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Bures geometry of the three-level quantum systems

Paul B. Slater*

ISBER, University of California, Santa Barbara, CA 93106-2150, USA

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Abstract

We compute — using a formula of Dittmann — the Bures metric tensor (g) for the eight-dimensional state space of three-level quantum systems, employing a newly developed Euler angle-based parameterization of the 3×3 density matrices. Most of the individual metric elements (g_{ij}) are found to be expressible in relatively compact form, many of them in fact being exactly *zero*. © 2001 Elsevier Science B.V. All rights reserved.

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1. Introduction

The Bures metric is a distinguished member — the *minimal* one — of the (nondenumerable) family of *monotone* metrics on the quantum systems [1]. Its contemporary study was pioneered by Uhlmann [2,3], along with several of his associates at the University of Leipzig [4–9]. In particular, Dittmann has derived several *explicit* formulas (ones not requiring knowledge of the eigenvalues of density matrices) for the Bures metric [8,9]. Slater [10] — interpreting the *volume element* of the metric as a natural (unnormalized) measure on the quantum systems — applied this work to certain low-dimensional subsets of the fifteen-dimensional set of 4×4 density matrices to obtain "exact Bures probabilities that two quantum bits are classically correlated" (cf. [11,12]).

* Fax: +1-805-893-7995.
E-mail address: slater@itp.ucsb.edu (P.B. Slater).

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The Bures metric on the three-dimensional convex set of the 2×2 density matrices (making use of Cartesian coordinates (x, y, z)),

$$\rho = \frac{1}{2}\begin{pmatrix} 1+z & x+\mathrm{i}y \\ x-\mathrm{i}y & 1-z \end{pmatrix} \quad (0 \leq x^2+y^2+z^2 \leq 1) \tag{1}$$

has been intensively studied. The corresponding metric tensor

$$g = \frac{1}{4(1-x^2-y^2-z^2)}\begin{pmatrix} 1-y^2-z^2 & xy & xz \\ xy & 1-x^2-z^2 & yz \\ xz & yz & 1-x^2-y^2 \end{pmatrix} \tag{2}$$

can be obtained by application of an (early) formula of Dittmann [8, Eq. (3.7)],

$$d_{\mathrm{Bures}}(\rho, \rho+\mathrm{d}\rho)^2 = \frac{1}{4}\mathrm{Tr}\{\mathrm{d}\rho\,\mathrm{d}\rho + \frac{1}{|\rho|}(\mathrm{d}\rho - \rho\,\mathrm{d}\rho)(\mathrm{d}\rho - \rho\,\mathrm{d}\rho)\}. \tag{3}$$

In spherical coordinates (r, θ, ϕ) the tensor (2) takes a *diagonal* form

$$g = \frac{1}{4}\begin{pmatrix} \frac{1}{1-r^2} & 0 & 0 \\ 0 & r^2 & 0 \\ 0 & 0 & r^2\sin^2\theta \end{pmatrix}. \tag{4}$$

The Bures metric can be viewed as the standard metric on the surface of a three-sphere [4,13]. As such, Hall [14, p. 128] has written that "the Bures metric for a two-dimensional system corresponds to the surface of a unit four-ball, i.e., to the maximally symmetric three-dimensional space of positive curvature (and may be recognized as the spatial part of the Robertson–Walker metric in general relativity). This space is homogeneous and isotropic, and hence the Bures metric does not distinguish a preferred location or direction in the space of density operators. Indeed, as well as rotational symmetry in Bloch coordinates (corresponding to unitary invariance), the metric has a further set of symmetries generated by the infinitesimal transformations

$$r \to r + \epsilon(1-r^2)^{1/2}a, \tag{5}$$

where a is an arbitrary three-vector and r the radial distance in the Bloch sphere of two-level quantum systems [13]." Petz and Sudár observed that in "the case of the [Bures] metric of the symmetric logarithmic derivative, the tangential component is independent of r" [1, p. 2667].

A principal goal of the present study is to determine any such symmetries possessed by the Bures metric when one proceeds from the study of the two-level quantum systems to that of the three-level quantum systems. One should be aware, though, that Dittmann has noted that in this case, the space "is not a space of constant curvature and not even a locally symmetric space, in contrast to what the case of two-dimensional density matrices might suggest" [8]. (In a locally symmetric space, the sectional curvature is invariant under parallel displacement, and the covariant derivative of the curvature tensor field vanishes

[6,15]. A formula for the scalar curvature of the monotone metrics for general n-level quantum systems is given in [16], cf. [17].) In other work [18], Dittmann has shown that the gauge field defining the Bures metric satisfies the source-free Yang–Mills equation. Petz [19, Theorem 3.4] has established that the Bures metric is the only monotone metric that is both "Fisher adjusted" and "Fubini-Study adjusted".

2. Methodology

Slater [20] (cf. [10, Eqs. (6) and (7)]) applied a formula (cf. (3)) of Dittmann [8, Eq. (3.8)] for the specific case of the three-level quantum systems,

$$g_\rho^B = \frac{1}{4}\mathrm{Tr}\left\{ \mathrm{d}\rho\,\mathrm{d}\rho + \frac{3}{1-\mathrm{Tr}\,\rho^3}(\mathrm{d}\rho - \rho\,\mathrm{d}\rho)(\mathrm{d}\rho - \rho\,\mathrm{d}\rho) \right. \\ \left. + \frac{3|\rho|}{1-\mathrm{Tr}\,\rho^3}(\mathrm{d}\rho - \rho^{-1}\mathrm{d}\rho)(\mathrm{d}\rho - \rho^{-1}\,\mathrm{d}\rho)\right\} \tag{6}$$

to the particular instance (a simple extension of the two-level quantum systems (1)) of a *four*-dimensional subset,

$$\rho = \frac{1}{2}\begin{pmatrix} v+z & 0 & x-\mathrm{i}y \\ 0 & 2-2v & 0 \\ x+\mathrm{i}y & 0 & v-z \end{pmatrix} \tag{7}$$

of the eight-dimensional convex set of 3×3 density matrices [21]. Now, in the present study, we apply this same formula (6) to the *full* eight-dimensional convex set of the three-level quantum systems itself. Of crucial and central importance here will be the use of a recently developed "Euler angle" parameterization of these density matrices [22,23]. In this parameterization, one takes an arbitrary density matrix (ρ) to be expressed in the ("Schur/Schatten") form ([9], Section 3; [24], p. 3725; [25], p. 53)

$$\rho = U\rho' U^\dagger. \tag{8}$$

Here

$$U = \mathrm{e}^{\mathrm{i}\lambda_3\alpha}\,\mathrm{e}^{\mathrm{i}\lambda_2\beta}\,\mathrm{e}^{\mathrm{i}\lambda_3\gamma}\,\mathrm{e}^{\mathrm{i}\lambda_5\theta}\,\mathrm{e}^{\mathrm{i}\lambda_3 a}\,\mathrm{e}^{\mathrm{i}\lambda_2 b} \tag{9}$$

is a member of $SU(3)$, the three immediately relevant (of the eight) Gell-Mann matrices [26] being

$$\lambda_2 = \begin{pmatrix} 0 & -\mathrm{i} & 0 \\ \mathrm{i} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \qquad \lambda_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \qquad \lambda_5 = \begin{pmatrix} 0 & 0 & -\mathrm{i} \\ 0 & 0 & 0 \\ \mathrm{i} & 0 & 0 \end{pmatrix}. \tag{10}$$

Making use of spherical coordinates (θ_1, θ_2),

$$\rho' = \begin{pmatrix} \cos^2\theta_1 & 0 & 0 \\ 0 & \sin^2\theta_1 \cos^2\theta_2 & 0 \\ 0 & 0 & \sin^2\theta_1 \sin^2\theta_2 \end{pmatrix}. \tag{11}$$

An appropriate set of ranges of the eight angles (by which all the 3×3 density matrices can be reproduced without duplication) is [22, Eqs. (11) and (12)]

$$0 \le \alpha, \gamma, a \le \pi, \quad 0 \le \beta, \theta, b \le \frac{\pi}{2}, \quad 0 \le \theta_1 \le \cos^{-1}\frac{1}{\sqrt{3}}, \quad 0 \le \theta_2 \le \frac{\pi}{4}. \tag{12}$$

We have inserted the so-parameterized 3×3 density matrix (8) into formula (6) to obtain the 8×8 Bures metric tensor. Since, by construction, we have explicit knowledge of the eigenvalues (λ's) and eigenvectors of ρ, we could alternatively have directly applied the *general* formula for the Bures metric in the n-dimensional case [4, Eq. (10)],

$$d_{\mathrm{Bures}}(\rho, \rho + \mathrm{d}\rho)^2 = \frac{1}{2}\sum_{i,j=1}^{n} \frac{|\langle i|\mathrm{d}\rho|j\rangle|^2}{\lambda_i + \lambda_j}, \tag{13}$$

or that given by Proposition 4 in [9].

3. Elements of the Bures metric tensor

Initially, all the entries of the tensor computed using (6) — implemented in MATHEMATICA — were given by extremely large complicated expressions. However, in a number of cases, both through exact computations and numerical experimentation, we were able to arrive at certain relatively compact (if not simply strictly *zero* themselves) expressions for the individual metric elements.

The first remarkable item to note is that (as repeated numerical experiments indicate) *all* the entries of the tensor are *independent* of the Euler angle α. Further numerical investigations have convinced us that many of the entries of the tensor are, in fact, zero (cf. [27,28]). (In the case of the two-level quantum systems, the off-diagonal entries of the Bures metric tensor (4) are zero, if spherical — as opposed to Cartesian — coordinates are employed.) For example, the spherical coordinates θ_1 and θ_2 are both orthogonal to the other seven coordinates. The diagonal entry ($g_{\theta_1\theta_1}$) of the Bures metric tensor (g) corresponding to the pairing (θ_1, θ_1) is simply 1, while the diagonal entry ($g_{\theta_2\theta_2}$) corresponding to the pairing (θ_2, θ_2) is $\sin^2\theta_1$.

Let us summarize our present state of explicit knowledge regarding the Bures metric elements (g_{ij}) for the three-level quantum systems. We write the corresponding (symmetric) matrix, using the ordering of coordinates (and hence rows and columns)

$$(\alpha, \gamma, a, \beta, b, \theta, \theta_1, \theta_2) \tag{14}$$

as

$$g = \begin{pmatrix} ? & ? & g_{13} & ? & g_{15} & g_{16} & 0 & 0 \\ \cdot & g_{22} & g_{23} & g_{24} & 0 & 0 & 0 & 0 \\ \cdot & \cdot & g_{33} & g_{34} & 0 & 0 & 0 & 0 \\ \cdot & \cdot & \cdot & g_{44} & g_{45} & g_{46} & 0 & 0 \\ \cdot & \cdot & \cdot & \cdot & g_{55} & 0 & 0 & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & g_{66} & 0 & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 1 & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \sin^2\theta_1 \end{pmatrix}. \tag{15}$$

Our specific element-by-element results are now presented.

- $g_{55} = g_{bb}$:
  We have (Fig. 1)

  $$g_{55} = g_{bb} = \frac{t^2}{16u_+}, \tag{16}$$

  where (cf. [30, Eq. (28)])

  $$t = 2 + 6\cos 2\theta_1 + \cos 2(\theta_1 - \theta_2) - 2\cos 2\theta_2 + \cos 2(\theta_1 + \theta_2), \tag{17}$$

  and

  $$u_\pm = 3 + \cos 2\theta_1 \pm 2\cos 2\theta_2 \sin^2\theta_1. \tag{18}$$

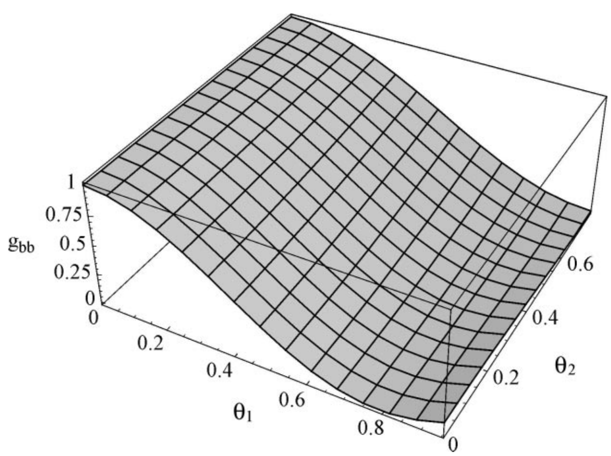

Fig. 1. Diagonal (5,5)-entry, corresponding to the Euler angle b, of the Bures metric tensor (15) for the three-level quantum systems. This term — which can be inverted (38) — enters as well into many of the expressions for the other metric elements.

- $g_{13} = g_{\alpha a}$:

$$g_{13} = g_{\alpha a} = \tfrac{1}{4} g_{55}\{(3+\cos 2\theta)\cos 2\beta \sin^2 2b + 2\cos 2(a+\gamma) \times \cos\theta \sin 4b \sin 2\beta\}. \tag{19}$$

- $g_{15} = g_{\alpha b}$:

$$g_{15} = g_{\alpha b} = g_{55} \cos\theta \sin 2\beta \sin 2(a+\gamma). \tag{20}$$

- $g_{16} = g_{\alpha\theta}$:

$$g_{16} = g_{\alpha\theta} = \frac{v}{32u_-} \sin 2b \sin 2\beta \sin 2(a+\gamma) \sin\theta, \tag{21}$$

where

$$v = 15 + 28\cos 2\theta_1 + 21\cos 4\theta_1 + 4(7+9\cos 2\theta_1)\cos 2\theta_2 \sin^2\theta_1 -4(5+3\cos 2\theta_1)\cos 4\theta_2 \sin^2\theta_1 + 8\cos 6\theta_2 \sin^4\theta_1. \tag{22}$$

In Fig. 2 we plot the Euler angle-independent part of g_{16}, that is $v/32u_-$.

- $g_{22} = g_{\gamma\gamma}$:

$$g_{22} = g_{\gamma\gamma} = \frac{1}{16\kappa}\{-g_{55}\kappa \cos^4 b(3+\cos 2\theta)^2 +4\cos^2 b(g_{55}\kappa + \mu\cos^2\theta + 4(\kappa+\upsilon)\cos^2 2\theta_2 \cos^4\theta \sin^2\theta_1) +16\kappa \cos^2 2\theta_2 \cos^2\theta \sin^2\theta_1 \sin^2\theta\}, \tag{23}$$

where

$$\kappa = 35 + 28\cos 2\theta_1 + \cos 4\theta_1 - 8\cos 4\theta_2 \sin^4\theta_1, \tag{24}$$

$$\upsilon = -4(1+3\cos 2\theta_1)(7+5\cos 2\theta_1)\sec 2\theta_2 - 16\cos 2\theta_2 \sin^4\theta_1, \tag{25}$$

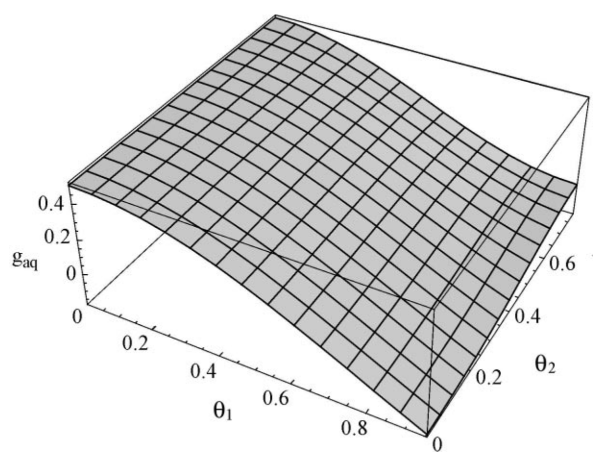

Fig. 2. Euler angle-independent factor of metric element corresponding to the (1,6)-entry of (15).

and

$$\begin{aligned}\mu = &-\sin^2\theta_1\{1621 + 125\cos 2\theta_2 + 46\cos 4\theta_2\\ &+4\cos 2\theta_1(261 + 49\cos 2\theta_2 + 10\cos 4\theta_2)\\ &+\cos 4\theta_1(151 + 63\cos 2\theta_2 + 42\cos 4\theta_2)\\ &-768\csc^2\theta_1 + 8(\cos 6\theta_2 - \cos 8\theta_2)\sin^4\theta_1\}.\end{aligned} \tag{26}$$

- $g_{23} = g_{\gamma a}$:

$$g_{23} = g_{\gamma a} = \tfrac{1}{4} g_{55}(3 + \cos 2\theta)\sin^2 2b. \tag{27}$$

- $g_{24} = g_{\gamma\beta}$:

$$g_{24} = g_{\gamma\beta} = \frac{3t\cos\theta\sin 2b\sin 2(a+\gamma)\sin^2\theta_1(\cos 2\theta - \mathrm{i}\sin 2\theta)}{256(-1 + \cos^6\theta_1 + \sin^6\theta_1(\cos^6\theta_2 + \sin^6\theta_2))}, \tag{28}$$

$$\begin{aligned}&\cos^2\theta_1(-p\cos 2b(-1 + 4\cos 2\theta_2 + \cos 4\theta_2)\\ &\quad +q(-1 + 7\cos 2\theta_2 - 3\cos 4\theta_2 + \cos 6\theta_2))\\ &\quad +2\cos^4\theta_1(p\cos 2b\cos^2\theta_2(3 + \cos 2\theta_2) + q(4 - 3\cos 2\theta_2 + \cos 4\theta_2)\sin^2\theta_2)\\ &\quad +(-p\cos 2b + q(-1 + 2\cos 2\theta_2))\sin^2 2\theta_2,\end{aligned}$$

where

$$p = 1 + 6\,\mathrm{e}^{2\mathrm{i}\theta} + \mathrm{e}^{4\mathrm{i}\theta}, \qquad q = (-1 + \mathrm{e}^{2\mathrm{i}\theta})^2.$$

- $g_{33} = g_{aa}$:

$$g_{33} = g_{aa} = g_{55}\sin^2 2b. \tag{29}$$

- $g_{34} = g_{a\beta}$:

$$g_{34} = g_{a\beta} = -\tfrac{1}{2} g_{55}\cos\theta\sin 4b\sin 2(a+\gamma). \tag{30}$$

- $g_{44} = g_{\beta\beta}$:

$$g_{44} = g_{\beta\beta} = -g_{55}\cos^2 b\cos^2\theta\sin^2 b\sin^2 2(a+\gamma) + \frac{\zeta}{32\kappa}, \tag{31}$$

where

$$\begin{aligned}\zeta = &-\csc^2\theta_1\{-101 + 12\cos 4\theta_1 + 64\cos 6\theta_1 + 25\cos 8\theta_1\\ &+16(61 + 100\cos 2\theta_1 + 31\cos 4\theta_1)\cos 2\theta_2\cos 2\theta\sin^4\theta_1\\ &-64(5 + 7\cos 2\theta_1)\cos 4\theta_2\sin^6\theta_1 + 128\cos 2\theta_2\cos 4\theta_2\cos 2\theta\sin^8\theta_1\\ &+2\cos^2 b\sin^2\theta_1(242 + 445\cos 2\theta_1 + 286\cos 4\theta_1 + 51\cos 6\theta_1\\ &+4((125 + 196\cos 2\theta_1 + 63\cos 4\theta_1)\cos 2\theta_2\\ &-2(29 + 28\cos 2\theta_1 + 7\cos 4\theta_1)\cos 4\theta_2)\sin^2\theta_1\\ &+32(\cos 6\theta_2 + \cos 8\theta_2)\sin^6\theta_1)\sin^2\theta\}.\end{aligned} \tag{32}$$

- $g_{45} = g_{\beta b}$:

$$g_{45} = g_{\beta b} = g_{55} \cos 2(a+\gamma) \cos\theta. \tag{33}$$

- $g_{46} = g_{\beta\theta}$:

$$g_{46} = g_{\beta\theta} = t \frac{\cos 2(a+\gamma) \sin 2b (2\cos 2\theta_1 - (\cos 4\theta_2 - 3\cos 2\theta_2)\sin^2\theta_1)\sin\theta}{8u_-}. \tag{34}$$

- $g_{66} = g_{\theta\theta}$:

$$\begin{aligned} g_{66} = g_{\theta\theta} = {} & \frac{32\cos^2 b \cos^4\theta_1}{6 + 2\cos 2\theta_1 + \cos 2(\theta_1 - \theta_2) - 2\cos 2\theta_2 + \cos 2(\theta_1+\theta_2)} \\ & + \frac{1}{4}\{-2 - 4\cos 2\theta_1 + (-\cos 2\theta_2 + \cos 4\theta_2)\sin^2\theta_1 - \cos 2b(6\cos^2\theta_1 \\ & + (\cos 2\theta_2 + \cos 4\theta_2)\sin^2\theta_1)\}. \end{aligned} \tag{35}$$

Since the Euler angles a and γ seem only to appear in the g_{ij}'s in the additive combination $a+\gamma$, we conducted a reparameterization of the form $\gamma = \tau - a$. Then, we found that the entries of the associated 8×8 Bures metric tensor (again computed using (6)) were not only independent of α, as before, but also of the parameter a.

4. Concluding remarks

We would like to express guarded optimism that, with sufficient expenditure of computational resources and/or added ingenuity and insight, the question marks in (15) can be effectively removed, and one proceed with supplementary analyses, such as inversion of the Bures metric tensor, for purposes of statistical estimation [29], [30, Eq. (7)] and computation of the volume element of the metric, that is the "quantum Jeffreys' prior" [20,31]. Let us note here that the inverse of the Bures metric tensor (2) for the *two*-level quantum systems takes the particularly simple form

$$g^{-1} = 4\begin{pmatrix} 1-x^2 & -xy & -xz \\ -xy & 1-y^2 & -yz \\ -xz & -yz & 1-z^2 \end{pmatrix}. \tag{36}$$

However, we have confirmed that the remaining not explicitly expressed g_{ij}'s in (15) are not simply products of two independent functions, one of the Euler angles $(\alpha, \gamma, a, \beta, b, \theta)$, and the other of the spherical angles (θ_1, θ_2). These three yet (relatively compactly) unexpressed elements (i.e., $g_{11} = g_{\alpha\alpha}$, $g_{12} = g_{\alpha\gamma}$ and $g_{14} = g_{\alpha\beta}$) are independent only of α, and not of the other seven parameters. If we set $\beta = b = 0$, then $g_{14} = 0$ and both g_{11} and g_{12} reduce to (cf. [30, Eq. (28)])

$$\frac{(-2 - 6\cos 2\theta_1 + \cos 2(\theta_1 - \theta_2) - 2\cos 2\theta_2 + \cos 2(\theta_1+\theta_2))^2 \sin^2 2\theta}{64(3 + \cos 2\theta_2 - 2\cos 2\theta_2 \sin^2\theta_1)}. \tag{37}$$

If we set $\beta = \theta = 0$, on the other hand, then both g_{11} and g_{12} reduce to g_{33}, i.e., $g_{55}\sin^2 2b$, while g_{44} reduces to $-\frac{1}{2}g_{55}\sin 4b \sin 2(a+\gamma)$.

We also cannot rule out the possibility that some of the more complicated expressions we have presented here — such as g_{22} and g_{44} — have, in fact, considerably simpler forms than have so far been uncovered. In addition to the transformation $\gamma = \tau - a$, which as we have already noted renders *all* the elements of the Bures metric tensor independent of a, as well as α, another quite interesting reparameterization would be based on the inversion of the relation (15), since the element g_{55} itself enters directly into the expressions for many of the other elements. That is, one has

$$\theta_2 = \sec^{-1}\frac{2\sqrt{2}\sin\theta_1}{\sqrt{4 + g_{55} + 4\cos 2\theta_2 + \sqrt{g_{55}}\sqrt{16 + g_{55} + 16\cos 2\theta_2}}}. \tag{38}$$

We have recomputed the Bures metric tensor, which we now denote $\tilde{g}$, again with (6), using τ and g_{55} as parameters, rather than γ and θ_2 as in our main analysis and, indeed, found that $\tilde{g}_{bb}$ has the expected form, i.e., equaling g_{55}, and, similar type results for $\tilde{g}_{\alpha a}$, $\tilde{g}_{\alpha b}$, $\tilde{g}_{aa}$, $\tilde{g}_{ab}$ and $\tilde{g}_{\beta b}$. Also, numerically $\tilde{g}_{\tau a} = g_{\gamma a}$.

Since Byrd has indicated that he will shortly present an Euler angle parameterization of $SU(4)$, parallel to that of $SU(3)$ [23] used here, it will, at that point, be of interest to similarly attempt to recreate the 15×15 Bures metric tensor for the *four*-level quantum systems — which are capable of describing the state of a pair of *qubits* (cf. [32]). For this task, rather than (6), it will be necessary to use one of the other "explicit formulae for the Bures metric" given by Dittmann in [9].

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