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# Calculation of the unitary part of the Bures measure for N-level quantum systems

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## Abstract

We use the canonical coset parameterization and provide a formula with the unitary part of the Bures measure for non-degenerate systems in terms of the product of even Euclidean balls. This formula is shown to be consistent with the sampling of random states through the generation of random unitary matrices.

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## 1. Introduction

The Bures measure is the volume element of the corresponding Bures metric that can be obtained from the infinitesimal form of the quantum fidelity between mixed quantum states [1–3], or from the statistical distance between mixed quantum states [4]. The Bures measure has been proposed as a prior distribution for implementation of quantum Bayes estimation [5, 6]. Other proposals and other measures also exist including monotonic Riemannian measures [6, 7]. The term monotonic is applied to stochastic maps, which are not allowed to increase the distance. Andai [8] calculated the volume of the whole state space according to the Lebesgue measure including a few monotonic Riemannian measures [7].

The quadratic form of the Bures metric can be written as

$$dB(\rho, \rho + d\rho)^2 = \frac{1}{2} \text{Tr} [G d\rho], \quad (1)$$

with  $G$  implicitly defined from  $d\rho = G\rho + \rho G$ . A more practical formula was found by Hübner [9] in terms of the eigenvalues (populations) of the state as

$$dB(\rho, \rho + d\rho)^2 = \frac{1}{2} \sum_{j=1}^N \sum_{k=1}^N \frac{|\langle \lambda_j | d\rho | \lambda_k \rangle|^2}{\lambda_j + \lambda_k}, \quad (2)$$

where  $\rho | \lambda_k \rangle = \lambda_k | \lambda_k \rangle$ . A general state can be parameterized by applying a unitary operator on the diagonal state  $\rho^{(D)} = \text{diag}(\lambda_1, \lambda_2, \dots, \lambda_N)$  as

$$\rho = \Omega \rho^{(D)} \Omega^\dagger, \quad (3)$$

with the unitary operator [10, 11] as the generalized flag manifold

$$\Omega \in \frac{U(N)}{U(m_1) \otimes U(m_2) \otimes \cdots \otimes U(m_q)}, \quad m_1 + m_2 + \cdots + m_q = N \quad (4)$$

where  $m_j$  is the degeneracy of the unique eigenvalue  $\lambda_j$ . The flag manifold can be decomposed as a product of cosets in order to develop a suitable parameterization. For example, the non-degenerate case can be decomposed as

$$\Omega \in \frac{U(N)}{U(1)^{\otimes N}} = \frac{U(N)}{U(N-1) \otimes U(1)} \frac{U(N-1)}{U(N-2) \otimes U(1)} \cdots \frac{U(2)}{U(1) \otimes U(1)}. \quad (5)$$

The eigenstates can be written as  $|\lambda_k\rangle = \Omega|k\rangle$  and the infinitesimal variation of  $\rho$  can be expanded as

$$d\rho = \Omega d\rho^{(D)} \Omega^\dagger + d\Omega \rho^{(D)} \Omega^\dagger + \Omega \rho^{(D)} d\Omega^\dagger. \quad (6)$$

Introducing this expression in Hübner's formula (2) we find

$$dB(\rho, \rho + d\rho)^2 = \frac{1}{4} \sum_{j=1}^N \frac{|\langle j|d\rho^{(D)}|j\rangle|^2}{\lambda_j} + \sum_{j=1}^N \sum_{k=j+1}^N \frac{|\langle j|[\Omega^\dagger d\Omega, \rho^{(D)}]|k\rangle|^2}{\lambda_j + \lambda_k} \quad (7)$$

$$= \frac{1}{4} \sum_{j=1}^N \frac{(d\lambda_j)^2}{\lambda_j} + \sum_{j=1}^N \sum_{k=j+1}^N \Lambda_{jk} |\Omega^\dagger d\Omega|_{jk}^2, \quad (8)$$

with  $\Lambda_{jk} = \frac{(\lambda_j - \lambda_k)^2}{\lambda_j + \lambda_k}$ , such that the volume element can be extracted to obtain Hall's formula [12] up to a scale factor. The volume element with the scale used in [13] is

$$dV_B = \delta(\lambda_1 + \lambda_2 + \cdots + \lambda_N - 1) \frac{d\lambda_1 d\lambda_2 \cdots d\lambda_N}{2^{N-2} \sqrt{\lambda_1 \lambda_2 \cdots \lambda_N}} \prod_{j < k}^N \Lambda_{jk} dx_{jk} dy_{jk}, \quad (9)$$

where  $dx_{jk} = \text{Re}(\Omega^\dagger d\Omega)_{jk}$  and  $dy_{jk} = \text{Im}(\Omega^\dagger d\Omega)_{jk}$ . The remarkable feature of this expression is that it separates the effect of the eigenvalues (populations) and the effect of the unitary operator,

$$dV_B = dV_B^{(\lambda)} dV_B^{(\Omega)}. \quad (10)$$

This paper is organized as follows. Section 2 reviews some results of the Euler parameterization and introduces some concepts and formulas to be used later in the paper. The main contribution of this paper is developed in section 3. Section 4 compares the results with the generation of random unitary matrices. Section 5 presents concluding remarks.

## 2. Euler parametrization

The generalized Euler parameterization was developed by Tilma and collaborators [14, 15] and was used in [16] to calculate the volume and measure of the unitary part of the Bures measure. In this section we review the three-level case in order to introduce some concepts and formulas that will be used in the next section. The unitary operator for a three-level system can be parameterized as [5, 15, 17]

$$\Omega = (e^{\phi^6 \lambda_3} e^{\phi^5 \lambda_2} e^{\phi^4 \lambda_3} e^{\phi^3 \lambda_5} =) (e^{\phi^2 \lambda_3} e^{\phi^1 \lambda_2}), \quad (11)$$

with the factors of  $\Omega$  as parameterization of  $\frac{U(3)}{U(2) \otimes U(1)}$  and  $\frac{U(2)}{U(1) \otimes U(1)}$  in terms of the Euler angles  $\phi^k$  and the Gell-Mann matrices  $\lambda_k$ . The measure of the unitary portion can be calculated as

the product of the measure of the corresponding cosets. For non-degenerate 3-level systems, the coset decomposition is

$$dV_B^{(\Omega)} = dV \left( \frac{U(3)}{U(2) \otimes U(1)} \right) dV \left( \frac{U(2)}{U(1) \otimes U(1)} \right). \quad (12)$$

The volume of the coset  $\frac{U(3)}{U(2) \otimes U(1)}$  can be obtained by calculating  $\Omega^\dagger d\Omega$  and selecting the matrix components where the corresponding Lie algebra lies. Thus, we may extract the coordinate transformation from the following terms:

$$\Omega^\dagger d\Omega \equiv \begin{pmatrix} \cdot & \cdot & dx^{3'} + i dx^{4'} \\ \cdot & \cdot & dx^{5'} + i dx^{6'} \\ \cdot & \cdot & \cdot \end{pmatrix} \quad (13)$$

to obtain

$$dV \left( \frac{U(3)}{U(2) \otimes U(1)} \right) = \cos \phi^3 \sin^3 \phi^3 \sin 2\phi^5 d\phi^3 d\phi^4 d\phi^5 d\phi^6. \quad (14)$$

A similar procedure can be carried out for the second coset.

The Haar measure of the coset  $\frac{U(n+1)}{U(n) \otimes U(1)}$  is topologically equivalent to an even sphere  $S^{2n}$  according to Gilmore [18, 19] with the corresponding volume

$$\text{Vol}_{\text{Haar}} \left( \frac{U(n+1)}{U(n) \otimes U(1)} \right) = \text{Vol}(S^{2n}). \quad (15)$$

However, the measure of the unitary section of the Bures measure is not the Haar measure. Some references refer to it as the *truncated* Haar Measure [15, 20]. Direct integration of the coset measure does not result in the volume of even spheres  $r^2 = 1$ , but instead in the volume of even balls  $r^2 \leq 1$ , with  $r$  as the radial coordinate, such that

$$\text{Vol} \left( \frac{U(n+1)}{U(n) \otimes U(1)} \right) = \text{Vol}(B^{2n}), \quad (16)$$

with

$$\text{Vol}(B^n) = \frac{2\pi^{n/2}}{n\Gamma(n/2)}, \quad (17)$$

which is in perfect agreement with the formulas found in [16, 21].

Consequently, the volume of the unitary section for non-degenerate systems is equal to the product of the volume of even balls

$$\text{Vol} \left( \frac{U(N)}{U(1)^{\otimes N}} \right) = \text{Vol}(B^{2N-2}) \text{Vol}(B^{2N-4}) \dots \text{Vol}(B^2) = \frac{\pi^{N(N-1)/2}}{\prod_1^N \Gamma(n)}. \quad (18)$$

This result is also consistent with the volume presented by Sommers and Życzkowski [3] as

$$\text{Vol}' \left( \frac{U(N)}{U(1)^{\otimes N}} \right) = \frac{(2\pi)^{N(N-1)/2}}{\prod_1^N \Gamma(n)}. \quad (19)$$

The discrepancy factor can be explained by a simple numerical scale factor of 1/2 on the Bures metric, because  $N(N - 1)$  is equal to the dimension of the Lie algebra occupied by the coset space. Equivalently,  $N(N - 1)$  is the number of degrees of freedom required to parameterize  $\frac{U(N)}{U(1)^{\otimes N}}$ . So far, we have shown that the volume of the coset (16) can be written as the volume of an even ball, but this does not imply that the measure of the coset is Euclidean defined on an even ball. This assertion is proved in the next section and further numerical tests are carried out in section 4.

### 3. Canonical coset parametrization

An important parameterization arises from the canonical coset, as presented by Gilmore [18] on page 351. The Bures metric was obtained for 3-level systems in [22] and a more general prescription in [11] for N-level systems, but the measure was not calculated in this formulation. The power of the canonical coset parameterization lies in the many possibilities to analytically express the exponential of the following typical block matrix:

$$\exp \begin{pmatrix} \mathbf{0} & B \\ -B^\dagger & 0 \end{pmatrix} = \begin{pmatrix} \cos \sqrt{B B^\dagger} & \frac{\sin \sqrt{B^\dagger B} B}{\sqrt{B^\dagger B}} \\ -\frac{\sin \sqrt{B^\dagger B} B}{\sqrt{B^\dagger B}} B^\dagger & \cos \sqrt{B^\dagger B} \end{pmatrix} \quad (20)$$

where the case of interest is such that  $B = \text{column}(z^1, z^2, \dots, z^{N-1})$  is a column vector of complex numbers. This exponential can also be expressed in terms of spherical coordinates  $x^j$  as

$$\exp \begin{pmatrix} \mathbf{0} & B \\ -B^\dagger & 0 \end{pmatrix} = \begin{pmatrix} [1 - X X^\dagger]^{1/2} & X \\ -X^\dagger & [1 - X^\dagger X]^{1/2} \end{pmatrix} \quad (21)$$

such that

$$X = \frac{\sin \sqrt{B^\dagger B} B}{\sqrt{B^\dagger B}} = \begin{pmatrix} x^1 + ix^2 \\ x^3 + ix^4 \\ \vdots \\ x^{2N-3} + ix^{2N-2} \end{pmatrix}. \quad (22)$$

This coordinate system is called spherical because the column vector is made of variables that range inside an even ball  $B^{2k}$ , where the radial coordinate is  $r^2 = X^\dagger X$ . The exponential in (21) is important because it provides a parameterization of the coset  $\frac{U(N)}{U(N-1) \otimes U(1)}$  as a  $N \times N$  matrix. The coset required to parameterize the unitary section of the Bures measure can be constructed in terms of products of layered cosets (5) that have form

$$\frac{U(2)}{U(1) \otimes U(1)} = \begin{pmatrix} \sqrt{1 - (x^1)^2 - (x^2)^2} & x^1 + ix^2 & 0 & 0 \dots 0 \\ -(x^1 - ix^2) & \sqrt{1 - (x^1)^2 - (x^2)^2} & 0 & 0 \dots 0 \\ 0 & 0 & 1 & 0 \dots 0 \\ \vdots & 0 & 0 & 1 \dots 0 \\ 0 & 0 & 0 & 0 \dots 1 \end{pmatrix}$$

$$\frac{U(3)}{U(2) \otimes U(1)} = \begin{pmatrix} W_{11}^{(2)} & W_{12}^{(2)} & x^3 + ix^4 & 0 \dots 0 \\ W_{21}^{(2)} & W_{22}^{(2)} & x^5 + ix^6 & 0 \dots 0 \\ -(x^3 - ix^4) & -(x^5 - ix^6) & \sqrt{1 - (x^3)^2 - \dots} & 0 \dots 0 \\ \vdots & 0 & 0 & 1 \dots 0 \\ 0 & 0 & 0 & 0 \dots 1 \end{pmatrix}$$

$$\vdots$$

with  $W_{jk}^{(n)} = (\sqrt{1 - X X^\dagger})_{jk}$ . With this background, we state the following theorem.

**Theorem 1.** *The measure of the following coset corresponds to an Euclidean measure defined inside of an even ball, such that*

$$dV \left( \frac{U(n+1)}{U(n) \otimes U(1)} \right) = dV_E(B^{2n}). \quad (23)$$

This theorem applied to 3-level systems results in

$$dV \left( \frac{U(3)}{U(2) \otimes U(1)} \right) = dx^3 dx^4 dx^5 dx^6, \quad (24)$$

such that  $(x^3)^2 + (x^4)^2 + (x^5)^2 + (x^6)^2 \leq 1$ , in terms of the variables of the corresponding canonical coset parameterization.

**Proof.** The strategy is based in the generalization of the proof initially provided for the simpler case  $dV \left( \frac{U(3)}{U(2) \otimes U(1)} \right)$ . The complex column  $X$  of interest is

$$X = \begin{pmatrix} x^3 + ix^4 \\ x^5 + ix^6 \end{pmatrix}, \quad (25)$$

such that the unitary operator becomes

$$\Omega = \begin{pmatrix} [\mathbf{1} - XX^\dagger]^{1/2} & X \\ -X^\dagger & [1 - X^\dagger X]^{1/2} \end{pmatrix} = \begin{pmatrix} \mathbf{1} + \frac{\sqrt{1-r^2}-1}{r^2} XX^\dagger & X \\ -X^\dagger & \sqrt{1-r^2} \end{pmatrix}, \quad (26)$$

with  $r^2 = X^\dagger X = (x^3)^2 + (x^4)^2 + (x^5)^2 + (x^6)^2$ . The measure is invariant under an orthonormal transformation  $\mathcal{O}$  applied to the coordinates  $(x^3, x^4, x^5, x^6)$ . This means that it is sufficient to consider the evaluation of  $\Omega^\dagger d\Omega$  at  $(x^3, x^4, x^5, x^6) = (r, 0, 0, 0)$ , which produces the following expression:

$$\Omega^\dagger d\Omega = \begin{pmatrix} -ir dx^4 & -\frac{(\sqrt{1-r^2}-1)(dx^5 - i dx^6)}{r} & \frac{dx^3 - i(r^2-1)dx^4}{\sqrt{1-r^2}} \\ \frac{(\sqrt{1-r^2}-1)(dx^5 + i dx^6)}{r} & 0 & dx^5 + i dx^6 \\ -\frac{dx^3 + i(r^2-1)dx^4}{\sqrt{1-r^2}} & -dx^5 + i dx^6 & ir dx^4 \end{pmatrix}. \quad (27)$$

The coordinate transformation can be extracted from  $(\Omega^\dagger d\Omega)_{13}$  and  $(\Omega^\dagger d\Omega)_{23}$ , as

$$\begin{pmatrix} dx^{3'} \\ dx^{4'} \\ dx^{5'} \\ dx^{6'} \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{1-r^2}} & 0 & 0 & 0 \\ 0 & \sqrt{1-r^2} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} dx^3 \\ dx^4 \\ dx^5 \\ dx^6 \end{pmatrix}, \quad (28)$$

which leads to the measure

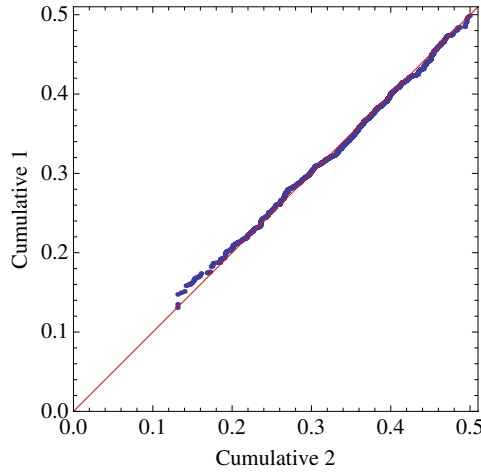
$$dV \left( \frac{U(3)}{U(2) \otimes U(1)} \right) = dx^3 dx^4 dx^5 dx^6, \quad (29)$$

with  $r \leq 1$ . The transformation matrix (28) changes with the application of an orthonormal operator  $\mathcal{O}$  on the coordinates  $(x^3, x^4, x^5, x^6)$ , but the determinant remains invariant as stated before. The only differentials without trivial transformation are  $dx^3$  and  $dx^4$  which were evaluated at  $x^3 = r$  and  $x^4 = 0$ . The rest of the differentials transform according to the identity. This means that by extending the coordinates to higher dimensions the extra differentials will transform according to the identity as well, thus, maintaining the determinant equal to 1 and proving the theorem.  $\square$

This theorem leads us to formulate the following formula of the Bures measure for a state with non-degenerate spectrum:

$$dV_B^{(\Omega)}(N) = dV(B^{2N-2}) dV(B^{2N-4}) \dots dV(B^2). \quad (30)$$

Some degenerate states including pure states and those without full-rank can be treated by reducing the degrees of freedom and the number of balls involved in the parameterization. For example, table 1 shows the characteristic diagonal states along with their corresponding measures in low dimensions.



**Figure 1.** Plot of the equivalent cumulatives of the component  $(\rho)_{33}$  for 1000 random states with spectrum  $\text{diag}(\frac{3}{8}, \frac{1}{8}, \frac{1}{2})$ .

(This figure is in colour only in the electronic version)

**Table 1.** Unitary part of the Bures measure for degenerate states with reduced rank, where  $\lambda_j \neq \lambda_k$ .

Diagonal state	$\Omega$	Measure
$\text{diag}(0, 0, 1)$	$\frac{U(3)}{U(2) \otimes U(1)}$	$dV(B^4)$
$\text{diag}(0, 0, 0, 1)$	$\frac{U(4)}{U(3) \otimes U(1)}$	$dV(B^6)$
$\text{diag}(0, 0, \lambda_2, \lambda_1)$	$\frac{U(4)}{U(3) \otimes U(1)} \frac{U(3)}{U(2) \otimes U(1)}$	$dV(B^6) dV(B^4)$
$\text{diag}(0, 0, 0, 0, 1)$	$\frac{U(5)}{U(4) \otimes U(1)}$	$dV(B^8)$
$\text{diag}(0, 0, 0, \lambda_2, \lambda_1)$	$\frac{U(5)}{U(4) \otimes U(1)} \frac{U(4)}{U(3) \otimes U(1)}$	$dV(B^8) dV(B^6)$
$\text{diag}(0, 0, \lambda_3, \lambda_2, \lambda_1)$	$\frac{U(5)}{U(4) \otimes U(1)} \frac{U(4)}{U(3) \otimes U(1)} \frac{U(3)}{U(2) \otimes U(1)}$	$dV(B^8) dV(B^6) dV(B^4)$

#### 4. Random sampling

The results from the previous sections can be used to compare the sampling distribution of the Euclidean spheres of the Bures measure against the sampling distribution obtained from a generation of random unitary matrices. The most efficient and transparent method to generate random unitary matrices is described by Mezzadri [23], which is based on the QR decomposition of complex random matrices. A random state  $\rho$  can be generated by two independent methods.

- 1: Through the generation of random unitary matrices.
- 2: Through the generation of random points on the even Euclidean balls  $B^{2k}$  and subsequent use of the canonical coset parameterization to obtain the state.

The alternative distributions seem to be equivalent as can be verified by plotting their cumulatives against each other and observing a linear one-to-one correspondence up to some

fluctuations. A specific test can be designed for states having the spectrum of the following non-degenerated diagonal state:

$$\rho^{(D)} = \text{diag}\left(\frac{3}{8}, \frac{1}{8}, \frac{1}{2}\right). \quad (31)$$

A plot of the two cumulatives against each other for the  $(\rho)_{33}$  component is shown in figure 1. This test was comprehensively carried out and verified for systems up to 5-levels.

## 5. Conclusions

We calculated the unitary part of the Bures measure for non-degenerate systems in terms of the canonical coset parameterization and found an expression as the product of Euclidean even balls. This result was shown to be in agreement with the numerical random sampling of unitary matrices and with the formulas of the volume found in the literature. These results are also relevant to monotone metrics other than the Bures metric including the Hilbert–Schmidt measure.

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