * \lambda_3 + \tfrac{1}{2\sqrt{3}}(-2+3x^2)y^2 * \lambda_8 \\ &\quad + \tfrac{1}{2\sqrt{6}}(-3+4y^2) * \lambda_{15}\Big) \cdots .\end{aligned} \tag{44}$$

Therefore, all density matrices in $SU(4)$ have the following form[7],

$$\begin{aligned}\rho = {} & e^{i\lambda_3\alpha_1}\, e^{i\lambda_2\alpha_2}\, e^{i\lambda_3\alpha_3}\, e^{i\lambda_5\alpha_4}\, e^{i\lambda_3\alpha_5}\, e^{i\lambda_{10}\alpha_6}\, e^{i\lambda_3\alpha_7}\, e^{i\lambda_2\alpha_8}\, e^{i\lambda_3\alpha_9}\, e^{i\lambda_5\alpha_{10}}\, e^{i\lambda_3\alpha_{11}}\, e^{i\lambda_2\alpha_{12}} \\ & \times \Big(\tfrac{1}{4}\mathbb{1}_4 + \tfrac{1}{2}(-1+2w^2)x^2y^2 * \lambda_3 + \tfrac{1}{2\sqrt{3}}(-2+3x^2)y^2 * \lambda_8 \\ & + \tfrac{1}{2\sqrt{6}}(-3+4y^2) * \lambda_{15}\Big)\, e^{-i\lambda_2\alpha_{12}}\, e^{-i\lambda_3\alpha_{11}}\, e^{-i\lambda_5\alpha_{10}}\, e^{-i\lambda_3\alpha_9}\, e^{-i\lambda_2\alpha_8} \\ & \times e^{-i\lambda_3\alpha_7}\, e^{-i\lambda_{10}\alpha_6}\, e^{-i\lambda_3\alpha_5}\, e^{-i\lambda_5\alpha_4}\, e^{-i\lambda_3\alpha_3}\, e^{-i\lambda_2\alpha_2}\, e^{-i\lambda_3\alpha_1}\end{aligned} \tag{45}$$

where

$$w^2 = \sin^2(\theta_1) \qquad x^2 = \sin^2(\theta_2) \qquad y^2 = \sin^2(\theta_3) \tag{46}$$

with the ranges for the 12 α parameters and the three θ parameters given by

$$\begin{aligned} & 0 \leqslant \alpha_1, \alpha_3, \alpha_5, \alpha_7, \alpha_9, \alpha_{11} \leqslant \pi \\ & 0 \leqslant \alpha_2, \alpha_4, \alpha_6, \alpha_8, \alpha_{10}, \alpha_{12} \leqslant \frac{\pi}{2} \\ & \frac{\pi}{4} \leqslant \theta_1 \leqslant \frac{\pi}{2} \qquad \cos^{-1}\left(\frac{1}{\sqrt{3}}\right) \leqslant \theta_2 \leqslant \frac{\pi}{2} \qquad \frac{\pi}{3} \leqslant \theta_3 \leqslant \frac{\pi}{2}. \end{aligned} \tag{47}$$

where the α are determined from calculating the volume for the group (explained in appendix B) and the θ from generalizing the work contained in [6].

In this manner all two-particle bipartite systems can be described by a ρ that is parametrized using 12 Euler angles, and three spatial rotations, and which by [20] majorizes

[7] One should be able to write only 12 matrices in the parametrization of U since the little group of ρ_d is generated by λ_3, λ_8 and λ_{15}.

all other density matrices of $SU(4)$[8]. Exploitations of this property, related to Birkhoff theorem concerning doubly stochastic matrices and convex sets [20], allow us to use this parametrization to find the subset of ranges that generate entangled density matrices and thus parametrize the convex polygon that describes the set of entangled two-qubit systems in terms of Euler angles and spatial rotations. In order to do this, we need to look at the partial transpose of equation (45)[9].

5. Reformulated partial transpose condition

To begin with, one could say that a particular operation provides *some* entanglement if the following condition holds. Let ρ be a density matrix composed of two pure separable qubit states. Then the following matrix will represent the two-qubit subsystems A and B,

$$\rho = \rho_A \otimes \rho_B. \tag{48}$$

Let $U \in SU(4)$ be a matrix transformation on two qubits. Therefore, if

$$\rho' = U\rho U^\dagger \tag{49}$$

is an entangled state then the operation is capable of producing entanglement [23, 24]. One way in which we can tell that the matrix ρ' is entangled, is to take the partial transpose of the matrix and see if it is positive (this is the Peres–Horodecki criterion [25, 26]). In other words we wish to see if

$$(\rho')^{T_A} \leqslant 0 \qquad \text{or} \qquad (\rho')^{T_B} \leqslant 0. \tag{50}$$

These relations imply that each of the partial transposes, T_A and T_B, leaves ρ non-negative. If either of these conditions is met then there is entanglement.

As an example of this we look at the situation where $\rho_d = \rho$ and U is given by equation (5). By taking the partial transpose of ρ' and finding the subset of the given ranges of ρ_d and U such that ρ' satisfies the above conditions for entanglement we will be able to derive the set of all matrices which describes the entanglement of two qubits. To do this, we look at the eigenvalues of the partial transpose of ρ'.

Using the Euler angle parametrization previously given, a numerical calculation of the eigenvalues of the partial transpose of ρ' has been attempted. Under the standard Peres–Horodecki criterion, if any of the eigenvalues of the partial transpose of ρ' is negative then we have an entangled ρ', otherwise the state ρ' is separable. As we have mentioned, we would like to derive a subset of the ranges of the Euler angle parameters involved that would yield such a situation, thus dividing the 15-parameter space into entangled and separable subsets. Unfortunately, due to the complicated nature of the parametrization, both numerical and symbolic calculations of the eigenvalues of the partial transpose of ρ' have become computationally intractable using standard mathematical software. Therefore, only a limited number of searches over the 15-parameter space of those parameter values that satisfy the Peres–Horodecki criterion have been attempted. These initial calculations, though, have shown that all possible combinations of the minimum and maximum values for the 12 α and three θ parameters do not yield entangled density matrices. Numerical work has also shown that with this parametrization, one, and only one, eigenvalue will be negative when the values

[8] The eigenvalues of the given ρ always satisfy $\nu_1 \geqslant (\nu_2, \nu_3, \nu_4)$ with an additional ordering between the ν_2, ν_3 and ν_4 eigenvalues. Therefore, one can always find an ordering of the ν_i that satisfies the majorization condition.

[9] It is worth noting that Englert and Metwally [21, 22] have shown that for certain purposes, nine parameters extracted from the density matrix are enough to describe certain important characteristics of the local and nonlocal properties of the density matrix. In such cases, one should use the density matrix representation discussed in section 6 which more clearly expresses their ideas.

of the parameters give entangled density matrices. This is a verification of Sanpera *et al* and Verstraete *et al* who have shown that the partial transpose of an entangled two-qubit state is always of full rank and has at most one negative eigenvalue [27, 28]. This result is important, for it allows us to move away from using the standard Peres–Horodecki criterion and substitute it with an expression that only depends on the sign of a determinant.

To begin with, the eigenvalue equation for a 4 by 4 matrix is of the form

$$(\lambda - \mu_1)(\lambda - \mu_2)(\lambda - \mu_3)(\lambda - \mu_4) \tag{51}$$

which generates

$$\lambda^4 + a\lambda^3 + b\lambda^2 + c\lambda + d = 0 \tag{52}$$

where

$$\begin{aligned} a &= -(\mu_1 + \mu_2 + \mu_3 + \mu_4) \\ b &= \mu_1\mu_2 + \mu_1\mu_3 + \mu_1\mu_4 + \mu_2\mu_3 + \mu_2\mu_4 + \mu_3\mu_4 \\ c &= -(\mu_1\mu_2(\mu_3 + \mu_4) + (\mu_1 + \mu_2)\mu_3\mu_4) \\ d &= \mu_1\mu_2\mu_3\mu_4. \end{aligned} \tag{53}$$

Now, since the μ_i are eigenvalues, there sum must be equal to 1. Thus coefficient a in equation (52) is -1. Therefore, the characteristic equation we must solve is given by

$$\lambda^4 - \lambda^3 + b\lambda^2 + c\lambda + d = 0 \tag{54}$$

which can be simplified by making the substitution $\tau = \lambda - 1/4$ which yields

$$\begin{aligned} &\tau^4 + p\tau^2 + q\tau + r = 0 \\ &p = b - \tfrac{3}{8} \\ &q = \frac{b}{2} - c - \frac{1}{8} \\ &r = \frac{b}{16} - \frac{c}{4} + d - \frac{3}{256}. \end{aligned} \tag{55}$$

The behaviour of the solutions of this equation depends on the cubic resolvent

$$\gamma^3 + 2p\gamma^2 + (p^2 - 4r)\gamma - q^2 = 0 \tag{56}$$

which has $\gamma_1\gamma_2\gamma_3 = q^2$ [29]. Recalling that the solution of a cubic equation can be obtained by using Cardano's formula [29] we can immediately write the roots for equation (56)

$$\begin{aligned} \gamma_1 &= \frac{-2p}{3} - \frac{2^{\frac{1}{3}}(-p^2 - 12r)}{3(2p^3 + 27q^2 - 72pr + \sqrt{4(-p^2 - 12r)^3 + (2p^3 + 27q^2 - 72pr)^2})^{\frac{1}{3}}} \\ &\quad + \frac{(2p^3 + 27q^2 - 72pr + \sqrt{4(-p^2 - 12r)^3 + (2p^3 + 27q^2 - 72pr)^2})^{\frac{1}{3}}}{32^{\frac{1}{3}}} \\ \gamma_2 &= \frac{-2p}{3} + \frac{(1 + \mathrm{i}\sqrt{3})(-p^2 - 12r)}{32^{\frac{2}{3}}(2p^3 + 27q^2 - 72pr + \sqrt{4(-p^2 - 12r)^3 + (2p^3 + 27q^2 - 72pr)^2})^{\frac{1}{3}}} \\ &\quad - \frac{(1 - \mathrm{i}\sqrt{3})(2p^3 + 27q^2 - 72pr + \sqrt{4(-p^2 - 12r)^3 + (2p^3 + 27q^2 - 72pr)^2})^{\frac{1}{3}}}{62^{\frac{1}{3}}} \\ \gamma_3 &= \frac{-2p}{3} + \frac{(1 - \mathrm{i}\sqrt{3})(-p^2 - 12r)}{32^{\frac{2}{3}}(2p^3 + 27q^2 - 72pr + \sqrt{4(-p^2 - 12r)^3 + (2p^3 + 27q^2 - 72pr)^2})^{\frac{1}{3}}} \\ &\quad - \frac{(1 + \mathrm{i}\sqrt{3})(2p^3 + 27q^2 - 72pr + \sqrt{4(-p^2 - 12r)^3 + (2p^3 + 27q^2 - 72pr)^2})^{\frac{1}{3}}}{62^{\frac{1}{3}}}. \end{aligned} \tag{57}$$

In terms of our original parameters b, c and d, we have for equation (56)

$$\gamma^3 + 2\left(\tfrac{-3}{8} - b\right)\gamma^2 + \left(\tfrac{3}{16} - b + b^2 + c - 4d\right)\gamma - \tfrac{1}{64}(1 - 4b + 8c)^2 \tag{58}$$

and therefore for its roots

$$\begin{aligned}
\gamma_1 = {} & -12(-1+8b)(-3+16b(1+b)-16c+64d) + [-54(1-8b)^2(1-4b+8c)^2 + 6\sqrt{3} \\
& \times \sqrt{27(1-8b)^4(1-4b+8c)^4 + 16(-1+8b)^3(-3+16b(1+b)-16c+64d)^3}]^{\frac{2}{3}} \\
& \times (12(-1+8b)[-54(1-8b)^2(1-4b+8c)^2 + 6\sqrt{3} \\
& \times \sqrt{27(1-8b)^4(1-4b+8c)^4 + 16(-1+8b)^3(-3+16b(1+b)-16c+64d)^3}]^{\frac{1}{3}})^{-1} \\
\gamma_2 = {} & 6(1+\mathrm{i}\sqrt{3})(-1+8b)(-3+16b(1+b)-16c+64d) \\
& + (-3)^{\frac{2}{3}}[-18(1-8b)^2(1-4b+8c)^2 + 2\sqrt{3} \\
& \times \sqrt{27(1-8b)^4(1-4b+8c)^4 + 16(-1+8b)^3(-3+16b(1+b)-16c+64d)^3}]^{\frac{2}{3}} \\
& \times (12(-1+8b)[-54(1-8b)^2(1-4b+8c)^2 + 6\sqrt{3} \\
& \times \sqrt{27(1-8b)^4(1-4b+8c)^4 + 16(-1+8b)^3(-3+16b(1+b)-16c+64d)^3}]^{\frac{1}{3}})^{-1} \\
\gamma_3 = {} & 12(1-\mathrm{i}\sqrt{3})(-1+8b)(-3+16b(1+b)-16c+64d) \\
& - 3^{\frac{1}{6}}(-3\mathrm{i}+\sqrt{3})[-18(1-8b)^2(1-4b+8c)^2 + 2\sqrt{3} \\
& \times \sqrt{27(1-8b)^4(1-4b+8c)^4 + 16(-1+8b)^3(-3+16b(1+b)-16c+64d)^3}]^{\frac{2}{3}} \\
& \times (24(-1+8b)[-54(1-8b)^2(1-4b+8c)^2 + 6\sqrt{3} \\
& \times \sqrt{27(1-8b)^4(1-4b+8c)^4 + 16(-1+8b)^3(-3+16b(1+b)-16c+64d)^3}]^{\frac{1}{3}})^{-1}.
\end{aligned} \tag{59}$$

Now, if all three γ solutions are real and positive, the quartic equation (55) has the following solutions:

$$\begin{aligned}
\tau_1 &= \frac{\sqrt{\gamma_1} + \sqrt{\gamma_2} + \sqrt{\gamma_3}}{2} & \tau_2 &= \frac{\sqrt{\gamma_1} - \sqrt{\gamma_2} - \sqrt{\gamma_3}}{2} \\
\tau_3 &= \frac{-\sqrt{\gamma_1} + \sqrt{\gamma_2} - \sqrt{\gamma_3}}{2} & \tau_4 &= \frac{-\sqrt{\gamma_1} - \sqrt{\gamma_2} + \sqrt{\gamma_3}}{2}.
\end{aligned} \tag{60}$$

Substitution of the γ values given in equation (59) into equation (60) creates the four eigenvalue equations that the standard Peres–Horodecki criterion would force us to evaluate. These are quite difficult and time consuming, especially when b, c and d are written in terms of the twelve α and three θ parameters, and can become computationally intractable even for modern mathematical software. But, from the previous discussion, it is obvious that with only one eigenvalue that changes sign, the only parameter that needs to be analysed is d. Therefore, instead of looking at solutions of (60) one may instead look at when d from equation (53) changes sign[10].

Now, the d parameter is the zeroth-order λ coefficient from the following equation:

$$\mathrm{Det}(\rho^{pt} - \mathbb{1}_4 * \lambda) \tag{61}$$

[10] Wang has proposed a general solution of the eigenvalue problem for the partial transpose of two qubits (see, for example, [30], equation (22)) in which he states that only one equation need be evaluated to determine entanglement. Unfortunately, in order to evaluate that one equation ([30], equation (22)), six other equations must first be evaluated ([30], equations (23)–(28)). In terms of the 15 parameters needed to represent the Hilbert space of a two-qubit density matrix, it is far easier to evaluate the zeroth order λ coefficient d given in equation (54) than to evaluate seven total equations. Even if one where to substitute and simplify, achieving one equation, its representation in terms of the 15 parameters needed to accurately describe the most general density matrix would still be more complicated to numerically and symbolically evaluate than the d parameter.

where ρ^{pt} is the partial transpose of equation (45). This is just the standard characteristic equation that yields the fourth-order polynomial from which the eigenvalues of the partial transpose of equation (45) are to be evaluated, and which equations (52) and (53) are generated from. Computationally, from the standpoint of our parametrization, it is easier to take this determinant than to explicitly solve for the roots of a fourth-order polynomial (as we have given above). The solution of equation (61) yields an expression for d in terms of the 12 α and three θ parameters that can be numerically evaluated by standard mathematical software packages with much greater efficiency than the full Peres–Horodecki criterion[11].

6. Conclusions

The aim of this paper has been to show an explicit Euler angle parametrization for the Hilbert space of all two-qubit density matrices. As we have stated, such a parametrization should be very useful for many calculations, especially numerical, concerning entanglement. This parametrization also allows for an in-depth analysis of the convex sets, subsets, and overall set boundaries of separable and entangled two-qubit systems without having to make any initial restrictions as to the type of parametrization and density matrix in question. We have also been able to use this parametrization as an independent verification to Marinov's $SU(4)$ volume calculation. The role of the parametrization in simplifying the Peres–Horodecki criteria for two-qubit systems has also been indicated.

Although one may generate or use other parametrizations of $SU(4)$ and two-qubit density matrices (see, for example, [31–34]), our parametrization does have the advantage of not naively overcounting the group, as well as generating an easily integrable Haar measure and having a form suited for generalization. Such a parametrization should also assist in providing a Bures distance for the space of two-qubits. Also, although previous work has been done on evaluating the eigenvalues of the partial transpose of the two-qubit density matrix (for example, the work done by Wang in [30]), our representation allows the user to effect both a reduction in the number of equations to be analysed for entanglement onset from 4 to 1 while still retaining the ability to analyse the little group and orbit space of the density matrix as well (see, for example, the work contained in [5]). We also believe that this research yields the following possibilities:

1. The partial transpose condition could be used to find the set of separable and entangled states by finding the ranges of the angles for which the density matrix is positive semi-definite.
2. The $SU(4)$ parametrization enables the calculation of the distance measure between density matrices and then uses the minimum distance to a completely separable matrix as a measure of separability. Applications to other measures of entanglement [35] are straightforward.
3. One could use ranges of the angles that correspond to entangled states to find the ranges of the parameters in the parametrization in terms of the Pauli basis states by using the following parametrization for the density matrix:

$$\rho = \frac{1}{4}(\mathbb{1}_4 + a_i\sigma_i \otimes \mathbb{1}_2 + \mathbb{1}_2 \otimes b_j\tau_j + c_{kl}\sigma_k \otimes \tau_l). \tag{62}$$

For more on this parametrization, see [21, 22] and references within.

[11] This greater efficiency is based on the observation that the kernel of the mathematical software package Mathematica ver. 4.0 rel. 3, running on an optimized 1.5 GHz Pentium 4 Linux box with 1 gigabyte of 333 MHz DDR, was unable to express equation (60) in terms of the 12 α and three θ parameters in a format suitable for encoding into a C++ program. On the other hand, it was quite easy to obtain all the coefficients of equation (54) in terms of our Euler parameters, simplify them and encode them into a C++ program for numerical evaluation. Also, since only one eigenvalue ever goes negative, we have reduced the number of equations to solve from 4 to 1 which is a definite improvement in calculatory efficiency.

4. Related to this last question is the question of the boundary between the convex set of entangled and separable states of the density matrices. For example, one could use the explicit parametrization to calculate specific measures of entanglement such as the entanglement of formation for different density matrices in different regions of the set of density matrices and see which regions of the convex set correspond to the greatest entanglement of formation. Another possibility is that given the boundary in the σ, τ form, we could recreate it in terms of the Euler angles.

There are obviously more, but for now, it is these areas that we believe offer the most interest to those wishing to develop a deeper understanding of bipartite entanglement. Also, since the methods here are quite general and rely primarily on the group-theoretical techniques developed here, we anticipate generalizations to higher-dimensional state spaces will be, in principle, straightforward.

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Appendix A. Commutation relations for $SU(4)$

We first note that the Gell–Mann-type basis for the Lie algebra of $SU(4)$ is given by the following set of matrices [18]:

$$\lambda_1 = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad \lambda_2 = \begin{pmatrix} 0 & -\mathrm{i} & 0 & 0 \\ \mathrm{i} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad \lambda_3 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

$$\lambda_4 = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad \lambda_5 = \begin{pmatrix} 0 & 0 & -\mathrm{i} & 0 \\ 0 & 0 & 0 & 0 \\ \mathrm{i} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad \lambda_6 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

$$\lambda_7 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & -\mathrm{i} & 0 \\ 0 & \mathrm{i} & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad \lambda_8 = \frac{1}{\sqrt{3}}\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -2 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad \lambda_9 = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \tag{A.1}$$

$$\lambda_{10} = \begin{pmatrix} 0 & 0 & 0 & -\mathrm{i} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \mathrm{i} & 0 & 0 & 0 \end{pmatrix} \quad \lambda_{11} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} \quad \lambda_{12} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\mathrm{i} \\ 0 & 0 & 0 & 0 \\ 0 & \mathrm{i} & 0 & 0 \end{pmatrix}$$

$$\lambda_{13} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \quad \lambda_{14} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\mathrm{i} \\ 0 & 0 & \mathrm{i} & 0 \end{pmatrix} \quad \lambda_{15} = \frac{1}{\sqrt{6}}\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -3 \end{pmatrix}.$$

Table A1. $[k_1, k_2] \in L(K)$.

	λ_1	λ_2	λ_3	λ_4	λ_5	λ_6	λ_7	λ_8	λ_{15}
λ_1	0	$2\mathrm{i}\lambda_3$	$-2\mathrm{i}\lambda_2$	$\mathrm{i}\lambda_7$	$-\mathrm{i}\lambda_6$	$\mathrm{i}\lambda_5$	$-\mathrm{i}\lambda_4$	0	0
λ_2	$-2\mathrm{i}\lambda_3$	0	$2\mathrm{i}\lambda_1$	$\mathrm{i}\lambda_6$	$\mathrm{i}\lambda_7$	$-\mathrm{i}\lambda_4$	$-\mathrm{i}\lambda_5$	0	0
λ_3	$2\mathrm{i}\lambda_2$	$-2\mathrm{i}\lambda_1$	0	$\mathrm{i}\lambda_5$	$-\mathrm{i}\lambda_4$	$-\mathrm{i}\lambda_7$	$\mathrm{i}\lambda_6$	0	0
λ_4	$-\mathrm{i}\lambda_7$	$-\mathrm{i}\lambda_6$	$-\mathrm{i}\lambda_5$	0	$\mathrm{i}(\lambda_3 + \sqrt{3}\lambda_8)$	$\mathrm{i}\lambda_2$	$\mathrm{i}\lambda_1$	$-\mathrm{i}\sqrt{3}\lambda_5$	0
λ_5	$\mathrm{i}\lambda_6$	$-\mathrm{i}\lambda_7$	$\mathrm{i}\lambda_4$	$-\mathrm{i}(\lambda_3 + \sqrt{3}\lambda_8)$	0	$-\mathrm{i}\lambda_1$	$\mathrm{i}\lambda_2$	$\mathrm{i}\sqrt{3}\lambda_4$	0
λ_6	$-\mathrm{i}\lambda_5$	$\mathrm{i}\lambda_4$	$\mathrm{i}\lambda_7$	$-\mathrm{i}\lambda_2$	$\mathrm{i}\lambda_1$	0	$\mathrm{i}(-\lambda_3 + \sqrt{3}\lambda_8)$	$-\mathrm{i}\sqrt{3}\lambda_7$	0
λ_7	$\mathrm{i}\lambda_4$	$\mathrm{i}\lambda_5$	$-\mathrm{i}\lambda_6$	$-\mathrm{i}\lambda_1$	$-\mathrm{i}\lambda_2$	$\mathrm{i}(\lambda_3 - \sqrt{3}\lambda_8)$	0	$\mathrm{i}\sqrt{3}\lambda_6$	0
λ_8	0	0	0	$\mathrm{i}\sqrt{3}\lambda_5$	$-\mathrm{i}\sqrt{3}\lambda_4$	$\mathrm{i}\sqrt{3}\lambda_7$	$-\mathrm{i}\sqrt{3}\lambda_6$	0	0
λ_{15}	0	0	0	0	0	0	0	0	0

Table A2. $[p_1, p_2] \in L(K)$.

	λ_9	λ_{10}	λ_{11}	λ_{12}	λ_{13}	λ_{14}
λ_9	0	$\mathrm{i}\left(\lambda_3 + \frac{1}{\sqrt{3}}\lambda_8 + 2\sqrt{\frac{2}{3}}\lambda_{15}\right)$	$\mathrm{i}\lambda_2$	$\mathrm{i}\lambda_1$	$\mathrm{i}\lambda_5$	$\mathrm{i}\lambda_4$
λ_{10}	$-\mathrm{i}\left(\lambda_3 + \frac{1}{\sqrt{3}}\lambda_8 + 2\sqrt{\frac{2}{3}}\lambda_{15}\right)$	0	$-\mathrm{i}\lambda_1$	$\mathrm{i}\lambda_2$	$-\mathrm{i}\lambda_4$	$\mathrm{i}\lambda_5$
λ_{11}	$-\mathrm{i}\lambda_2$	$\mathrm{i}\lambda_1$	0	$\mathrm{i}\left(-\lambda_3 + \frac{1}{\sqrt{3}}\lambda_8 + 2\sqrt{\frac{2}{3}}\lambda_{15}\right)$	$\mathrm{i}\lambda_7$	$\mathrm{i}\lambda_6$
λ_{12}	$-\mathrm{i}\lambda_1$	$-\mathrm{i}\lambda_2$	$\mathrm{i}\left(\lambda_3 - \frac{1}{\sqrt{3}}\lambda_8 - 2\sqrt{\frac{2}{3}}\lambda_{15}\right)$	0	$-\mathrm{i}\lambda_6$	$\mathrm{i}\lambda_7$
λ_{13}	$-\mathrm{i}\lambda_5$	$\mathrm{i}\lambda_4$	$-\mathrm{i}\lambda_7$	$\mathrm{i}\lambda_6$	0	$2\mathrm{i}\left(-\frac{1}{\sqrt{3}}\lambda_8 + \sqrt{\frac{2}{3}}\lambda_{15}\right)$
λ_{14}	$-\mathrm{i}\lambda_4$	$-\mathrm{i}\lambda_5$	$-\mathrm{i}\lambda_6$	$-\mathrm{i}\lambda_7$	$2\mathrm{i}\left(\frac{1}{\sqrt{3}}\lambda_8 - \sqrt{\frac{2}{3}}\lambda_{15}\right)$	0

In order to develop the Cartan decomposition of $SU(4)$ it is helpful to look at the commutator relationships between the 15 elements of its Lie algebra. In tables A1–A3 we list the commutator solutions of the corresponding ith row and jth column Gell–Mann matrices corresponding to the following definitions:

$$[\lambda_i, \lambda_j] = 2\mathrm{i} f_{ijk}\lambda_k \qquad f_{ijk} = \frac{1}{4\mathrm{i}} \mathrm{Tr}[[\lambda_i, \lambda_j] \cdot \lambda_k].$$

Table A1 corresponds to the $L(K)$ subset of $SU(4)$, $\{\lambda_1, \ldots, \lambda_8, \lambda_{15}\}$ and shows that for $k_1, k_2 \in L(K), [k_1, k_2] \in L(K)$. Table A2 corresponds to the $L(P)$ subset of $SU(4)$, $\{\lambda_9, \ldots, \lambda_{14}\}$ and shows that for $p_1, p_2 \in L(P), [p_1, p_2] \in L(K)$. Table A3 corresponds to the commutator solutions for the situation when $k_1 \in L(K)$ and $p_2 \in L(P), [k_1, p_2] \in L(P)$.

Appendix B. Invariant volume element normalization calculations

Before integrating $\mathrm{d}V_{SU(4)}$ we need some group theory. We begin with a digression concerning the centre of a group [36, 37]. If S is a subset of a group G, then the centralizer $C_G(S)$ of S in G is defined by

$$C(S) \equiv C_G(S) = \{x \in G \mid \text{ if } s \in S \text{ then } xs = sx\}. \tag{B1}$$

Table A3. $[k_1, p_2] \in L(P)$.

	λ_1	λ_2	λ_3	λ_4	λ_5	λ_6	λ_7	λ_8	λ_9	λ_{10}	λ_{11}	λ_{12}	λ_{13}	λ_{14}	λ_{15}
λ_1									$i\lambda_{12}$	$-i\lambda_{11}$	$i\lambda_{10}$	$-i\lambda_9$	0	0	
λ_2									$i\lambda_{11}$	$i\lambda_{12}$	$-i\lambda_9$	$-i\lambda_{10}$	0	0	
λ_3									$i\lambda_{10}$	$-i\lambda_9$	$-i\lambda_{12}$	$i\lambda_{11}$	0	0	
λ_4									$i\lambda_{14}$	$-i\lambda_{13}$	0	0	$i\lambda_{10}$	$-i\lambda_9$	
λ_5									$i\lambda_{13}$	$i\lambda_{14}$	0	0	$-i\lambda_9$	$-i\lambda_{10}$	
λ_6									0	0	$i\lambda_{14}$	$-i\lambda_{13}$	$i\lambda_{12}$	$-i\lambda_{11}$	
λ_7									0	0	$i\lambda_{13}$	$i\lambda_{14}$	$-i\lambda_{11}$	$-i\lambda_{12}$	
λ_8									$\frac{i}{\sqrt{3}}\lambda_{10}$	$-\frac{i}{\sqrt{3}}\lambda_9$	$\frac{i}{\sqrt{3}}\lambda_{12}$	$-\frac{i}{\sqrt{3}}\lambda_{11}$	$-\frac{i}{\sqrt{3}}\lambda_{14}$	$\frac{i}{\sqrt{3}}\lambda_{13}$	
λ_9	$-i\lambda_{12}$	$-i\lambda_{11}$	$-i\lambda_{10}$	$-i\lambda_{14}$	$-i\lambda_{13}$	0	0	$-\frac{i}{\sqrt{3}}\lambda_{10}$							$-i\sqrt{\frac{8}{3}}\lambda_{10}$
λ_{10}	$i\lambda_{11}$	$-i\lambda_{12}$	$i\lambda_9$	$i\lambda_{13}$	$-i\lambda_{14}$	0	0	$\frac{i}{\sqrt{3}}\lambda_9$							$i\sqrt{\frac{8}{3}}\lambda_9$
λ_{11}	$-i\lambda_{10}$	$i\lambda_9$	$i\lambda_{12}$	0	0	$-i\lambda_{14}$	$-i\lambda_{13}$	$-\frac{i}{\sqrt{3}}\lambda_{12}$							$-i\sqrt{\frac{8}{3}}\lambda_{12}$
λ_{12}	$i\lambda_9$	$i\lambda_{10}$	$-i\lambda_{11}$	0	0	$i\lambda_{13}$	$-i\lambda_{14}$	$\frac{i}{\sqrt{3}}\lambda_{11}$							$i\sqrt{\frac{8}{3}}\lambda_{11}$
λ_{13}	0	0	0	$-i\lambda_{10}$	$i\lambda_9$	$-i\lambda_{12}$	$i\lambda_{11}$	$\frac{i}{\sqrt{3}}\lambda_{14}$							$-i\sqrt{\frac{8}{3}}\lambda_{14}$
λ_{14}	0	0	0	$i\lambda_9$	$i\lambda_{10}$	$i\lambda_{11}$	$i\lambda_{12}$	$-\frac{i}{\sqrt{3}}\lambda_{13}$							$i\sqrt{\frac{8}{3}}\lambda_{13}$
λ_{15}									$i\sqrt{\frac{8}{3}}\lambda_{10}$	$-i\sqrt{\frac{8}{3}}\lambda_9$	$i\sqrt{\frac{8}{3}}\lambda_{12}$	$-i\sqrt{\frac{8}{3}}\lambda_{11}$	$i\sqrt{\frac{8}{3}}\lambda_{14}$	$-i\sqrt{\frac{8}{3}}\lambda_{13}$	0

For example, if $S = \{y\}$, $C(y)$ will be used instead of $C(\{y\})$. Next, the centralizer of G in G is called the centre of G and is denoted by $Z(G)$ or Z.

$$Z(G) \equiv Z = \{z \in G \mid zx = xz \text{ for all } x \in G\} = C_G(G). \tag{B2}$$

Another way of writing this is

$$Z(G) = \cap\{C(x) \mid x \in G\} = \{z \mid \text{if } x \in G \text{ then } z \in C(x)\}. \tag{B3}$$

In other words, the centre is the set of all elements z that commutes with all other elements in the group. Finally, the commutator $[x, y]$ of two elements x and y of a group G is given by the equation

$$[x, y] = x^{-1}y^{-1}xy. \tag{B4}$$

Now what we want to find is the number of elements at the centre of $SU(N)$ for $N = 2, 3$ and 4. Begin by defining the following

$$Z_n = \text{cyclic group of order } n \cong \mathbb{Z}_n \cong Z(SU(N)). \tag{B5}$$

Therefore, the set of all matrices which comprise the centre of $SU(N)$, $Z(SU(N))$, is congruent to Z_N since we know that if G is a finite linear group over a field F, then the set of matrices of the form $\Sigma c_g g$, where $g \in G$ and $c_g \in F$, forms an algebra (in fact, a ring) [37, 15]. For example, for $SU(2)$ we would have

$$\begin{aligned} &Z_2 = \{x \in SU(2) \mid [x, y] \in Z_1 \text{ for all } y \in SU(2)\} \\ &[x, y] = \omega \mathbb{1}_2 \qquad Z_1 = \{\mathbb{1}_2\}. \end{aligned} \tag{B6}$$

This would be the set of all 2 by 2 matrix elements such that the commutator relationship would yield the identity matrix multiplied by some non-zero coefficient. In general, this can be written as

$$Z_N = \{x \in SU(N) \mid [x, y] \in Z_1 \text{ for all } y \in SU(N)\} \qquad Z_1 = \{\mathbb{1}_N\}. \tag{B7}$$

This is similar to the result from [36], which shows that the centre of the general linear group of real matrices, $GL_N(\Re)$ is the group of scalar matrices, that is, those of the from $\omega\mathbb{I}$, where $\mathbb{I}$ is the identity element of the group and ω is some multiplicative constant. For $SU(N)$, $\omega\mathbb{I}$ is an Nth root of unity.

To begin our actual search for the normalization constant for our invariant volume element, we first again look at the group $SU(2)$. For this group, every element can be written as

$$\begin{pmatrix} a & b \\ -\bar{b} & \bar{a} \end{pmatrix} \tag{B8}$$

where $|a|^2 + |b|^2 = 1$. Again, following [36] we can make the following parametrization:

$$a = y_1 - \mathrm{i}y_2 \qquad b = y_3 - \mathrm{i}y_4 \qquad 1 = y_1^2 + y_2^2 + y_3^2 + y_4^2. \tag{B9}$$

The elements $(1, 0, 0, 0)$ and $(-1, 0, 0, 0)$ are anti-podal points, or polar points if one pictures the group as a three-dimensional unit sphere in a four-dimensional space parameterized by y, and thus comprise the elements for the centre group of $SU(2)$ (i.e. $\pm\mathbb{1}_2$). Therefore, the centre for $SU(2)$ is comprised of two elements.

In our parametrization, the general $SU(2)$ elements are given by

$$D(\mu, \nu, \xi) = \mathrm{e}^{\mathrm{i}\lambda_3\mu}\,\mathrm{e}^{\mathrm{i}\lambda_2\nu}\,\mathrm{e}^{\mathrm{i}\lambda_3\xi} \qquad \mathrm{d}V_{SU(2)} = \sin(2\nu)\,\mathrm{d}\mu\,\mathrm{d}\nu\,\mathrm{d}\xi \tag{B10}$$

with corresponding ranges

$$0 \leqslant \mu, \xi \leqslant \pi \qquad 0 \leqslant \nu \leqslant \frac{\pi}{2}. \tag{B11}$$

Integrating over the volume element $dV_{SU(2)}$ with the above ranges yields the volume of the group $SU(2)/Z_2$. In other words, the $SU(2)$ group with its two centre elements identified. In order to get the full volume of the $SU(2)$ group, all one needs to do is multiply the volume of $SU(2)/Z_2$ by the number of removed centre elements, in this case 2.

This process can be extended to the $SU(3)$ and $SU(4)$ parametrizations. For $SU(3)$ [6, 8–10] (here recast as a component of the $SU(4)$ parametrization)

$$SU(3) = e^{i\lambda_3\alpha_7}\, e^{i\lambda_2\alpha_8}\, e^{i\lambda_3\alpha_9}\, e^{i\lambda_5\alpha_{10}} D(\alpha_{11}, \alpha_{12}, \alpha_{13})\, e^{i\lambda_8\alpha_{14}}. \tag{B12}$$

Now, we get an initial factor of two from the $D(\alpha_{11}, \alpha_{12}, \alpha_{13})$ component. We shall now prove that we get another factor of two from the $e^{i\lambda_3\alpha_9}\, e^{i\lambda_5\alpha_{10}}$ component as well.

From the commutation relations of the elements of the Lie algebra of $SU(3)$ (see [8], for details) we see that $\{\lambda_3, \lambda_4, \lambda_5, \lambda_8\}$ form a closed subalgebra $SU(2) \times U(1)$.[12]

$$\begin{array}{lll} [\lambda_3, \lambda_4] = i\lambda_5 & [\lambda_3, \lambda_5] = -i\lambda_4 & [\lambda_3, \lambda_8] = 0 \\ [\lambda_4, \lambda_5] = i(\lambda_3 + \sqrt{3}\lambda_8) & [\lambda_4, \lambda_8] = -i\sqrt{3}\lambda_5 & [\lambda_5, \lambda_8] = i\sqrt{3}\lambda_4. \end{array} \tag{B13}$$

Observation of the four λ matrices with respect to the Pauli spin matrices of $SU(2)$ shows that λ_4 is the $SU(3)$ analogue of σ_1, λ_5 is the $SU(3)$ analogue of σ_2 and both λ_3 and λ_8 are the $SU(3)$ analogues of σ_3

$$\begin{aligned} \sigma_1 &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \implies \lambda_4 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \\ \sigma_2 &= \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \implies \lambda_5 = \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix} \\ \sigma_3 &= \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \implies \lambda_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad \text{and} \quad \lambda_8 = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}. \end{aligned} \tag{B14}$$

Thus one may use either $\{\lambda_3, \lambda_5\}$ or $\{\lambda_3, \lambda_5, \lambda_8\}$ to generate an $SU(2)$ subgroup of $SU(3)$. The volume of this $SU(2)$ subgroup of $SU(3)$ must be equal to the volume of the general $SU(2)$ group, $2\pi^2$. If we demand that any element of the $SU(2)$ subgroup of $SU(3)$ has similar ranges as its $SU(2)$ analogue[13], then a multiplicative factor of 2 is required for the $e^{i\lambda_3\alpha_9}\, e^{i\lambda_5\alpha_{10}}$ component[14].

Finally, $SU(3)$ has a Z_3 whose elements have the generic form

$$\begin{pmatrix} \eta_1 & 0 & 0 \\ 0 & \eta_2 & 0 \\ 0 & 0 & \eta_1^{-1}\eta_2^{-1} \end{pmatrix} \tag{B15}$$

where

$$\eta_1^3 = \eta_2^3 = 1. \tag{B16}$$

[12] Georgi [38] has stated that λ_2, λ_5 and λ_7 generate an $SU(2)$ subalgebra of $SU(3)$. This fact can be seen in the commutator relationships between these three λ matrices contained in [8] or in appendix A.

[13] This requires a normalization factor of $\frac{1}{\sqrt{3}}$ on the maximal range of λ_8 that is explained by the removal of the Z_3 elements of $SU(3)$.

[14] When calculating this volume element, it is important to remember that the closed subalgebra being used is $SU(2) \times U(1)$ and therefore the integrated kernel, be it derived either from $e^{i\lambda_3\alpha}\, e^{i\lambda_5\beta}\, e^{i\lambda_3\gamma}$ or from $e^{i\lambda_3\alpha}\, e^{i\lambda_5\beta}\, e^{i\lambda_8\gamma}$, will require contributions from both the $SU(2)$ and $U(1)$ elements.

Solving for η_1 and η_2 yields the following elements for Z_3

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad -\begin{pmatrix} (-1)^{\frac{1}{3}} & 0 & 0 \\ 0 & (-1)^{\frac{1}{3}} & 0 \\ 0 & 0 & (-1)^{\frac{1}{3}} \end{pmatrix} \qquad \begin{pmatrix} (-1)^{\frac{2}{3}} & 0 & 0 \\ 0 & (-1)^{\frac{2}{3}} & 0 \\ 0 & 0 & (-1)^{\frac{2}{3}} \end{pmatrix} \tag{B17}$$

which are the three cube roots of unity. Combining these $SU(3)$ centre elements, a total of three, with the 2 factors of 2 from the previous discussion, yields a total multiplication factor of 12. The volume of $SU(3)$ is then

$$V_{SU(3)} = 2 \times 2 \times 3 \times V(SU(3)/Z_3) = \sqrt{3}\pi^5 \tag{B18}$$

using the ranges given above for the general $SU(2)$ elements, combined with $0 \leqslant \alpha_{14} \leqslant \frac{\pi}{\sqrt{3}}$. Explicitly,

$$0 \leqslant \alpha_7, \alpha_9, \alpha_{11}, \alpha_{13} \leqslant \pi \qquad 0 \leqslant \alpha_8, \alpha_{10}, \alpha_{12} \leqslant \frac{\pi}{2} \qquad 0 \leqslant \alpha_{14} \leqslant \frac{\pi}{\sqrt{3}}. \tag{B19}$$

These are modifications of [6, 8–10, 39] and take into account the updated Marinov group volume values [19].

For $SU(4)$ the process is similar to that used for $SU(3)$, but now with two $SU(2)$ subgroups to worry about. For $SU(4)$,

$$U = \mathrm{e}^{\mathrm{i}\lambda_3\alpha_1}\,\mathrm{e}^{\mathrm{i}\lambda_2\alpha_2}\,\mathrm{e}^{\mathrm{i}\lambda_3\alpha_3}\,\mathrm{e}^{\mathrm{i}\lambda_5\alpha_4}\,\mathrm{e}^{\mathrm{i}\lambda_3\alpha_5}\,\mathrm{e}^{\mathrm{i}\lambda_{10}\alpha_6}[SU(3)]\,\mathrm{e}^{\mathrm{i}\lambda_{15}\alpha_{15}}. \tag{B20}$$

Here, the two $SU(2)$ subalgebras in $SU(4)$ that we are concerned with are $\{\lambda_3, \lambda_4, \lambda_5, \lambda_8, \lambda_{15}\}$ and $\{\lambda_3, \lambda_9, \lambda_{10}, \lambda_8, \lambda_{15}\}$. Both of these $SU(2) \times U(1) \times U(1)$ subalgebras are represented in the parametrization of $SU(4)$ as $SU(2)$ subgroup elements, $\mathrm{e}^{\mathrm{i}\lambda_3\alpha_3}\,\mathrm{e}^{\mathrm{i}\lambda_5\alpha_4}$ and $\mathrm{e}^{\mathrm{i}\lambda_3\alpha_5}\,\mathrm{e}^{\mathrm{i}\lambda_{10}\alpha_6}$. We can see that λ_{10} is the $SU(4)$ analogue of σ_2[15] and λ_{15} is the $SU(4)$ analogue to σ_3.[16] The demand that all $SU(2)$ subgroups of $SU(4)$ must have a volume equal to $2\pi^2$ is equivalent to having the parameters of the associated elements of the $SU(2)$ subgroup run through similar ranges as their $SU(2)$ analogues[17]. As with $SU(3)$, this restriction yields an overall multiplicative factor of 4 from these two elements[18]. Recalling that the $SU(3)$ element yields a multiplicative factor of 12, all that remains is to determine the multiplicative factor equivalent to the identification of the $SU(4)$ centre, Z_4.

The elements of the centre of $SU(4)$ are similar in form to the ones from $SU(3)$;

$$\begin{pmatrix} \eta_1 & 0 & 0 & 0 \\ 0 & \eta_2 & 0 & 0 \\ 0 & 0 & \eta_3 & 0 \\ 0 & 0 & 0 & \eta_1^{-1}\eta_2^{-1}\eta_3^{-1} \end{pmatrix} \tag{B21}$$

where

$$\eta_1^4 = \eta_2^4 = \eta_3^4 = 1. \tag{B22}$$

[15] We have already discussed λ_5 in the previous section on $SU(3)$.

[16] It is the $SU(4)$ Cartan subalgebra element.

[17] This requires a normalization factor of $\frac{1}{\sqrt{6}}$ on the maximal range of λ_{15} that is explained by the removal of the Z_4 elements of $SU(4)$.

[18] When calculating these volume elements, it is important to remember that the closed subalgebra being used is $SU(2) \times U(1) \times U(1)$ and therefore, as in the $SU(3)$ case, the integrated kernels will require contributions from appropriate Cartan subalgebra elements. For example, the $\mathrm{e}^{\mathrm{i}\lambda_3\alpha_3}\,\mathrm{e}^{\mathrm{i}\lambda_5\alpha_4}$ component is an $SU(2)$ sub-element of the parametrization of $SU(4)$, but in creating its corresponding $SU(2)$ subgroup volume kernel (see the $SU(3)$ discussion), one must remember that it is a $SU(2) \subset SU(3) \subset SU(4)$ and therefore the kernel only requires contributions from the λ_3 and λ_8 components. On the other hand, the $\mathrm{e}^{\mathrm{i}\lambda_3\alpha_5}\,\mathrm{e}^{\mathrm{i}\lambda_{10}\alpha_6}$ element corresponds to a $SU(2) \subset SU(4)$ and therefore, the volume kernel will require contributions from all three Cartan subalgebra elements of $SU(4)$.

Solving yields the four roots of unity: $\pm\mathbb{1}_4$ and $\pm\,\mathrm{i}\mathbb{1}_4$, where $\mathbb{1}_4$ is the 4×4 identity matrix. So we can see that Z_4 gives another factor of 4, which, when combined with the factor of 4 from the two $SU(2)$ subgroups, and the factor of 12 from the $SU(3)$ elements, gives a total multiplicative factor of 192. Integration of the volume element given in equation (34) with the following ranges

$$
\begin{aligned}
&0 \leqslant \alpha_1, \alpha_3, \alpha_5, \alpha_7, \alpha_9, \alpha_{11}, \alpha_{13} \leqslant \pi \qquad 0 \leqslant \alpha_2, \alpha_4, \alpha_6, \alpha_8, \alpha_{10}, \alpha_{12} \leqslant \frac{\pi}{2} \\
&0 \leqslant \alpha_{14} \leqslant \frac{\pi}{\sqrt{3}} \qquad 0 \leqslant \alpha_{15} \leqslant \frac{\pi}{\sqrt{6}}
\end{aligned}
\tag{B23}
$$

gives

$$
V_{SU(4)} = 2\times 2\times 2\times 2\times 3\times 4\times V(SU(4)/Z_4) = \frac{\sqrt{2}\pi^9}{3}. \tag{B24}
$$

This calculated volume for $SU(4)$ agrees with that from Marinov [19].

Appendix C. Modified parameter ranges for group covering

In order to be complete, we list the modifications to the ranges given in appendix B that affect a covering of $SU(2)$, $SU(3)$ and $SU(4)$ without jeopardizing the calculated group volumes.

To begin with, in our parametrization, the general $SU(2)$ elements are given by

$$
D(\mu,\nu,\xi) = \mathrm{e}^{\mathrm{i}\lambda_3\mu}\,\mathrm{e}^{\mathrm{i}\lambda_2\nu}\,\mathrm{e}^{\mathrm{i}\lambda_3\xi} \qquad \mathrm{d}V_{SU(2)} = \sin(2\nu)\,\mathrm{d}\mu\,\mathrm{d}\nu\,\mathrm{d}\xi \tag{C1}
$$

with the corresponding ranges for the volume of $SU(2)/Z_2$ given as

$$
0 \leqslant \mu, \xi \leqslant \pi \qquad 0 \leqslant \nu \leqslant \frac{\pi}{2}. \tag{C2}
$$

In order to generate a covering of $SU(2)$, the ξ parameter must be modified to take into account the uniqueness of the two central group elements, $\pm\mathbb{1}_2$, under spinor transformations[19]. This modification is straightforward enough; ξ range is multiplied by the number of central group elements in $SU(2)$. The new ranges are thus

$$
0 \leqslant \mu \leqslant \pi \qquad 0 \leqslant \nu \leqslant \frac{\pi}{2} \qquad 0 \leqslant \xi \leqslant 2\pi. \tag{C3}
$$

These ranges yield both a covering of $SU(2)$, as well as the correct group volume for $SU(2)$.[20]

For $SU(3)$, here given as a component of the $SU(4)$ parametrization, we know we have two $SU(2)$ components (from appendix B),

$$
SU(3) = \mathrm{e}^{\mathrm{i}\lambda_3\alpha_7}\,\mathrm{e}^{\mathrm{i}\lambda_2\alpha_8}\,\mathrm{e}^{\mathrm{i}\lambda_3\alpha_9}\,\mathrm{e}^{\mathrm{i}\lambda_5\alpha_{10}}\,D(\alpha_{11},\alpha_{12},\alpha_{13})\,\mathrm{e}^{\mathrm{i}\lambda_8\alpha_{14}}. \tag{C4}
$$

Therefore, the ranges of α_9 and α_{13} should be modified just as ξ was done in the previous discussion for $SU(2)$. Remembering the discussion in appendix B concerning the central group of $SU(3)$, we can deduce that α_{14} ranges should be multiplied by a factor of 3. This yields the following, corrected, ranges for $SU(3)$[21]

$$
0 \leqslant \alpha_7, \alpha_{11} \leqslant \pi \qquad 0 \leqslant \alpha_8, \alpha_{10}, \alpha_{12} \leqslant \frac{\pi}{2} \qquad 0 \leqslant \alpha_9, \alpha_{13} \leqslant 2\pi \qquad 0 \leqslant \alpha_{14} \leqslant \sqrt{3}\pi. \tag{C5}
$$

[19] For specific examples of this, see either [12] or [40].

[20] One may interchange μ and ξ ranges without altering either the volume calculation, or the final orientation of a two-vector under operation by D. This interchange is beneficial when looking at Euler parametrizations beyond $SU(2)$.

[21] Earlier representations of these ranges for $SU(3)$, for example in [6, 8–10, 16, 39], were incorrect in that they failed to take into account the updated $SU(N)$ volume formula in [19].

These ranges yield both a covering of $SU(3)$, as well as the correct group volume for $SU(3)$.

For $SU(4)$, we have two $SU(2)$ subgroup components

$$SU(4) = \mathrm{e}^{\mathrm{i}\lambda_3\alpha_1}\,\mathrm{e}^{\mathrm{i}\lambda_2\alpha_2}\,\mathrm{e}^{\mathrm{i}\lambda_3\alpha_3}\,\mathrm{e}^{\mathrm{i}\lambda_5\alpha_4}\,\mathrm{e}^{\mathrm{i}\lambda_3\alpha_5}\,\mathrm{e}^{\mathrm{i}\lambda_{10}\alpha_6}[SU(3)]\,\mathrm{e}^{\mathrm{i}\lambda_{15}\alpha_{15}}. \tag{C6}$$

As with the $SU(2)$ subgroup ranges in $SU(3)$, the ranges for α_3 and α_5 each get multiplied by 2 and α_{15} ranges get multiplied by 4 (the number of $SU(4)$ central group elements). The remaining ranges are either held the same, or modified in the case of the $SU(3)$ element;

$$\begin{aligned} &0 \leqslant \alpha_1, \alpha_7, \alpha_{11} \leqslant \pi \qquad 0 \leqslant \alpha_2, \alpha_4, \alpha_6, \alpha_8, \alpha_{10}, \alpha_{12} \leqslant \frac{\pi}{2} \\ &0 \leqslant \alpha_3, \alpha_5, \alpha_9, \alpha_{13} \leqslant 2\pi \qquad 0 \leqslant \alpha_{14} \leqslant \sqrt{3}\pi \qquad 0 \leqslant \alpha_{15} \leqslant 2\sqrt{\frac{2}{3}}\pi. \end{aligned} \tag{C7}$$

These ranges yield both a covering of $SU(4)$, as well as the correct group volume for $SU(4)$.

In general, we can see that by looking at $SU(N)/Z_N$ not only can we arrive at a parametrization of $SU(N)$ with a logically derivable set of ranges that gives the correct group volume, but we can also show how those ranges can be logically modified to cover the entire group as well without any arbitrariness in assigning values to the parameters. It is this work that will be the subject of a future paper.

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