Bures Measures over the Spaces of Two and Three-Dimensional Density Matrices

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Abstract

Due to considerable recent interest in the use of density matrices for a wide variety of purposes, including quantum computation, we present a general method for their parameterizations in terms of Euler angles. We assert that this is of more fundamental importance than (as several people have remarked to us) “just another parameterization of the density matrix.” There are several uses to which this methodology can be put. One that has received particular attention is in the construction of certain distinguished (Bures) measures on the $(n^2 - 1)$-dimensional convex sets of $n \times n$ density matrices.

Key words: Density matrix; Euler angles; Bures metric; Haar measure

1 Introduction

The density matrix [1] — having origins in early (independent) work of Landau and von Neumann — has proved to be a very useful concept in physics. Researchers have devoted substantial efforts in describing the spaces defined by density matrices [2], in using them to analyze the separability of quantum systems [3,4], in comparing information-theoretic properties of various probability distributions over them [5], as well as studying the question of parallel transport in this context [6]. There is, of course, a quite straightforward manner in which to parameterize density matrices — simply in terms of the real and complex parts of the entries of these Hermitian matrices. A more indirect approach, but one of particular interest, relies upon Euler angle parameterizations of the special unitary matrices. It has been known for quite some time...
that one can parameterize density matrices with the help of such angles. To do so, we take a diagonal density matrix, $\rho$, which represents our quantum system in a particular basis. We then perform a unitary transformation in Hilbert space that takes $\rho$ to an arbitrary basis. This unitary transformation can be assumed to have a determinant equal to one since an overall phase does not affect the physics. Now when we apply the unitary transformation, we operate in the following manner,

$$\rho' = U\rho U^\dagger,$$

where $U \in SU(n)$ for an $n$-state system. The diagonal matrix $\rho$ can be parameterized by its $n - 1$ eigenvalues, and the unitary transformation by $n^2 - 1$ variables. At this point, however, we have parameterized $\rho'$ using too many, that is $n^2 + n - 2$ parameters, since the density matrices for the $n$-state systems comprise only an $(n^2 - 1)$-dimensional convex set. A primary objective here will be to demonstrate how such an “over-parameterization” can be avoided, by the elimination (from the unitary transformation) of $n - 1$ of the set of $n^2 + n - 2$ parameters.

Below, we will show that the density matrices for the 2-state and 3-state systems can be conveniently and insightfully parameterized in terms of Euler angle coordinates. In doing so, we take full advantage of the group properties associated with the unitary transformation. In particular, we obtain useful (Bures) measures on the spaces of density matrices, which can be used in the integration of functions over spaces and subspaces of quantum systems. Specifically, in Section 2.1 we exhibit the Euler angle-based parameterization of the 2-state quantum systems. In Section 2.2 we present the Euler angle-based parameterization of the 3-state systems. In Section 2.3 we discuss their straightforward generalization to $n$-state systems. In Section 3.1 we show how to use this to write down the Bures measures on the space of density matrices for 2-state systems and in Section 3.2 its counterpart for 3-state systems. Finally, we discuss ongoing work which is intended to yield the explicit generalization to 4-state systems. This, we anticipate will be highly useful in analyzing the (fifteen-dimensional) space occupied by pairs of qubits (cf. [7]).

2 Parametrization of Density Matrices

2.1 2-state Density Matrices

In this section we review certain properties of density matrices for the 2-state systems and demonstrate how to parameterize the 2-state density matrix in Euler angles. This should make the extension to 3-state systems in the
following section more transparent.

Much is known about 2-state density matrices. One of the more obvious properties is that a 2-state system can be spanned by two pure state density matrices of the following form:

\[
\rho_1 = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad \rho_2 = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}.
\] (1)

(These can be denoted by antipodal points on a two-sphere, making use of the elegant Riemann sphere representation [11].) For a mixed state diagonal density matrix, we write the linear combination of these two density matrices as

\[
\rho = \sum \rho_i a^i,
\] (2)

where \( \sum a^i = 1 \). The \( a^i \) may be represented in several ways. One common way is to let \( a^1 = a \) and \( a^2 = 1 - a \). What we wish to emphasize in this paper is that they are better represented by \( a^1 = \cos^2 \theta \) and \( a^2 = \sin^2 \theta \). Why this is true will be more obvious in the next section.

To take \( \rho \) to an arbitrary configuration (basis) we act with a unitary transformation \( U \in SU(2) \), in the manner

\[
\rho \rightarrow \rho' = U \rho U^{-1} = U \rho U^\dagger.
\] (3)

One may note that an \( n \)-state density matrix should have \( n^2 - 1 \) parameters, whereas this one appears to have 4, that is 3 (from \( SU(2) \)) + 1 (from the diagonal). However, in the Euler angle parameterization of \( SU(2) \), given by

\[
U = e^{i\sigma_3 \alpha} e^{i\sigma_2 \beta} e^{i\sigma_3 \gamma},
\] (4)

where the \( \sigma \)s are the Pauli matrices, we see that the parameter \( \gamma \) drops out since \( \sigma_3 \) is diagonal and so the matrix exponential \( e^{i\sigma_3 \gamma} \) commutes with \( \rho \) leaving precisely three parameters, as is appropriate and desired.

An important part of this parameterization is the ranges of the angles. For the 2-state case these are well-known (up to normalization given in eg., [12]). They are

\[
0 \leq \alpha \leq \pi, \quad 0 \leq \beta \leq \pi/2, \quad 0 \leq \theta \leq \pi/4.
\] (5)
2.2 3-state Density Matrices

For 3-state density matrices we can achieve a similar parameterization. The pure states are spanned by

\[ \rho_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \rho_2 = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \rho_3 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \] (6)

We can then obtain a mixed state by the linear combination \( \sum \rho_i a^i \), with \( \sum a^i = 1 \). Here again we use the squared components of a sphere. In this case, it is a two-sphere, thus for a 3-state system we take a generic mixed state to be

\[ \rho = \begin{pmatrix} \cos^2 \theta_1 \sin^2 \theta_2 & 0 & 0 \\ 0 & \sin^2 \theta_1 \sin^2 \theta_2 & 0 \\ 0 & 0 & \cos^2 \theta_2 \end{pmatrix}. \] (7)

We then can take this to an arbitrary configuration (basis) by the process

\[ \rho \rightarrow \rho' = U \rho U^\dagger, \] (8)

where \( U \in SU(3) \). In the Euler angle parameterization of \( SU(3) \), \( U \) is given by [13]

\[ U = e^{i\lambda_3 a} e^{i\lambda_2 b} e^{i\lambda_3 c} e^{i\lambda_5 \phi} e^{i\lambda_3 a} e^{i\lambda_2 b} e^{i\lambda_3 c} e^{i\lambda_8 \phi/\sqrt{3}} \] (9)
where the Gell-Mann matrices have been used;

\[
\lambda_1 = \begin{pmatrix}
0 & 1 & 0 \\
1 & 0 & 0 \\
0 & 0 & 0
\end{pmatrix}, \quad \lambda_2 = \begin{pmatrix}
0 & -i & 0 \\
i & 0 & 0 \\
0 & 0 & 0
\end{pmatrix}, \quad \lambda_3 = \begin{pmatrix}
1 & 0 & 0 \\
0 & -1 & 0 \\
0 & 0 & 0
\end{pmatrix},
\]

\[
\lambda_4 = \begin{pmatrix}
0 & 0 & 0 \\
0 & 0 & -i \\
1 & 0 & 0
\end{pmatrix}, \quad \lambda_5 = \begin{pmatrix}
0 & 0 & 0 \\
i & 0 & 0 \\
0 & 0 & 0
\end{pmatrix}, \quad \lambda_6 = \begin{pmatrix}
0 & 0 & 1 \\
0 & 1 & 0
\end{pmatrix}, \quad \lambda_7 = \begin{pmatrix}
0 & 0 & 0 \\
0 & -i & 0 \\
0 & i & 0
\end{pmatrix}, \quad \lambda_8 = \begin{pmatrix}
1/\sqrt{3} & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & -2
\end{pmatrix}.
\]

(10)

Since \(\lambda_3\), and \(\lambda_8\) appear on the right in (9), they commute with the diagonal matrix \(\rho\) and drop out of the parameterization. Thus we are left with \(3^2 - 1 = 8\) parameters for the 3-state case, as we should expect [2].

As in the 2-state case, the ranges of the angles in the parameterization are very important. For the case of three states we have

\[
0 \leq \alpha, \gamma, a \leq \pi, \quad 0 \leq \beta, \theta, b \leq \pi/2,
\]

\[
0 \leq \theta_1 \leq \pi/4, \text{ and } 0 \leq \theta_2 \leq \cos^{-1}(1/\sqrt{3}).
\]

(11)

(12)

Here one should note that using \(a, b\) and \(1 - a - b\) for the diagonal elements of the density matrix would give rise to a domain of integration that is non-rectangular. For density matrices of higher dimensional systems this could be extremely awkward. Here however, we see that the domain is indeed a rectangular solid with the final angle for a density matrix of \(n\)-dimensions having the range \(0 \leq \theta_{n-1} \leq \cos^{-1}(1/\sqrt{n})\).

2.3 \textit{n-state Density Matrices}

Though there is now no explicit parameterization of \(SU(n)\) in terms of Euler angles, the generalization is rather obvious. The difficulty in manipulating the one-forms to calculate the volume elements increases as \(n^2\) so unless some substantial progress is made in getting computers to manipulate trigonometric functions symbolically, it appears that progress will be quite
slow. It is anticipated that the density-matrix-parameterization program advanced here will not be achievable for groups much higher in dimensionality than $\text{dim}(SU(4)) = 15$. Perhaps, however, with sufficient interest and effort it could be accomplished for the Lie group $SU(8)$, in order to effectively describe the 63-dimensional space of three entangled qubits.

3 Bures Measures on the Convex Sets of Density Matrices

3.1 2-state Systems

The parameterization of the space of density matrices by Euler angles immediately leads to a particularly simple procedure for integrating over the space. A natural (Bures) measure on the space is given by the product of the (Hall) measure [15, eqs. (24, 25)] [16] on the space of eigenvalues $(\lambda_1, \ldots, \lambda_n)$, that is

$$du = \frac{d\lambda_1 \ldots d\lambda_n}{(\lambda_1 \ldots \lambda_n)^{\frac{n}{2}}} \prod_{j<k} \frac{4(\lambda_j - \lambda_k)^2}{\lambda_j + \lambda_k}$$

and the measure on the space of unitary matrices, the (modified/truncated) Haar measure. The geometry of the three-dimensional space is obvious from the parameterization. We have a solid section of the two-sphere and the space $SU(2)/U(1) \cong S^2$. In other words, our measure is given by

$$DV = du \times dS^2,$$

where $DV$ is the Bures measure on the space of density matrices, $dS^2$ is the standard measure on $S^2$, i.e. $dS^2 = d(G/H)$, with $G = SU(2)$ and $H = U(1)$ [8] and $du$ is given by (13) with $n = 2$.

3.2 3-state Systems

The measure on the eight-dimensional space of density matrices describing 3-states is a generalization of the previous case. We have

$$DV = du \times d(G/H),$$

where $DV$ is the Bures measure on the space of density matrices, with $G = SU(3)$ and $H = U(1) \times U(1)$ [8] and $du$ is given by (13) with $n = 3$. The
ranges of the Euler angles are given in Section 2.2. This is a new result. In the past the ranges of the angles were not properly specified when using the Haar measure. Additionally, the problem of overparameterization [3] was not clarified until recently [10].

In [16], it has been shown how the Bures measures for the 2- and 3-state systems can be normalized to form probability distributions.

4 Applications/Conclusions

The point of this note has been to clarify that: (1) the Euler angle parameterization eliminates any naive over-parameterization ([3]) of the density matrix using a unitary group representation; and (2) doing so helps in providing a natural (Bures) measure on the space of density matrices, which incorporates the (truncated) Haar measure on the group manifold of $SU(n)$.

So this is not “just another parameterization of the density matrix”, while proving very useful for many calculations. We find that people often do not appreciate the point of view of Feynman, who wrote that “every theoretical physicist who is any good knows six or seven different theoretical representations for exactly the same physics” [9].

In addition this gives rise to a rather natural (Bures) measure on the space of density matrices, using which one can integrate functions of quantum-mechanical interest (such as the von Neumann entropy, $-\text{Tr} \rho \log \rho$) over spaces and subspaces of the group with relative ease. Much of the geometry of the space can then be seen in terms of the moduli of the group space [10], a point apparently not appreciated by a number of readers of [10].

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References
[1] K. Blum, Density matrix theory and applications, Plenum Press, 1996.

[2] F. J. Bloore, “Geometrical description of the convex sets of states for systems with spin-1/2 and spin-1,” Journal of Physics A, 9 (12) (1976) 2059-2067.

[3] K. Życzkowski, P. Horodecki, A. Sanpera, and M. Lewenstein, Physical Review A, 58 (2) (1998) 883-892.

[4] P. B. Slater, “A priori probabilities of separable quantum states”, Journal of Physics A, 32 (28) (1999) 5261-5275.

[5] P. B. Slater, “Comparative noninformativities of quantum priors based on monotone metrics,” Physics Letters A, 247 (1-2) (1998) 1-8.

[6] M. Hübner, “Computation of Uhlmann’s parallel transport for density matrices and the Bures metric on three-dimensional Hilbert space,” Physics Letters A, 179 (4-5) (1993), 226-230.

[7] P. B. Slater, Exact Bures Probabilities that Two Quantum Bits are Classically Correlated, quant-ph/9911058.

[8] T. Bröcker and T. tom Dieck, Representations of Compact Lie Groups. Springer, New York 1985.

[9] R. P. Feynman, “The Character of Physical Law,” MIT Press, 1965.

[10] L. J. Boya, M. Byrd, M. Mims and E. C. G. Sudarshan, “Density Matrices and Geometric Phases for n-state Systems”, quant-ph/9810084.

[11] R. Penrose, “The Emperor’s New Mind: Concerning Computers, Minds, and the Laws of Physics”, Penguin, 1991.

[12] L. C. Biedenharn, and J. D. Louck, Angular Momentum in Quantum Physics Theory and Application, Cambridge University Press, 1977.

[13] M. Byrd, “Differential Geometry on SU(3) with Applications to Three State Systems,” Journal of Mathematical Physics, 39 (11) (1998) 6125-6136 and “Erratum: Differential geometry on SU(3) with applications to three state systems” J. Math. Phys. 41, (2000) 1026-1030.

[14] M. Byrd and E. C. G. Sudarshan, “SU(3) Revisited,” Journal of Physics A, 31 (1998) 9255-9268.

[15] M. J. W. Hall, “Random Quantum Correlations and Density Operator Distributions,” Physics Letters A, 242 (3) (1998) 123-129.

[16] P. B. Slater, “Hall Normalization Constants for the Bures Volumes of the n-State Quantum Systems,” Journal of Physics A, 32 (1999) (47) 8231-8246.