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Exact Bures probabilities that two quantum bits are classically correlated

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Abstract. In previous studies, we have explored the *ansatz* that the volume elements of the *Bures* metrics over quantum systems might serve as *prior* distributions, in analogy with the (classical) *Bayesian* role of the volume elements ("Jeffreys' priors") of *Fisher information* metrics. Continuing this work, we obtain *exact* Bures prior probabilities that the members of certain *low*-dimensional subsets of the *fifteen*-dimensional convex set of 4×4 density matrices are *separable* or *classically correlated*. The main analytical tools employed are *symbolic* integration and a formula of Dittmann (J. Phys. A **32**, 2663 (1999)) for Bures metric tensors. This study complements an earlier one (J. Phys. A **32**, 5261 (1999)) in which numerical (randomization) – but *not* integration – methods were used to estimate Bures separability probabilities for *unrestricted* 4×4 and 6×6 density matrices. The exact values adduced here for pairs of quantum bits (qubits), typically, well exceed the estimate (≈ 0.1) there, but this disparity may be attributable to our focus on special low-dimensional subsets. Quite remarkably, for the $q = 1$ and $q = \frac{1}{2}$ states inferred using the principle of maximum nonadditive (Tsallis) entropy, the Bures probabilities of separability are *both* equal to $\sqrt{2} - 1$. For the Werner *qubit-qutrit* and *qutrit-qutrit* states, the probabilities are vanishingly small, while in the *qubit-qubit* case it is $\frac{1}{4}$.

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1 Introduction

1.1 Background

In a previous study [1], we exploited certain *numerical* methods to estimate the *a priori* probability – based on the volume element of the Bures metric [2–6] – that, a member of the fifteen-dimensional convex set (R) of 4×4 density matrices is *separable* (classically correlated), that is, expressible as a convex combination of tensor products of pairs of 2×2 density matrices. (Ensembles of separable states, as well as of *bound entangled* states can not be "distilled" to obtain pairs in singlet states for *quantum* information processing [7,8].) This Bures probability estimate ≈ 0.1 was rather unstable in character ([1], Tab. 1) due, in part it appeared, to difficult-to-avoid "over-parameterizations" of R, as well as to the unavailability, in that context, of numerical *integration* methods. But now in Sections 2.1, 2.2 and 2.3 below, we are able to report *exact* probabilities of separability by restricting consideration to certain low-dimensional subsets of R, for which *symbolic* integration can be performed. Then, in the subsequent body of the paper, we investigate analogous questions when R is replaced by the convex sets of 9×9 and 6×6 density matrices. (We have also elsewhere studied, using numerical methods, the Bures probability of separability of the two-party *Gaussian* states [9] (*cf.* [10])).

Preliminarily though, we investigate in Section 1.2 certain relevant motivating issues, first having arisen in the context of the 3×3 density matrices. These quantum-theoretic entities belong to an eight-dimensional convex set (Q), which we parameterize in the manner,

$$\rho_Q = \frac{1}{2} \begin{pmatrix} v+z & u-\mathrm{i}w & x-\mathrm{i}y \\ u+\mathrm{i}w & 2-2v & s-\mathrm{i}t \\ x+\mathrm{i}y & s+\mathrm{i}t & v-z \end{pmatrix} \cdot \qquad (1)$$

The feasible range of the eight parameters – defined by the boundary of Q – is determined by the requirements imposed on density matrices, in general, that they be Hermitian, nonnegative definite (all eigenvalues nonnegative), and have unit trace [11].

Dittmann ([2], Eq. (3.8)) (*cf.* [3]) has presented an "explicit" formula (one not requiring the computation of eigenvalues and eigenvectors) for the Bures metric [2–6]

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over the 3×3 density matrices. It takes the form

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

If we implement this formula, using ρ_Q for ρ, we obtain an 8×8 matrix – the Bures metric tensor, which we will denote by g.

It has been proposed [1,12–16] that the square root of the determinant of g, that is, $|g|^{1/2}$, which gives the *volume element* of the metric, be taken as a prior distribution (to speak in terms of the specific instance presently before us) over the 3×3 density matrices (*cf.* [17]). This *ansatz* is based on an analogy with Bayesian theory [18,19], in which the volume element of the *Fisher information* [20] matrix is used as a *reparameterization-invariant* prior, termed "Jeffreys' prior".

Unfortunately, the ("brute force") computation of the determinant of such 8×8 symbolic matrices appears to exceed present capabilities [21,22]. In light of this limitation, we pursued a strategy of fixing (in particular, setting to zero) a certain number (four) of the eight parameters, thus, leading to an achievable calculation. A similar course was followed in a brief exercise in ([14], Eqs. (31, 32)), but using a quite different parameterization of Q – one based on the expected values with respect to a set of four mutually unbiased (orthonormal) bases of three-dimensional Hilbert space [23,24].

In [16] we have reported exact results for the "Hall normalization constants" for the Bures volumes of the n-state quantum systems, $n = 2, \ldots, 6$. These analyses utilized certain parameterizations (of Schur form) of the $n \times n$ density matrices [25], in which the eigenvalues and eigenvectors of these density matrices are *explicitly* given. It was established there ([16], Sect. 2.2), among other things, that the Bures volume for the 3×3 density matrices is, in fact, *normalizable* over Q, forming a *probability distribution*. Since it appears to be highly problematical to find an explicit transformation from this eigen-parameterization of Boya *et al.* [25] to that used in equation (1), we can not conveniently utilize the results of [16] for our specific purposes here. For the n-level systems, $n > 3$, the analogous task would appear to be even more challenging, since the appropriate parameterizations of $SU(n)$ and the associated invariant (Haar) measures seem not yet to have been developed (*cf.* [26–29]).

1.2 Two forms of conditional Bures priors for a certain four-parameter three-level quantum system

Since we aim to reexamine the specific findings in [12], we will cast our analyses specifically in terms of the parameterized form (1). We have computed, using the formula (2), the 8×8 Bures metric tensor (g) associated with (1). Then – only subsequent to this computation – we set the four parameters s, t, u and v all equal to zero in g, obtaining what we denote by $\tilde{g}$. (Actually, this "conditioning" on P can be performed immediately after the determination of the differential element $\mathrm{d}\rho$, thus simplifying the further calculations in (2).) Then,

$$|\tilde{g}|^{\frac{1}{2}} = \frac{1}{64v(1-v)^{\frac{1}{2}}(v^2-x^2-y^2-z^2)^{\frac{1}{2}}(x^2+y^2+z^2-(v-2)^2)}, \tag{3}$$

which could be considered to constitute the (unnormalized) conditional Bures prior over P.

On the other hand, if we *ab initio* nullify the same four parameters (s, t, u, v) in ρ_Q, we get the family of density matrices, defined over a four-dimensional convex subset (P) of Q,

$$\rho_P = \frac{1}{2}\begin{pmatrix} v+z & 0 & x-\mathrm{i}y \\ 0 & 2-2v & 0 \\ x+\mathrm{i}y & 0 & v-z \end{pmatrix}, \tag{4}$$

which was the specific object of study in [12].

Now, let us describe two ways in which an alternative to the presumptive conditional prior (3), that is,

$$\frac{1}{16v(1-v)^{\frac{1}{2}}(v^2-x^2-y^2-z^2)^{\frac{1}{2}}}, \tag{5}$$

has been derived. We obtain the outcome (5) if we either: (a) employ ρ_P directly in Dittmann's formula (2), and generate the corresponding 4×4 metric tensor and compute the square root of its determinant (the procedure followed in [12]); or (b) extract from $\tilde{g}$ the 4×4 submatrix with rows and columns associated with (the four *non*-nullified parameters) v, x, y and z, that is

$$\frac{1}{4(v^2-x^2-y^2-z^2)} \times \begin{pmatrix} \frac{v-x^2+y^2+z^2}{1-v} & -x & -y & -z \\ -x & \frac{v^2-y^2-z^2}{v} & \frac{xy}{v} & \frac{xz}{v} \\ -y & \frac{xy}{v} & \frac{v^2-x^2-z^2}{v} & \frac{yz}{v} \\ -z & \frac{xz}{v} & \frac{yz}{v} & \frac{v^2-x^2-y^2}{v} \end{pmatrix} \tag{6}$$

and calculate the square root of its determinant. The matrix (6) is *not* exactly the same as (14) there – a result which was presumably also obtained by the use of ρ_P in (2). The four diagonal entries there are the *negatives* of the ones in (6), that is, we had there ([12], Eq. (14))

$$\frac{1}{4(v^2-x^2-y^2-z^2)} \times \begin{pmatrix} \frac{v-x^2+y^2+z^2}{1-v} & -x & -y & -z \\ -x & \frac{y^2+z^2-v^2}{v} & \frac{xy}{v} & \frac{xz}{v} \\ -y & \frac{xy}{v} & \frac{x^2+z^2-v^2}{v} & \frac{yz}{v} \\ -z & \frac{xz}{v} & \frac{yz}{v} & \frac{x^2+y^2-v^2}{v} \end{pmatrix}. \tag{7}$$

In any case, the determinants of these two nonidentical 4×4 matrices are the same, so the substantive conclusions of [12] regarding Bures priors are unchanged.

Hall has pointed out that the result (3) is, in fact, an eight-dimensional volume element rather that the four-dimensional one desired here. In addition, a referee has remarked there can be "two different sets of basis one-forms that are used to compute the volume element. This happens, for example, in $SU(n)$ when one uses $A^{-1}\mathrm{d}A$ as the matrix of left invariant one-forms. There exist n^2 invariant forms in this matrix. One must choose an independent set. This set is thus not unique".

It is interesting to compare the form of (6) with the Bures metric tensor for the 2×2 systems ([12], Eq. (4))

$$\frac{1}{4(1-x^2-y^2-z^2)} \times \begin{pmatrix} 1-y^2-z^2 & xy & xz \\ xy & 1-x^2-z^2 & yz \\ xz & yz & 1-x^2-y^2 \end{pmatrix}, \quad (8)$$

obtained by the application of Dittmann's formula ([2], Eq. (3.7) (*cf.* (2)),

$$d_{\mathrm{Bures}}(\rho, \rho+\mathrm{d}\rho)^2 = \frac{1}{4}\mathrm{Tr}\{\mathrm{d}\rho\mathrm{d}\rho + \frac{1}{|\rho|}(\mathrm{d}\rho - \rho\mathrm{d}\rho)(\mathrm{d}\rho - \rho\mathrm{d}\rho)\}. \quad (9)$$

(Of course, in the limit $v \to 1$, ρ_P, in effect, degenerates to a two-level system, and it is of interest to keep this in mind in examining the results presented here. In the opposite limit $v \to 0$, one simply leaves the domain of quantum considerations.)

We note that (3) differs from (5) in that it has an additional factor,

$$f = \frac{1}{4(x^2+y^2+z^2-(v-2)^2)} \cdot \quad (10)$$

Since v can be no greater than 1 and $x^2+y^2+z^2$ no greater than v if ρ_P is to meet the nonnegativity requirements of a density matrix, f must be *negative* over the feasible range (P) of parameters of ρ_P. In fact, the square root of the determinant of the "complementary" 4×4 submatrix of $\tilde{g}$ – the one associated with the *nullified* parameters, s, t, u, w, rather than v, x, y, z – is equal to f.

Now, it is interesting to note – transforming the Cartesian coordinates (x, y, z) to spherical ones (r, θ, ϕ) – that while the previous result (5) of [12] can be normalized to a (proper) probability distribution over P,

$$p(v, r, \theta, \phi) = \frac{3r^2 \sin\theta}{4\pi^2 v(1-v)^{\frac{1}{2}}(v^2-r^2)^{\frac{1}{2}}}, \quad (11)$$

the new prior (3) is itself *not* normalizable over P, that is, it is *improper*. However, we can (partially) integrate (3) over the three spherical coordinates to obtain the *univariate* marginal over the variable v,

$$q(v) = \frac{\pi^2}{64v}(-1 - \frac{2}{(1-v)^{\frac{1}{2}}} + \frac{1}{-1+v}). \quad (12)$$

The integral of (12) over $v \in [0,1]$ diverges, however. We can compare (12) with the univariate marginal *probability distribution* of (11) ([12], Eq. (19))

$$p(v) = \frac{3v}{4(1-v)^{\frac{1}{2}}} \cdot \quad (13)$$

(In [30,31] $p(v)$ was interpreted as a density-of-states or structure function, for thermodynamic purposes, and the associated partition function reported.) The behaviors of (12) and (13) are quite distinct, the latter monotonically increasing as v increases, while the [negative] of the former has a minimum at $v \approx 0.618034$.

Let us also observe that the factor f, given in (10), the added presence of which leads to the non-normalizability of (3), takes the form in the spherical coordinates,

$$f = \frac{1}{4(r+2-v)(r+v-2)} = \frac{1}{4(r^2-(v-2)^2)} \cdot \quad (14)$$

The eight eigenvalues (λ) of the nullified form of the Bures metric tensor g, that is $\tilde{g}$, come in pairs. They are

$$\lambda_{1,2} = \frac{1}{4v}, \quad \lambda_{3,4} = \frac{1}{4+2r-2v}, \quad \lambda_{5,6} = -\frac{1}{2(r+v-2)},$$
$$\lambda_{7,8} = \frac{1}{-2(r^2+(v-2)v)+2(r^4+v^4+2r^2(2+(v-4)v))^{\frac{1}{2}}} \cdot \quad (15)$$

Of course, the product of these eight eigenvalues gives us $|\tilde{g}|$, the square root of which – that is (3) – constitutes the new (but unnormalizable/improper) possibility here for the conditional Bures/quantum Jeffreys' prior over the four-dimensional convex subset P of the eight-dimensional convex set Q composed of the 3×3 density matrices.

2 Bures priors and separability probabilities for various composite quantum systems

2.1 One-parameter $2 \otimes 2$ systems

Now, let us seek to extend the comparative form of analysis in Section 1.2 to the 4×4 density matrices. For the Bures metric in this setting we rely upon Proposition 1 in the recent paper of Dittmann [3], which presents an explicit formula in terms of the characteristic polynomials of the density matrices. (Let us point out that in the earlier preprint versions, in particular `quant-ph/9911058v4`, of our paper here, a number of "anomalous" results were reported. These turned out to be attributable to our misinterpretation of the symbol Y' in [3] as the transpose of Y, rather than the conjugate transpose of Y. We have since amended our analyses in this regard.) We apply it to several *one*-dimensional convex subsets of the fifteen-dimensional convex set (R) of 4×4 density matrices. These subsets – unless otherwise indicated – are (partially) characterized by having their associated two 2×2 reduced systems described by the fully mixed (diagonal) density matrix, having $\frac{1}{2}$ for its two diagonal entries. Or to put it equivalently, the three Stokes/Bloch parameters for each of the two subsystems are all zero. (A complete characterization of the inseparable $2 \otimes 2$ systems with maximally disordered subsystems has been presented within the Hilbert-Schmidt space formalism [32].)

2.1.1 The three intra-directional correlations are all equal

For our first scenario, we stipulate *zero* correlation between the spins of these two reduced (fully mixed) systems in *different* directions, but identical non-zero (in general) correlation between them in the *same* (x, y or z) directions. We denote this common correlation parameter by ζ. In terms of the parameterization of the coupled two-level systems given in [33] (*cf.* [34,35]), the feasible range of ζ is $[-\frac{1}{4}, \frac{1}{12}]$. [The parameterization in [33] is based on the superposition of sixteen 4×4 matrices – which are the pairwise direct products of the four 2×2 Pauli matrices, including among them, the identity matrix. Since the six Stokes/Bloch parameters have all been set to zero, the nine correlation parameters ($\zeta_{ij}, i, j = x, y, z$) must all lie between -1 and 1, and the nine-fold sum of their squares can not exceed 3 [33]. It has been shown that all the tangent vectors corresponding to a basis of the Lie algebra – corresponding to two copies of $SU(2)$ – span six dimensions, and thus there are, in fact, nine *nonlocal* parameters [36]. A referee has suggested that the use of "local orbits would simplify the picture especially for physicists dealing professionally with entanglement. It is because then the reader knows that one deals with what is of the main importance (orbit parameters – like Schmidt coefficients for pure states) from the point of view of say quantum information transmission (like *e.g.* teleportation)" (*cf.* [37,38]).]

If we implement the formula of Dittmann ([3], Eq. (9)) using a general (fifteen-parameter) 4×4 density matrix [33], then nullify twelve of the parameters of the resultant Bures metric tensor, and set the indicated remaining three (ζ_{ii}) all equal to one value ζ, we obtain as the conditional Bures prior (the counterpart of $|\tilde{g}|^{\frac{1}{2}}$ in Sect. 1.2),

$$\frac{32768}{(1-4\zeta)^3(1+4\zeta)^{\frac{9}{2}}\sqrt{1-12\zeta}}\,. \tag{16}$$

On the other hand, if we set the fifteen parameters in precisely this same fashion *before* employing the formula of Dittmann, we obtain for the volume element

$$\frac{2\sqrt{3}}{(1-8\zeta-48\zeta^2)^{\frac{1}{2}}}\,. \tag{17}$$

The former prior is *non-normalizable* over $\zeta \in [-\frac{1}{4}, \frac{1}{12}]$, while the latter is *normalizable*, its integral over this interval equalling $\frac{\pi}{2}$. In Figure 1, we display this probability distribution. The pair of outcomes ((16) and (17)) is, thus, fully analogous in terms of normalizability, to what we found above ((3) and (5)) for the particular four-dimensional case (P) of the three-level quantum systems (Q) investigated above.

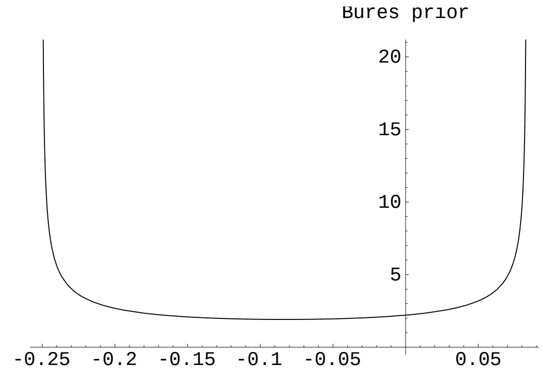

Fig. 1. Normalized conditional Bures prior (17) for one-parameter four-level scenario 1.

Now, for $\zeta \in [-\frac{1}{12}, \frac{1}{12}]$, the associated one-parameter density matrix is *separable* or *classically correlated* (a necessary and *sufficient* condition for which for the 4×4 and 6×6 density matrices is that their partial transposes have nonnegative eigenvalues [39]). So, if we integrate the normalized form of (17) over this interval, we obtain the conditional Bures probability of separability (*cf.* [1,9,40,41]). This probability turns out to be precisely $\frac{1}{2}$. Contrastingly, in [1], for *arbitrary* coupled two-level systems in the fifteen-dimensional convex set R, it was necessary to rely upon numerical (randomization) simulations for estimates of the Bures probability of separability, so this *exact* result appears quite novel in nature. (In [1], the (unconditional) Bures probability of separability was estimated to be ≈ 0.1.)

2.1.2 One intra-directional correlation equals the negative of the other two

A closely related scenario in which the probability of separability is also precisely $\frac{1}{2}$ is one for which the only non-nullified parameters are again the three intra-directional correlations, but now two of them (say, for the x- and y-directions) are set equal to ζ and the third to $-\zeta$. Then, the conditional Bures probability distribution (computed in the analogous manner) is (Fig. 2)

$$\frac{4\sqrt{3}}{\pi(1+8\zeta-48\zeta^2)^{\frac{1}{2}}}\,. \tag{18}$$

The region of feasibility is $[-\frac{1}{12}, \frac{1}{4}]$ and of separability, $[-\frac{1}{12}, \frac{1}{12}]$.

2.1.3 The six inter-directional correlations are all equal

Let us now examine another one-parameter scenario in which the pair of two-level systems is still composed of fully mixed states, but for which the correlations (ζ_{ii})

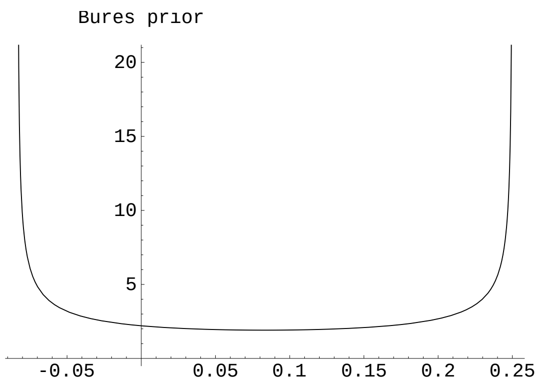

Fig. 2. Normalized conditional Bures prior (18) for one-parameter four-level scenario 2.

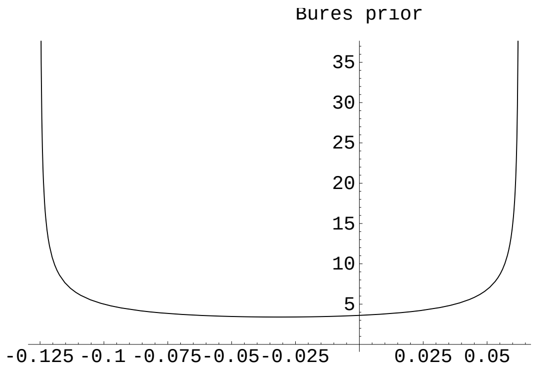

Fig. 3. Normalized conditional Bures prior (19) for one-parameter four-level scenario 3.

in the same directions are zero, while the correlations in different directions ($\zeta_{ij}, i \neq j$) are not necessarily zero and all equal. Thus, we *ab initio* set the (six) interdirectional correlations to ζ, the other nine parameters all to zero, and employ the formula of Dittmann [3] (in the manner we have settled upon for this and all subsequent analyses here). We obtain the conditional Bures *probability distribution* (Fig. 3),

$$\frac{8\sqrt{2}}{\pi(1-8\zeta-128\zeta^2)^{\frac{1}{2}}}, \tag{19}$$

over the feasible range, $\zeta \in [-\frac{1}{8}, \frac{1}{16}]$. The range of separability is $[-\frac{1}{16}, \frac{1}{16}]$. The associated conditional Bures probability of separability is then $\frac{1}{2} + \frac{\sin^{-1}\frac{1}{3}}{\pi} \approx 0.608173$.

2.1.4 The six inter-directional correlations all equal the negative of the three intra-directional correlations

Another one-dimensional scenario of possible interest is one in which we set the intra-directional correlations to ζ and the inter-directional ones to $-\zeta$. Now, the range of feasibility is $\zeta \in [-\frac{1}{20}, \frac{1}{12}]$ and the interval of separability is $\zeta \in [-\frac{1}{20}, \frac{1}{20}]$. Now, application of the Dittmann formula

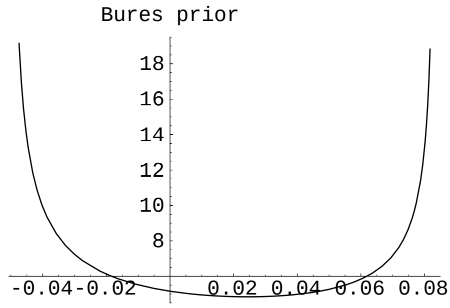

Fig. 4. Normalized conditional Bures prior for one-parameter four-level scenario 4.

yields

$$12\frac{3-20\zeta}{(4\zeta-1)(12\zeta-1)(1+20\zeta)}, \tag{20}$$

the square root of which gives us the unnormalized Bures prior. Since the integrations involved yield various elliptic functions, we have to resort to numerical methods to obtain the Bures probability of separability, that is, 0.702675. In Figure 4, we plot the associated Bures probability density function.

2.1.5 Three scenarios for which the probabilities of separability are simply 1

If we set all nine (inter- and intra-) directional correlations to one value ζ, and the other six (Stokes/Bloch) parameters to zero, so that again the two reduced systems are fully mixed in nature, then proceeding along the same lines as above, we obtain the particularly simple conditional Bures probability distribution,

$$\frac{12}{\pi(1-144\zeta^2)^{\frac{1}{2}}}, \tag{21}$$

over the feasible range $\zeta \in [-\frac{1}{12}, \frac{1}{12}]$. However, all the states in this range are separable, so the associated probability (Bures or otherwise) of separability is simply 1.

If we (formally, but somewhat unnaturally) set all fifteen parameters to ζ, say, then the conditional Bures prior is proportional to

$$\frac{2(3-20\zeta)^{\frac{1}{2}}}{(1+12\zeta-336\zeta^2+576\zeta^3)^{\frac{1}{2}}}\,. \tag{22}$$

Though version 3 of MATHEMATICA failed (exceeding its iteration limit of 4096) to integrate over $\zeta \in [-\frac{1}{4(3+2\sqrt{3})} \approx -0.0386751, \frac{1}{12}]$, version 4 (as shown by M. Trott) yielded

$$\frac{1}{3}\sqrt{\frac{2}{33}(6+\sqrt{3})}\,\Pi(\frac{5}{33}(6+\sqrt{3}); \sin^{-1}(\sqrt{\frac{1}{11}(13-4\sqrt{3})})|\frac{1}{11}(13+4\sqrt{3})). \tag{23}$$

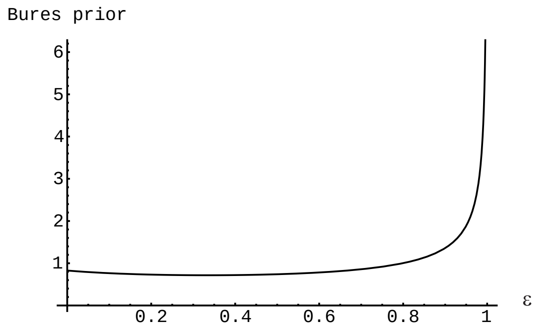

Fig. 5. Bures conditional probability distribution (25) over the two-qubit Werner states.

In any case, all the 4 × 4 density matrices in this one-dimensional set are separable, as well. Another scenario in which the probability of separability is unity, is one in which the three intra-directional correlations (ζ_{ii}) are all zero, and the two systems are *anti*-correlated in different directions, that is $\zeta_{ij} = -\zeta_{ji}$.

2.1.6 Rains-Smolin entangled states

On page 182 of [42], Rains presents a one-parameter (x) set of 4×4 density matrices, apparently communicated to him by Smolin. The corresponding normalized Bures prior for this set of states – defined over the range of feasibility $x \in [-u, u], u = \sqrt{807599}/175 \approx 5.13523$ – is

$$\frac{175}{\pi(807599 - 30625x^2)^{\frac{1}{2}}}\,. \tag{24}$$

None of the members of this set is separable.

2.1.7 Two-qubit Werner states

It is of some interest that all the Bures conditional probabilities of separability we obtained in the various one-dimensional scenarios above are substantially larger than the approximate estimate of 0.1 for the fifteen-dimensional set of 4 × 4 density matrices, obtained on the basis of (unfortunately, but perhaps unavoidably, rather crude) *numerical* methods in [1]. One does, however, obtain a (somewhat smaller) probability of separability of $\frac{1}{4}$ for the two-qubit "Werner states" [43]. These are mixtures of the fully mixed state and a maximally entangled state, with weights $1 - \epsilon$ and ϵ, respectively. (In terms of our other set of parameters, the three intra-directional correlations are all equal to $-\epsilon/4$, while the remaining twelve parameters are zero. A referee has suggested that the parameter ϵ is comparable to the *visibility* in optics [44], that is $(I_{\max} - I_{\min})/(I_{\max} + I_{\min})$, where I is the intensity.) The range of feasibility is $\epsilon \in [0, 1]$ and of separability, $[0, \frac{1}{3}]$. The Bures conditional probability distribution (Fig. 5) is

$$\frac{3\sqrt{3}}{\pi(4 + 8\epsilon - 12\epsilon^2)^{\frac{1}{2}}}\,. \tag{25}$$

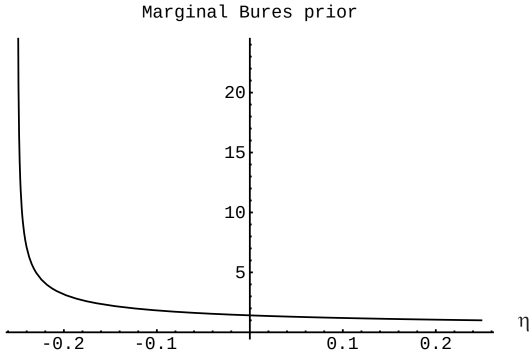

Fig. 6. Univariate marginal Bures prior probability distribution for two-parameter four-level scenario.

2.2 Two-parameter 2 ⊗ 2 systems

2.2.1 Two intra-directional correlations are equal and the third one, free

Now we modify scenario 2 of Section 2.1.2, in that we set two intra-directional correlations again to a common value, call it ζ, and the third, not to $-\zeta$ this time, but to an independent parameter, call it η. (The remaining parameters – the six Stokes/Bloch ones and the six inter-directional correlations stay fixed at zero.) The normalized conditional Bures prior is then

$$\frac{8\sqrt{2}}{\pi((1 + 4\eta)((1 - 4\eta)^2 - 64\zeta^2))^{\frac{1}{2}}}\,. \tag{26}$$

The (triangular-shaped) range of *feasibility* over which we integrated to normalize the (conditional) Bures volume element extends in the η-direction from $-\frac{1}{4}$ to $\frac{1}{4}$. In this triangle, we integrated first over ζ from $\frac{(-1+4\eta)}{8}$ to $\frac{(1-4\eta)}{8}$. The part of the (rhombus-shaped) range of *separability* for $\eta \in [0, \frac{1}{4}]$ coincides with the feasible domain, and for $\eta \in [-\frac{1}{4}, 0]$ extends over $\zeta \in [-\frac{(1+4\eta)}{8}, \frac{(1+4\eta)}{8}]$. The univariate marginal probability distribution (Fig. 6) of (26) over η is $\sqrt{2}/\sqrt{1+4\eta}$.

The probability of separability for this two-parameter four-level scenario is, then, remarkably simply, $\sqrt{2} - 1 \approx 0.414214$ – being somewhat less than the $\frac{1}{2}$ of the related scenario 2 of Section 2.1.2. (Of this total figure, $1 - \frac{1}{\sqrt{2}} \approx 0.292893$ comes from the integration over $\eta > 0$ and $\frac{3}{\sqrt{2}} - 2 \approx 0.12132$ from the other half of the rhomboidal separability region, that is for $\eta < 0$. This second result required the use of version 4 of MATHEMATICA, and I thank Michael Trott for his assistance.)

2.2.2 States inferred by the principle of maximum nonadditive (Tsallis) entropy

Here the two variables parameterizing the 4×4 density matrices are the q-expected value (b_q – "internal energy") and the q-variance (σ_q^2) of the Bell–Clauser- Horne- Shimony- Holt (Bell-CHSH)

$$\frac{8}{((-1+4\zeta-4\eta-4\kappa)(1+4\zeta+4\eta-4\kappa)(1+4\zeta-4\eta+4\kappa)(-1+4\zeta+4\eta+4\kappa))^{\frac{1}{2}}}\,. \tag{29}$$

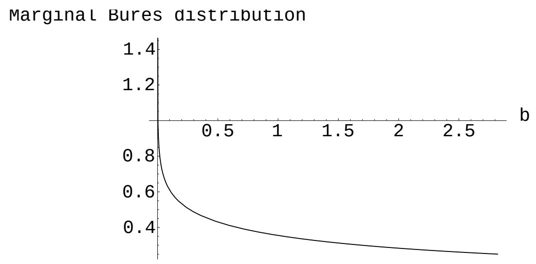

Fig. 7. Marginal Bures prior probability distribution over the expected value b_1.

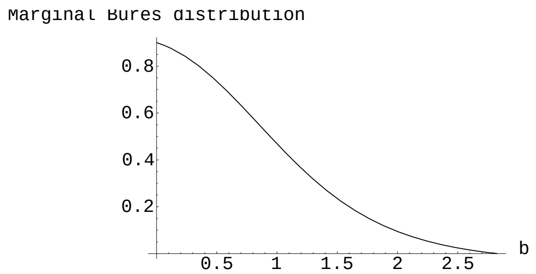

Fig. 8. Marginal Bures prior probability distribution over the expected value $b_{\frac{1}{2}}$.

observable [45] or "Hamiltonian" used by Abe and Rajagopal [46] (*cf.* [47]) in their effort to avoid *fake* entanglement when only b_q is employed in the Jaynes maximum entropy inference scheme [48]. We know from [46] that the feasible region is determined by $0 \leq b_q \leq 2\sqrt{2}$ and $2\sqrt{2}b_q \leq \sigma_q^2 \leq 8$.

Let us, first, set the positive parameter q indexing the Tsallis entropy to 1. ("It is of interest to note that for $q > 1$, indicating the subadditive feature of the Tsallis entropy, the entangled region is small and enlarges as ones goes into the superadditive regime, where $q < 1$" [46].) Then, the corresponding Bures prior probability distribution – again applying the formula of Dittmann – is

$$\frac{1}{\pi(8-\sigma_1^2)^{\frac{1}{2}}(\sigma_1^2-8b_1^4)^{\frac{1}{2}}}\,. \tag{27}$$

In Figure 7, we show the univariate marginal probability distribution of (27) – having integrated it over the parameter σ_1^2 – for the expected value b_1. The region of *separability* is determined ([47], Eqs. (11, 12)) by the supplementary requirements that $\sigma_1^2 \leq 8 - 2\sqrt{2}b_1$ and $b_1 \leq \sqrt{2}$. The probability of separability is, then, $\sqrt{2}-1 \approx 0.414214$ (*cf.* [46], Fig. 1d).

For $q = \frac{1}{2}$, the corresponding Bures probability distribution is (*cf.* (27))

$$\frac{32}{\pi(32+4{b_{\frac{1}{2}}}^2+(\sigma_{\frac{1}{2}}^2-8)\sigma_{\frac{1}{2}}^2)^{\frac{3}{2}}}\,. \tag{28}$$

In Figure 8, we show the marginal probability distribution of (28) over the q-expectation value $b_{\frac{1}{2}}$.

The probability of separability is then again, quite remarkably, $\sqrt{2}-1$. (The domain of integration is now determined by the supplementary requirements that $\sigma_{\frac{1}{2}}^2 \leq 8+2\sqrt{2}b_{\frac{1}{2}} - 2\sqrt{2}\sqrt{b_{\frac{1}{2}}(4\sqrt{2}+b_{\frac{1}{2}})}$ and $b_{\frac{1}{2}} \leq 4-2\sqrt{2}$.) So, it would appear from our two analyses that the probability of separability is *independent* of the particular choice of q. (Certainly, whether or not this is so bears further investigation. However, we have encountered initial computational difficulties in obtaining results for other choices of the index q.)

Of course, it would be of interest to consider the index of the Tsallis entropy q as a third intrinsic variable parameterizing the joint states of the two qubits, in addition to b_q and σ_q^2, but doing so would appear to exceed current computational capabilities.

2.3 Three-parameter $2 \otimes 2$ systems

2.3.1 The three intra-directional correlations are independent

If we now modify the scenario immediately above by letting all three intra-directional correlations be independent of one another – while maintaining the other twelve (Stokes/Bloch and inter-directional correlation) parameters of the four-level systems at zero – the conditional Bures prior takes the form (symmetric in the three free parameters)

see equation (29) above.

The normalization factor, by which this must be divided to yield a probability distribution is $\frac{\pi^2}{8}$. The Bures probability of separability is $\frac{2}{\pi}-\frac{1}{2} \approx 0.13662$.

To obtain these results, we employed the change-of-variables, $\kappa = -\frac{1}{4}+\zeta-\eta-\frac{\upsilon}{4}$, that is, $\upsilon = -1+4\zeta-4\eta-4\kappa$. The integration over the domain of feasibility was obtained using the ordered limits, $\zeta \in [-1/4, 1/4]$; $\upsilon \in [2(-1+4\zeta), 0]$; and $\eta \in [(-2-\upsilon)/8, (8\zeta-\upsilon)/8]$. For the domain of separability, we employed $\zeta \in [0, 1/4]$; $\upsilon \in [2(-1+4\zeta), 0]$; and $\eta \in [(-2+8\zeta-\upsilon)/8, -\upsilon/8]$. The univariate marginal probability distribution of (29) over $\zeta \in [-1/4, 1/4]$ is the uniform one.

2.3.2 Diagonal density matrices

As a simple exercise of interest, we have analyzed – again with the use of Dittmann's general formula for the Bures metric tensor – four-level *diagonal* density matrices, having entries denoted $x, y, z, 1-x-y-z$. (All such density matrices are separable.) The Bures prior probability distribution over the three-dimensional simplex spanned by these entries is, then, simply the Dirichlet distribution

$$\frac{1}{\pi^2(xyz(1-x-y-z))^{\frac{1}{2}}}, \tag{30}$$

which serves as the prior probability distribution ("Jeffreys' prior") based on the Fisher information metric for a quadriinomial distribution [18,19]. This result is, thus, consistent with the study of Braunstein and Caves [6], in which the Bures metric was obtained by maximizing the Fisher information over all quantum measurements, not just ones described by one-dimensional orthogonal projectors.

2.4 A four-parameter $2 \otimes 2$ system

2.4.1 One-parameter unitary transformation of diagonal density matrices

If we transform the (three-parameter) diagonal density matrices discussed immediately above by a (*one*-parameter) 4×4 unitary matrix,

$$U_1 = \mathrm{e}^{\mathrm{i}wP} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos w & \sin w & 0 \\ 0 & -\sin w & \cos w & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \tag{31}$$

where P is a traceless Hermitian matrix (one of the standard generators of $SU(4)$ [49]) with its only nonzero entries being i in the (3,2) cell and $-i$ in the (2,3) cell, we find that the (unnormalized) Bures prior is (*cf.* (30))

$$\frac{\sqrt{(y-z)^2}}{8(xyz(y+z)(1-x-y-z))^{\frac{1}{2}}}, \tag{32}$$

being independent of the fourth (unitary) parameter w. To normalize this prior over the product of the three-dimensional simplex and the interval $w \in [0, 2\pi]$, we need to multiply it by $\frac{3}{\pi^2}$. The additional separability requirement is that $w \in [-u, u]$, where

$$u = \frac{\sin^{-1}\left(\frac{2\sqrt{x-x^2-xy-xz}}{\sqrt{y^2-2yz+z^2}}\right)}{2}\cdot \tag{33}$$

The approximate Bures probability of separability is, then, 0.112, similar to the (unrestricted) estimate in [1].

2.5 One-parameter $3 \otimes 3$ systems – the two-qutrit Werner states

Caves and Milburn ([50], Sect. 3) have constructed two-*qutrit* Werner states. (Such states violate the partial transposition criterion for separability, while satisfying a certain reduction criterion, the violation of which implies distillability [51]). Again applying Proposition 1 of Dittman [3] to this one-dimensional set of 9×9 density matrices, we obtained for the (unnormalized) conditional Bures prior, the *square root* of the ratio of

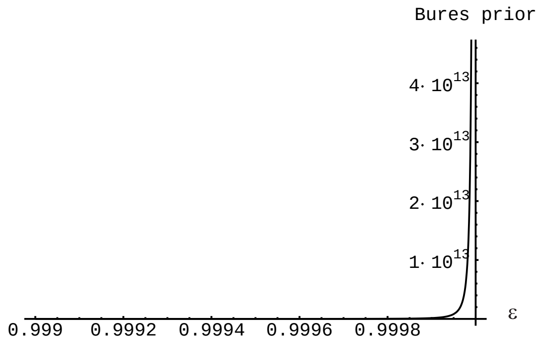

Fig. 9. Bures conditional (unnormalized) measure – that is, the square root of the ratio (34) – over the two-qutrit Werner states.

$$\begin{aligned} &-16(2+7\epsilon)(496+14384\epsilon+179472\epsilon^2+1269568\epsilon^3 \\ &\quad +5676488\epsilon^4+16753596\epsilon^5+31419646\epsilon^6 \\ &\quad +31863023\epsilon^7+14859999\epsilon^8) \end{aligned} \tag{34}$$

to

$$3(-1+\epsilon)^5(1+8\epsilon)(31+161\epsilon) \times (31+603\epsilon+3993\epsilon^2+8981\epsilon^3).$$

The range of separability is $[0, \frac{1}{4}]$ [50]. (If the maximally entangled component of the Werner state is replaced by an arbitrary 9×9 density matrix, the range of separability for the resulting mixture must include $[0, \frac{1}{28}]$ [50].) The integral of the square root of the ratio (34) over this range is 1.05879, while over $[0, 0.999999]$, it is 9.62137×10^9. The conditional Bures probability of separability of the two-qutrit Werner states, thus, appears to be vanishingly small (*cf.* [9,10]). The "maximally entangled states of two qutrits are more entangled than maximally entangled states of two qubits" [50]. The two-qutrit Bures prior (Fig. 9) is much more steeply rising than the two-qubit one displayed in Figure 5. (Note, of course, the difference in the scale employed in the two plots.)

2.6 One-parameter $2 \otimes 3$ systems

It clearly constitutes a challenging task to extend (*cf.* Sect. 2.2) the series of one-dimensional analyses in Section 2 to m-dimensional ($m > 1$) subsets of the fifteen-dimensional set of 4×4 density matrices, and *a fortiori* to $n \times n$ density matrices, $n > 4$. Only in highly special cases, does it appear that the use of *exact* integration methods, such as exploited above, will succeed, and recourse will have to be had to *numerical* techniques, such as were advanced in [1,9]. We should note, though, that in those two studies, numerical *integration* procedures were not readily applicable. They would be available if one has, as here, *explicit* forms for the Bures prior, and can suitably define the limits of integration – that is, the boundaries of the sets of density matrices (and separable density matrices) under analysis.

$$\frac{1}{6}\begin{pmatrix} 1+2\sqrt{3}\nu & 0 & 6\nu & 0 & 0 & 0 \\ 0 & 1+2\sqrt{3}\nu & 0 & 0 & 0 & -12i\nu \\ 6\nu & 0 & 1-4\sqrt{3}\nu & 0 & 0 & 0 \\ 0 & 0 & 0 & 1-2\sqrt{3}\nu & 0 & -6\nu \\ 0 & 0 & 0 & 0 & 1-2\sqrt{3}\nu & 0 \\ 0 & 12i\nu & 0 & -6\nu & 0 & 1+4\sqrt{3}\nu \end{pmatrix}, \quad (35)$$

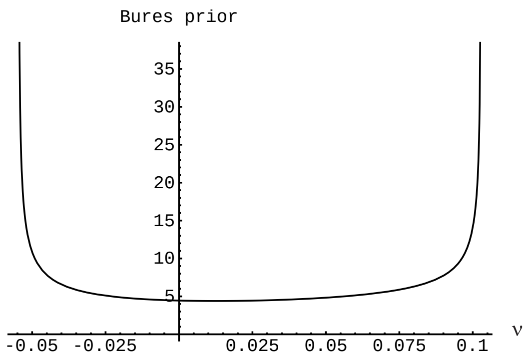

Fig. 10. Normalized conditional Bures prior over the single parameter (ν) of the *six*-level system (35).

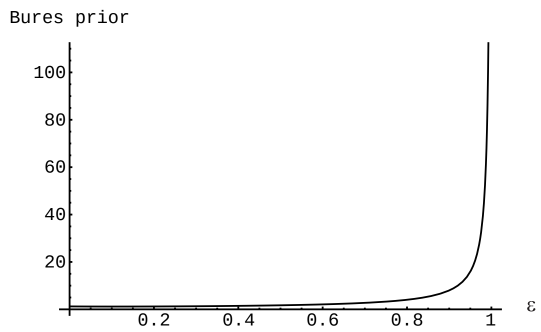

Fig. 11. Bures conditional (unnormalized) measure – that is, the square root of the ratio (36) – over the qubit-qutrit Werner states.

2.6.1 Scenario 1

As an illustration of the application of numerical integration techniques to such a higher-dimensional scenario, we have considered the one-parameter (ν) family of 6×6 density matrices,

see equation (35) above

the 2×2 and 3×3 reduced systems of which are fully mixed. The range of feasibility is $\nu \in [-0.0546647, 0.10277]$ and that of separability is $\nu \in [-0.0546647, 0.0546647]$. (Again, we apply the positive partial transposition Peres-Horodecki condition, sufficient as well as necessary for both the $2 \otimes 2$ and $2 \otimes 3$ systems [39].) We have determined the corresponding (conditional) Bures prior, again based on Proposition 1 in [3]. The probability of separability is the ratio of the integrals of the prior over these two intervals. This turns out to be 0.607921 – as seems plausible from the plot of the (conditional) Bures prior over the feasibility range in Figure 10. This figure displays a minimum at $\nu = 0$ (*cf.* Fig. 4). For $\nu < 0$, we numerically integrate, as well as plot, the absolute value of the (imaginary) Bures prior in this part of the parameter range.

2.6.2 The qubit-qutrit Werner states

The probability of separability also appears to be vanishingly small for the "hybrid" qubit-qutrit Werner states (*cf.* [9]). The greatest degree of entanglement one can hope to achieve is to have the qubit in a fully mixed state, and the qutrit in a degenerate state, with spectrum $\frac{1}{2}$, $\frac{1}{2}$ and 0. The range of separability can then be shown to be $[0, \frac{1}{4}]$ [52]. (For the analysis of *multi*-qubit Werner states, see [53].) The (unnormalized) conditional Bures prior (Fig. 11) is the *square root* of the ratio of

$$10(1+2\epsilon)(26+286\epsilon+1236\epsilon^2+2506\epsilon^3+2021\epsilon^4) \quad (36)$$

to

$$(-1+\epsilon)^2(1+5\epsilon)(13+32\epsilon)(13+126\epsilon+429\epsilon^2+512\epsilon^3).$$

3 Concluding remarks

We believe the main contribution of this study is that it emphatically reveals – through its remarkably simple results of an exact nature – the existence of an intimate connection between two major (but, heretofore, rather distinct) areas of study in quantum physics. By this is meant the study of: (1) metric structures on quantum systems [54]; and (2) entanglement of quantum systems (*cf.* [55]). It should be noted, however, that the several *exact* Bures probabilities of separability adduced above are all for certain qubit-qubit systems (representable by 4×4 density matrices). It would be of interest to see if exact results are obtainable for qubit-qutrit (representable by 6×6 density matrices) and even larger-sized systems, as well as for qubit-qubit systems parameterized by more than three variables (the maximum possible being fifteen). Such investigations would, undoubtedly, demand considerable computational resources and sophistication. (Let us also direct the reader's attention to our study [9], in which we employ numerical methods to estimate the Bures probability of separability of the two-party *Gaussian* states, forms of continuous variable systems. For this purpose, we employed an analogue [57] (*cf.* [58]) of the Peres-Horodecki criterion for separability [39].)

We also intend to use the Bures probabilities as weights for the *entanglement of formation* [56]. By doing so, we should be able to order different scenarios by the total amount of entanglement they involve. As a first example, we have found this figure to be equal to 0.0441763 for the first (one-parameter) scenario we have analyzed above (Sect. 2.1), that of three equal intra-directional correlations (and all other parameters fixed at zero).

One of the clearer findings of [1] was that the Bures (minimal monotone) probability of separability provides an *upper* bound on the related probability for any monotone metric. So, it would appear that the results reported above might also be interpreted as providing upper bounds on any acceptable measure of the probability of separability.

Let us also remark that a quite distinct direction perhaps worthy of exploration is the use of Bures priors as densities-of-states or structure functions for thermodynamic purposes (*cf.* [30,31,59–61]). (However, our initial efforts to find explicit forms for the partition functions corresponding to the results above have not succeeded.)

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