Silver mean conjectures for 15-dimensional volumes and 14-dimensional hyperareas of the separable two-qubit systems

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Abstract

Extensive numerical integration results lead us to conjecture that the *silver mean*, that is, $\sigma_{Ag} = \sqrt{2} - 1 \approx 0.414214$ plays a fundamental role in certain geometries (those given by monotone metrics) imposable on the 15-dimensional convex set of two-qubit systems. For example, we hypothesize that the volume of separable two-qubit states, as measured in terms of (four times) the minimal monotone or Bures metric is $\sigma_{Ag}/3$, and $10\sigma_{Ag}$ in terms of (four times) the Kubo–Mori monotone metric. Also, we conjecture, in terms of (four times) the Bures metric, that part of the 14-dimensional boundary of separable states consisting generically of rank-*four* 4×4 density matrices has volume ("hyperarea") $55\sigma_{Ag}/39$, and that part composed of rank-*three* density matrices, $43\sigma_{Ag}/39$, so the *total* boundary hyperarea would be $98\sigma_{Ag}/39$. While the Bures *probability* of separability (≈ 0.07334) dominates that (≈ 0.050339) based on the Wigner–Yanase metric (and all other monotone metrics) for rank-four states, the Wigner–Yanase (≈ 0.18228) strongly dominates the Bures (≈ 0.03982) for the rank-three states.
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1. Introduction

1.1. Background

An arbitrary state of two quantum bits (qubits) is describable by a 4×4 density matrix (D_4)—an Hermitian, nonnegative definite matrix having trace unity. The convex set of all such density matrices is 15-dimensional in nature [1,2]. Endowing this set with the statistical distinguishability (SD) metric [3] (identically *four* times the Bures [minimal monotone] metric [3]), we addressed in [4] the question (first essentially raised in the pioneering study [5], and investigated further in [6–8]) of what proportion of the 15-dimensional convex set (now a Riemannian manifold) is separable (classically correlated) in nature [9]. This pertains to the question of manifest interest "Is the world more classical or more quantum?" [5].

The Peres–Horodecki partial transposition criterion [10,11] provides a convenient necessary *and* sufficient condition for testing for separability in the cases of qubit–qubit (as well as qubit–qutrit) pairs [12]. That is, if one transposes in place the four 2×2 blocks of D_4, then in the case that the four eigenvalues of the resultant matrix are *all* nonnegative—or more simply, if its determinant is nonnegative [13, Theorem 5]—D_4 itself is separable.

Sommers and Życzkowski [14, Eq. (4.12)] have recently established (confirming en passant certain conjectures of Slater [15]) that the Bures volume of the $(N^2 - 1)$-dimensional convex set of complex density matrices (D_N) of size N is equal to

$$\frac{2^{1-N^2} \pi^{N^2/2}}{\Gamma(N^2/2)}. \tag{1}$$

For the only specific case of interest here, $N = 4$, this gives us for the total Bures volume,

$$V_{\text{Bures}}^{s+n} = \frac{\pi^8}{165150720} \approx 5.74538 \times 10^{-5}, \tag{2}$$

where superscript *s* denotes the set of separable and the superscript *n* the (complementary) set of nonseparable 4×4 density matrices. (The comparable volume based on the *Hilbert–Schmidt* metric—which induces the *flat*, Euclidean geometry into the set of mixed quantum states—is $V_{\text{HS}}^{s+n} = \pi^6/851350500 \approx 1.12925 \times 10^{-6}$ [16, Eq. (4.5)].) The volume V_{Bures}^{s+n} is *exactly* equal to that of a 15-dimensional *half* sphere with radius $1/2$ [14]. Now, additionally,

$$V_{\text{SD}}^{s+n} = 2^{15} V_{\text{Bures}}^{s+n} = \frac{\pi^8}{5040} \approx 1.882645. \tag{3}$$

So, V_{SD}^{s+n} is itself exactly equal to one-half the volume ("surface area") of a 15-dimensional sphere of radius 1. (The full sphere of total surface area $\pi^8/2520 = 2V_{\text{SD}}^{s+n}$ sits in 16-dimensional Euclidean space and bounds the unit ball there.)

One of the objectives in this study is to accurately estimate the included volume V_{SD}^s. Then, we could, in turn, obtain a good estimate of the SD/Bures probability of separability.

$$P_{\text{SD}}^s = \frac{V_{\text{SD}}^s}{V_{\text{SD}}^{s+n}} = P_{\text{Bures}}^s = \frac{V_{\text{Bures}}^s}{V_{\text{Bures}}^{s+n}}. \tag{4}$$

Also, we could gain evidence as to possible *exact* values, which on the basis of previous lower dimensional analyses [8], we have been led to believe is a distinct possibility.

We had already undertaken this task in [4] (seeking there to exploit the then just-developed Euler angle parameterization of the 4×4 density matrices [17]). The analysis was, however, in retrospect, based on a relatively small number (65 million) of points, generated in the underlying quasi-Monte Carlo procedure (scrambled Halton sequences) (cf. [18,19]). (Substantial computer assets were required, nonetheless. Numerical integration in high-dimensional spaces is a particularly challenging computational task.) One of the classical "low-discrepancy" sequences is the *van der Corput* sequence in base b, where b is any integer greater than one. The uniformity of the van der Corput numbers can be further improved by permuting/scrambling the coefficients in the digit expansion of N in base b. The scrambled Halton sequence in N-dimensions—which we employed in [4] and in our auxiliary analyses below (Section 4)—is constructed using the so-scrambled van der Corput numbers for b's ranging over the first N prime numbers [19, p. 53].

To facilitate comparisons with the results of Sommers and Życzkowski [14], which were reported subsequent to our analysis in [4], we need to both divide the estimates given in [4] by $4! = 24$ to take into account the strict ordering of the four eigenvalues of D_4 employed by Sommers and Życzkowski [14, Eq. (3.23)], as well as to multiply them by 8, since we (due to a confusion of scaling constants) only, in effect, used a factor of 2^{12} in [4, Eqs. (5)–(7)] rather than one of 2^{15}, as indicated above in (3) is required. These two independent adjustments together amount to a multiplication by $8/24 = 1/3$. This means that the estimate of V_{SD}^{s+n} (the true value of which, as given above, is known to be ≈ 1.882645) from the quasi-Monte Carlo analysis in [4], should be taken to be $1.88284 = 5.64851/3$; the estimate of V_{SD}^{s} from [4] should, similarly, be considered to be $0.138767 = 0.416302/3$; and of P_{SD}^{s} (for which no adjustment is needed, being a ratio), 0.0737012.

We had been led in [4]—if only for numerical rather than any clear conceptual reasons—to formulate a conjecture that (after adjustment by the indicated factor of $1/3$) can be expressed here as

$$V_{SD}^{s} = \frac{\pi^6}{6930} = 0.138729, \tag{5}$$

as well as that

$$P_{SD}^{s} \equiv P_{Bures}^{s} = \frac{8}{11\pi^2} \approx 0.0736881 \tag{6}$$

(suggesting that the [quantum] "world"—even in the case of only two qubits—is considerably "more quantum than classical"). We now must view (5) and (6), but approximations to the revised conjectures (15) and (16) below, obtained on the basis of such larger quasi-Monte Carlo calculations.

1.2. Monotone metrics and quasi-Monte Carlo procedures

The Bures metric plays the role of the *minimal* monotone metric. The monotone metrics comprise an infinite (nondenumerable) class [20–22], generalizing the (classically *unique*) Fisher information metric [23]. The Bures metric has certainly been the most widely studied

member of this class [3,14,24–27]. For the infinitesimal distance element between two states D_4 and $D_4 + \delta D_4$, we have

$$(ds_{\text{Bures}})^2 = \tfrac{1}{2} \Sigma_{j,k} (\lambda_j + \lambda_k)^{-1} |\langle j|\delta D_4|k\rangle|^2, \tag{7}$$

where D_4 is diagonal in the orthonormal basis $\{|j\rangle\}$ with eigenvalues $\{\lambda_j\}$.

Two other prominent members are the *maximal* monotone metric [28] and the *Kubo–Mori* (KM) [29–31] (also termed Bogoliubov–Kubo–Mori and Chentsov [32]) monotone metric. The Kubo–Mori metric (or canonical correlation stemming from differentiation of the relative entropy) is, up to a scale factor, the *unique* monotone Riemannian metric with respect to which the exponential and mixture connections are *dual* [32], and as such, certainly merits further attention.

In this study, we will utilize additional computer power recently available to us, together with *another* advanced quasi-Monte Carlo procedure (scrambled Faure–Tezuka sequences [33]—the use of which was recommended to us by G. Ökten, who provided a corresponding MATHEMATICA code). Faure and Tezuka were guided "by the construction $C^{(i)} = A^{(i)} P^{(i-1)}$ and by some possible extensions of the generator formal series in the framework of Neiderreiter". ($A^{(i)}$ is an arbitrary nonsingular lower triangular [NLT] matrix, P is the Pascal matrix [34] and $C^{(i)}$ is a generator matrix of a sequence X.) Their idea was to multiply from the right by nonsingular upper triangular (NUT) random matrices and get the new generator matrices $C^{(i)} = P^{(i-1)} U^{(i)}$ for $(0, s)$-sequences [33]. "Faure–Tezuka scrambling scrambles the digits of i before multiplying by the generator matrices ... The effect of the Faure–Tezuka scrambling can be thought of as reordering the original sequence, rather than permuting its digits like the Owen scrambling ... Scrambled sequences often have smaller discrepancies than their nonscrambled counterparts. Moreover, random scramblings facilitate error estimation" [35, p. 107].

The Faure–Tezuka procedure appears to us to be exceptionally successful in generating a highly uniform (low discrepancy [36]) distribution of points over the hypercube—as judged by its yielding an estimate of 1.88264 for $V_{\text{SD}}^{s+n} \approx 1.882645$. However, at this stage, the procedure *does* have the arguable shortcoming that it does not readily lend itself to the use of "error bars" for the estimates it produces, as quite naturally do (the generally considerably less efficient) Monte Carlo methods (which, of course, distribute points on the basis of pseudorandom, rather than deterministic, methods).

"It is easier to estimate the error of Monte Carlo methods because one can perform a number of replications and compute the variance. Clever randomizations of quasi-Monte Carlo methods combine higher accuracy with practical error estimates" [35, p. 95]. G. Ökten is presently developing a MATHEMATICA version of the scrambled Faure–Tezuka sequence in which there will be a random generating matrix for each dimension— rather than one for all [15] dimensions—which will then be susceptible to statistical testing [35].

1.3. Morozova–Chentsov functions

To study such monotone metrics *other* than the SD/Bures one, we will utilize a certain ansatz (cf. [7]). Contained in the formula [14, Eq. (3.18)] of Sommers and Życzkowski for the "Bures volume of the set of mixed quantum states" is the subexpression

(following their notation),

$$Q_N = \Pi_{\nu<\mu}^{1...N} \frac{(\rho_\nu - \rho_\mu)^2}{\rho_\nu + \rho_\mu}, \tag{8}$$

where ρ_μ, ρ_ν ($\mu, \nu = 1, \ldots, N$) denote the eigenvalues of an $N \times N$ density matrix (D_N). The term (8) can equivalently be rewritten using the "Morozova–Chentsov" function for the Bures metric [14, Eq. (2.18)],

$$c_{\text{Bures}}(\rho_\mu, \rho_\nu) = \frac{2}{\rho_\nu + \rho_\mu}, \tag{9}$$

as

$$Q_N = \tfrac{1}{2} \Pi_{\nu<\mu}^{1...N} (\rho_\nu - \rho_\mu)^2 c_{\text{Bures}}(\rho_\mu, \rho_\nu). \tag{10}$$

A Morozova–Chentsov function is a positive continuous function $c(\lambda, \mu)$ that is symmetric in its two variables and for which $c(\lambda, \lambda) = C\lambda^{-1}$, for some constant C, and $c(t\lambda, t\mu) = t^{-1}c(\lambda, \mu)$ [21, Theorem 1.1]. There exist one-to-one correspondences between Morozova–Chentsov functions, monotone metrics and operator means. [21, Corollary 6]. "Operator means are binary operations on positive operators which fulfill the main requirements of monotonicity and the transformer inequality" [21].

The ansatz we employ is that the replacement of $c_{\text{Bures}}(\rho_\mu, \rho_\nu)$ in the formulas for the Bures volume element by the particular Morozova–Chentsov function corresponding to a given monotone metric (g) will yield the volume element corresponding to that particular g. We have been readily able to validate this for a number of instances in the case of the *two-level* quantum systems [$N = 2$], using the general formula for the monotone metrics over such systems of Petz and Sudár [20, Eq. (3.17)]. One can argue that the joint distribution of the eigenvalues of D_N is the product of Q_N—pertaining to the off-diagonal elements of the density matrix—-and an additional factor H_N—pertaining to the diagonal elements. Now, H_N is equal to the reciprocal of the square root of the determinant of the density matrix for *all* [Fisher-adjusted] monotone metrics—so we need not be concerned with its variation across metrics in this study—and simply unity in the case of the [flat] Hilbert–Schmidt metric (cf. [37]).

1.4. Outline of the study

In addition to studying the SD/Bures metric, we ask analogous questions in relation to a number of other monotone metrics of interest. We study two of these metrics, in addition to the SD metric, in our "main analysis" (Section 3) and two more in our "auxiliary analysis" (Section 4), which is based on the same scrambled Halton procedure employed in [4]—but with more than five times the number of points generated there, but also many fewer points than in the primary (main) analysis here. (In hindsight, we might have better consolidated the several monotone metrics into a *single* investigation, from the very outset, but our initial/tentative/exploratory analyses grew, and we were highly reluctant to discard several weeks worth of demanding and apparently revealing computations. Also, we had been using two different sets of processors [Macs and Suns] for our computations and for a number of reasons—too involved and idiosyncratic to make the subject of discussion

here—it proved convenient to conduct *two* distinct analyses.) Also, we include analyses in Section 5 pertaining to the *maximal* monotone metric, and a number of metrics interpolated between the minimal and maximal ones. (The "average" monotone metric—studied in our main analysis (Section 3)—is obtained by such an interpolation.) In Section 6 we apply Monte Carlo methods in a limited study of the questions raised before. In Section 7, we undertake studies concerned with the values of volumes ("surface areas") of the 14-dimensional *boundary* of the 15-dimensional convex set of two-qubit states, as measured in terms of the various monotone metrics under investigation here.

To begin with (Section 2), we will seek to determine V_{KM}^{s+n}. A wiggly line over the acronym for a metric will denote that we have ab initio multiplied that metric by 4, in order to facilitate comparisons with results presented in terms of the SD, rather than the Bures metric, which is one-fourth of the SD metric. (This, perhaps fortuitously, gives us a quite appealing *scale* of numerical results.) The probabilities themselves—being computed as *ratios*—are, of course, invariant under such a scaling, so the "wiggle" is irrelevant for them.

2. Preliminary analysis of the Kubo–Mori metric

The Morozova–Chentsov function for the Kubo–Mori metric is [14, Eq. (2.18)]

$$c_{\mathrm{KM}}(\rho_\mu, \rho_v) = \frac{\log \rho_v - \log \rho_\mu}{\rho_v - \rho_\mu}. \tag{11}$$

To proceed in the study of the KM metric, we first wrote a MATHEMATICA program, using the numerical integration command, that succeeded to a high degree of accuracy in reproducing the formula [14, Eq. (4.11)],

$$C_N = \frac{2^{N^2-N}\Gamma(N^2/2)}{\pi^{N/2}\Gamma(1)\dots\Gamma(N+1)} \tag{12}$$

for the Hall/Bures normalization constants [37,15] for various N. (These constants form one of the two factors—along with the volume of the flag manifold [14, Eqs. (3.22) and (3.23)]—in determining the total Bures volume.) Then, in the MATHEMATICA program, we replaced the Morozova–Chentsov function (9) for the Bures metric in the product formula (10) by the one (11) for the Kubo–Mori function. For the cases $N = 3$ and 4, we found that the new numerical results were to several decimal places of accuracy (and in the case $N = 2$, exactly) equal to $2^{N(N-1)/2}$ times the comparable result for the Bures metric, given by (12). This immediately implies that the KM volumes of mixed states are also $2^{N(N-1)/2}$ times the corresponding Bures volumes (and the same for the KM̃ and SD volumes), since the remaining factors involved, that is, the volumes of the flag manifolds are common to both the Bures and KM cases (as well as to all the monotone metrics). Thus, we arrive at our first *conjecture* (cf. [14]),

$$V_{\widetilde{\mathrm{KM}}}^{s+n} = 64V_{\mathrm{SD}}^{s+n} = \frac{4\pi^8}{315} \approx 120.489, \tag{13}$$

Table 1
Estimates based on (four times) the Bures, "average" and Kubo–Mori metrics, using a scrambled Faure–Tezuka sequence composed of 2 billion points distributed over the 15-dimensional unit hypercube, for quasi-Monte Carlo numerical integration

Metric	V^{s+n}_{metric}	V^s_{metric}	$P^s_{\text{metric}} = V^s/V^{s+n}$
Bures	1.88264(1.88264)	0.137884 (0.137817)	0.0732398 (0.0732042)
Average	28.0801(28.0803)	1.33504 (1.33436)	0.0475438 (0.0475194)
Kubo–Mori	120.504(120.531)	4.1412 (4.14123)	0.0343654 (0.0343583)

The results based on the first 1 billion points are given in parentheses.

for which we will obtain some further support in our *main* numerical analysis (Section 3), yielding Table 1.

3. Main analysis

Associated with the minimal (Bures) monotone metric is the operator monotone function, $f_{\text{Bures}}(t) = (1 + t)/2$, and with the *maximal* monotone metric, the operator monotone function, $f_{\max}(t) = 2t/(1 + t)$ [14, Eq. (2.17)]. The *average* of these two functions, that is, $f_{\text{average}}(t) = (1 + 6t + t^2)/(4 + 4t)$, is also necessarily operator monotone [21, Eq. (20)] and thus yields a monotone metric (apparently previously uninvestigated). Again employing our basic ansatz, we used the associated Morozova–Chentsov function—given by the general formula [20, p. 2667], $c(x, y) = 1/yf(x/y)$:

$$c_{\text{average}}(\rho_\mu, \rho_\nu) = \frac{4(\rho_\mu + \rho_\nu)}{\rho_\mu^2 + 6\rho_\mu\rho_\nu + \rho_\nu^2}. \tag{14}$$

For our main quasi-Monte Carlo analysis, we (simultaneously) numerically integrated the SD, K̃M and aṽg volume elements over a 15-dimensional *hypercube* using two billion points for evaluation, with the points forming a scrambled *Faure–Tezuka* sequence [33]. (As in [4], the 15 original variables—12 Euler angles and 3 angles for the eigenvalues [17, Eq. (38)]—parameterizing the 4×4 density matrices were first linearly transformed so as to all lie in the range [0, 1].) This "low-discrepancy" sequence is designed to give a close-to-*uniform* coverage of points over the hypercube, and accordingly yield relatively accurate numerical integration results.

The results of Table 1 suggest that rejecting the previous conjecture (5)—based on a much smaller number (65 million) of data points than the 2 billion here—and replacing it by (perhaps the more "elegant")

$$V^s_{\text{SD}} = \tfrac{1}{3}\sigma_{\text{Ag}} \equiv \tfrac{1}{3}(\sqrt{2} - 1) \approx 0.138071, \tag{15}$$

where σ_{Ag} denotes the "silver mean" [38]. (As we proceed from 1 billion to 2 billion points, some apparent convergence—0.137817 to 0.137884—of the numerical estimate to the conjecture (15) is observed. It is interesting to note the occurrence of the *first* three positive integers in (15)—a property which obviously the much-studied *golden mean*,

($\sqrt{5} - 1$)/2 lacks.) By implication then, the conjecture (6) is replaced by

$$P^s_{\text{SD/Bures}} = \frac{V^s_{\text{SD}}}{V^{s+n}_{\text{SD}}} = \frac{1680\sigma_{\text{Ag}}}{\pi^8} \approx 0.0733389. \tag{16}$$

In addition to simplify our numerical results, we were also encouraged to advance this conjecture (15) on the basis of certain earlier results. In [8], a number of quite surprisingly simple *exact* results were obtained using *symbolic* integration, for certain specialized [low-dimensional] two-qubit scenarios. This had led us to first investigate in [4] the possibility of an exact probability of separability also in the *full* 15-dimensional setting. (Unfortunately, as far as we can perceive, the full 15-dimensional problem is not at all amenable—due to its complexity—to the use of the currently available symbolic integration programs and, it would appear, possibly for the foreseeable future.)

In particular in [8], a Bures *probability* of separability equal to σ_{Ag} had been obtained for both the $q = 1$ and $q = 1/2$ states [39] inferred using the principle of maximum nonadditive [Tsallis] entropy—and also for an additional *low*-dimensional scenario [8, Section II.B.1]. (We have recently reanalyzed this last scenario, but with the *maximal* monotone metric, and also found a probability of separability equal to σ_{Ag}. The value σ_{Ag} also arises as the amount by which Bell's inequality is violated [40, Eq. (8)].) Christos and Gherghetta [38] took the silver mean, as in our study here, to be the positive solution of the equation $x + 2 = 1/x$—since having a "mean" value less than 1 was useful in their investigation of trajectory scaling functions—while others (perhaps more) [41,42] [43, Chapter 22] have defined it as the positive solution of $x - 2 = 1/x$, that is, $\sqrt{2} + 1$, the *reciprocal* of our σ_{Ag}. (The square root of two minus one is also apparently a form of "Pisot number" [44]. Similar definitional, but perhaps not highly significant, ambiguities occur in the (more widespread) usage of the term "golden mean", that is ($\sqrt{5} \pm 1$)/2 [45]. ("The characteristic sequence of ($\sqrt{5} - 1$)/2 (respectively, $\sqrt{2} - 1$) is called the *golden mean sequence* (respectively, *Pell sequence*)" [46]. This line of analysis—concerned with the alignment of two words over an alphabet—originated, apparently, from a 1963 unpublished talk of the prominent [Nobelist] physicist, D.R. Hofstadter [46].) In [47], demonstrating a conjecture of Gromov, the *minimal volume* of $\boldsymbol{R}^2$ (the infinite Euclidean plane) was shown to be $2\pi/\sigma_{\text{Ag}}$. (An exposition of this result is given in [48].) In [49] the value of $1/2\sigma_{\text{Ag}}$ was obtained for a certain supremum of *volumes*.

Further conjectures that $V^s_{\text{avg}} = 29\sigma_{\text{Ag}}/9 \approx 1.33469$ and $V^s_{\tilde{\text{KM}}} = 10\sigma_{\text{Ag}} \approx 4.14214$ seem worth investigating, based on the results in Table 1. (Our estimate of the ratio $V^s_{\tilde{\text{KM}}}/V^s_{\text{SD}}$ from Table 1 is 30.0339.) So, we have an implied conjecture that

$$P^s_{\tilde{\text{KM}}} = \frac{V^s_{\tilde{\text{KM}}}}{V^{s+n}_{\tilde{\text{KM}}}} = \frac{1575\sigma_{\text{Ag}}}{2\pi^8} \approx 0.0343776. \tag{17}$$

It would then follow that $P^s_{\tilde{\text{KM}}}/P^s_{\text{SD/Bures}} = 15/32 = 0.46875$.

The convergence to the *known* value of V^{s+n}_{SD} in Table 1 seems more pronounced than any presumptive convergence to the conjectured values of the separable volumes alone, but the latter are based on considerably smaller samples (roughly, one-quarter the number) of points than the former (for which, of course, *all* the 2 billion systematically generated
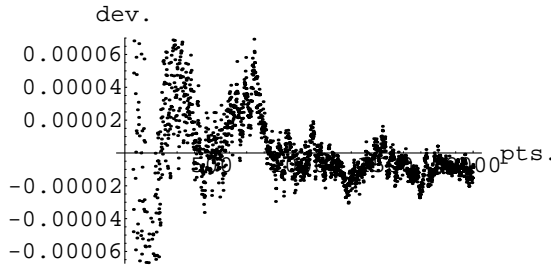
Fig. 1. Deviations of the estimated values of V_{SD}^{s+n} from the *known* value—as shown by Sommers and Życzkowski—of $\pi^8/5040 \approx 1.882645$, as the number of points in the scrambled Faure–Tezuka sequence increases from 1 million to 2000 million.

points are used). Clearly, our conjecture (15) can be reexpressed as $V_{SD}^n = V_{SD}^{s+n} - V_{SD}^s = \pi^8/5040 - \sigma_{Ag}/3 \approx 1.74457$. Our sample estimate for V_{SD}^n is, then, 1.74475.

In Figs. 1–5, we show the *deviations* from our conjectured and known values of the estimates provided by the Faure–Tezuka sequence as the number of points in the sequence increases from 1 million to 2000 million (i.e., 2 billion).
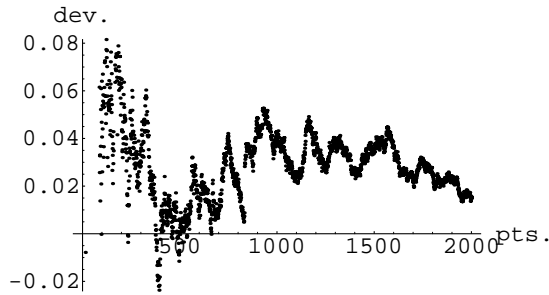

Fig. 2. Deviations of the estimated values of V_{KM}^{s+n} from the *conjectured* value of $4\pi^8/315 \approx 120.489$, as the number of points in the scrambled Faure–Tezuka sequence increases from 1 million to 2000 million.
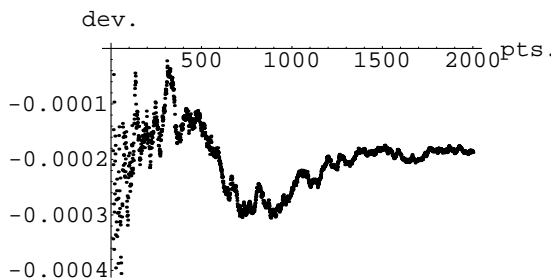

Fig. 3. Deviations of the estimated values of V_{SD}^s from the *conjectured* value of $\sigma_{Ag}/3 \approx 0.138729$, as the number of points in the scrambled Faure–Tezuka sequence increases from 1 million to 2000 million.
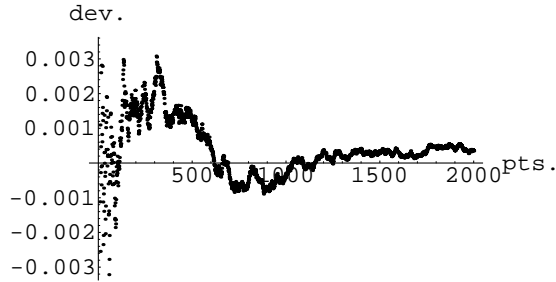
Fig. 4. Deviations of the estimated values of $V_{a\tilde{v}g}^{s}$ from the *conjectured* value of $29\sigma_{Ag}/9 \approx 1.33469$, as the number of points in the scrambled Faure–Tezuka sequence increases from 1 million to 2000 million.
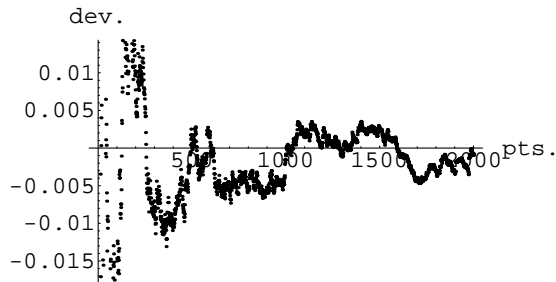

Fig. 5. Deviations of the estimated values of $V_{K\tilde{M}}^{s}$ from the *conjectured* value of $10\sigma_{Ag} \approx 4.14214$, as the number of points in the scrambled Faure–Tezuka sequence increases from 1 million to 2000 million.

In Fig. 6, additionally, we show *together* the *relative* deviations of V_{SD}^{s+n} and of $V_{K\tilde{M}}^{s+n}$ from the known and conjectured values. In other words, we *divide* the estimated values by the known/conjectured values and subtract 1. The SD curve is extraordinarily better behaved ("hugging" the *x*-axis) than is the KM curve. Perhaps this difference is attributable to the "simpler" (more numerically stable?) nature of the Morozova–Chentsov function in the SD case (9) than in the KM case (11).

Further plotting of our various results yielded one of particular interest. In Fig. 7 we show the estimates of $V_{a\tilde{v}g}^{n} - V_{SD}^{n}$. Of course, this figure (the scale of which was internally
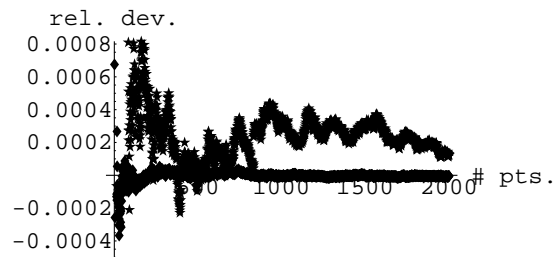

Fig. 6. Joint plot of *relative* deviations of estimates of V_{SD}^{s+n} and $V_{K\tilde{M}}^{s+n}$ from their known and conjectured values of $\pi^{8}/5040$ and $4\pi^{8}/315$. The more rugged curve corresponds to $V_{K\tilde{M}}^{s+n}$.
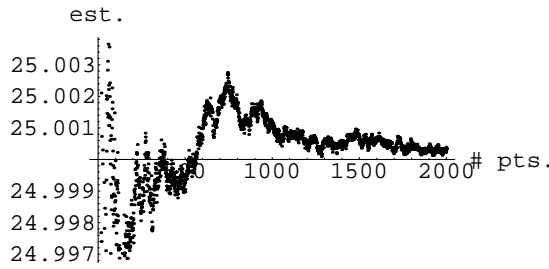
Fig. 7. Estimates of the difference, $V_{\text{a}\tilde{\text{v}}\text{g}}^{n} - V_{\text{SD}}^{n}$, as the number of points in the scrambled Faure–Tezuka sequence increases from 1 million to 2000 million. Note the strong suggestion that the true value is 25 (or close thereto).
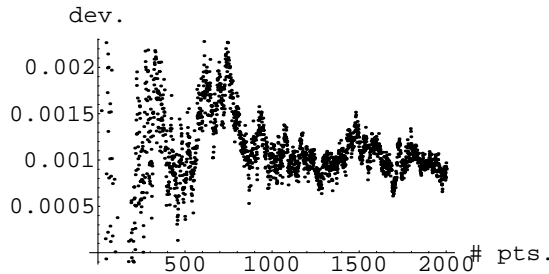

Fig. 8. Deviations of the estimated values of $V_{\text{a}\tilde{\text{v}}\text{g}}^{s+n}$ from the conjectured value of $25\pi^8/8448$, as the number of points in the scrambled Faure–Tezuka sequence increases from 1 million to 2000 million.

chosen by MATHEMATICA, based on the data, and not exogeneously imposed) strongly suggests that $V_{\text{a}\tilde{\text{v}}\text{g}}^{n} - V_{\text{SD}}^{n} = 25$. Now, we found that if we posit

$$V_{\text{a}\tilde{\text{v}}\text{g}}^{s+n} = \frac{25\pi^8}{8448} \approx 28.0792, \tag{18}$$

(with $8448 = 2^8 \cdot 3 \cdot 11$), it would follow that

$$V_{\text{a}\tilde{\text{v}}\text{g}}^{n} - V_{\text{SD}}^{n} = \frac{2449\pi^8}{887040} - \frac{26}{9}\sigma_{\text{Ag}} \approx 24.99996094, \tag{19}$$

(with $887040 = 2^8 \cdot 3^2 \cdot 5 \cdot 7 \cdot 11$), being *strikingly* close to the indicated value of 25.

In Fig. 8, we plot the deviations of the estimates of $V_{\text{a}\tilde{\text{v}}\text{g}}^{s+n}$ from its conjectured value (18).

4. Auxiliary analysis

In an *independent* set of computations (Table 2), employing 415 million points of a scrambled *Halton* sequence (as opposed to the scrambled Faure–Tezuka sequence used in Section 3), we sought to obtain estimates of the probability of separability of two arbitrarily coupled qubits based on three monotone metrics of interest. The specific method employed

Table 2
Estimates based on (four times) the Grosse–Krattenthaler–Slater, Wigner–Yanase and Kubo–Mori monotone metrics, using a scrambled Halton sequence consisting of 415 million points

Metric	V^{s+n}_{metric}	$V^{s}_{\tilde{\text{metric}}}$	$P^{s}_{\text{metric}} = V^{s}/V^{s+n}$
GKS	5.4237	0.330827	0.0609965
WY	14.5129	0.730567	0.0503391
KM	120.504	4.1791	0.0346801

was that of scrambled Halton sequences [19]. (While there are different scrambled Faure–Tezuka sequences depending upon the particular random generating matrices used, the scrambled Halton sequence is unique in nature.)

These correspond to the operator monotone functions,

$$f_{\text{GKS}}(t) = \frac{t^{t/(t-1)}}{e}; \qquad f_{\text{WY}}(t) = \frac{1}{4}(\sqrt{t}+1)^2; \qquad f_{\text{KM}}(t) = \frac{t-1}{\log t}. \qquad (20)$$

The subscript GKS denotes the Grosse–Krattenthaler–Slater ("quasi-Bures") metric (which yields the common asymptotic minimax and maximin redundancies for *universal* quantum coding [50, Section IV.B, 51]), the subscript WY, the Wigner–Yanase information metric [52, Section 4] [53,54], and the subscript KM, the Kubo–Mori metric already studied in Sections 2 and 3. (We had, in fact, intended to study the "Noninformative" monotone metric [55] here instead of the KM metric, but there was a programming oversight that was only uncovered at the end of the computations). It appears conjecturable that, in terms of the separable states, $V^{s}_{\text{G}\tilde{\text{K}}\text{S}} = 4\sigma_{\text{Ag}}/5 \approx 0.331371$. (The evidence is somewhat of a weaker nature that $V^{s}_{\text{W}\tilde{\text{Y}}} = 7\sigma_{\text{Ag}}/4 \approx 0.724874$.) Also, in terms of the combined separable and nonseparable states, it seems possible that $V^{s+n}_{\text{GKS}} = \pi^8/1750 \approx 5.42202$, with $1750 = 2 \cdot 5^3 \cdot 7$. If so, we would have $P^{s}_{\text{GKS}} = 1400\sigma_{\text{Ag}}/\pi^8 \approx 0.0611158$.

We had hoped to further extend the scrambled Halton sequence used here, but doing so has so far proved problematical, in terms of available computer resources.

5. Maximal monotone metric

As to the *maximal* monotone metric, numerical, together with some analytical evidence, strongly indicate that V^{s+n}_{max} is infinite (unbounded) (as well as V^{s}_{max}). The supporting *analytical* evidence consists in the fact that for the three-dimensional convex set of 2×2 density matrices, parameterized by spherical coordinates $[r, \theta, \phi]$ in the "Bloch ball", the volume element of the maximal monotone metric is $r^2 \sin \theta (1 - r^2)^{-3/2}$, the integral of which *diverges* over the ball. Contrastingly, the volume element of the minimal monotone metric is $r^2 \sin \theta (1 - r^2)^{-1/2}$, the integral over the ball of which is *finite*, namely π^2. For $s \geq 1$ the integral of $r^2 \sin \theta (1 - r^2)^{-s}$ diverges, so the divergence associated with the monotone metric itself is not simply marginal or "borderline" in character.

To gain further evidence in these regards, one can engage in numerical estimation for the one-parameter family of *interpolating* metrics given by the operator monotone functions

$$f_a(t) = (1 - a) f_{\text{max}}(t) + a f_{\text{Bures}}(t), \qquad (21)$$

Table 3
Estimates based on the first 96 million points of a scrambled Faure–Tezuka sequence of (four times) a number of metrics obtained by interpolating between the maximal ($a = 0$) and minimal ($a = 1$) monotone metrics

a	1	10^{-1}	10^{-2}	10^{-3}	10^{-4}	10^{-5}	0
V_a^{s+n}	1.88258	7951.27	9.3254×10^6	6.0345×10^9	3.049×10^{12}	1.2825×10^{15}	8.0858×10^{39}
V_a^s	0.13786	148.569	63659	2.0972×10^7	6.502×10^9	2.2084×10^{12}	5.229×10^{36}
P_a^s	0.073229	0.01868	0.006827	0.003475	0.0021325	0.0017219	0.00064669

for which the Morozova–Chentsov functions are of the form

$$c_a(\rho_\mu, \rho_v) = \frac{2(\rho_\mu + \rho_v)}{a(\rho_\mu - \rho_v)^2 + 4\rho_\mu \rho_v}. \tag{22}$$

Then, one could plot the results as a function of the parameter a and study the limit $a \to 0$. (Of course, for $a = 1/2$, one would recover the "average" monotone metric, studied in Section 3.)

A preliminary investigation along these lines is reported in Table 3. Based on the first 96 million points of a scrambled Faure–Tezuka sequence, we obtain estimates of V_a^{s+n}, V_a^s and $P_a^s = V_a^s / V_a^{s+n}$ for (four times) the metrics interpolating between the maximal ($a = 0$) and minimal ($a = 1$) monotone metrics for several values of a, increasingly close to $a = 0$. So, P_{max}^s would seem quite close to being 0. (However, some clearly numerically anomalous behavior occurred in passing from 96 million points to 97 million points. The estimates of V_{max}^{s+n}, V_{max}^s and P_{max}^s jumped to 8.27999×10^{40}, 7.48026×10^{40} and 0.903414, respectively.)

It would be interesting to *formally* test the hypothesis that $P_{max}^s = 0$. (More specifically, we might ask the question if the *limit* of P_a^s as $a \to 0$ is 0.) If it can, in fact, be established that P_{max}^s is zero, this might serve as something in the nature of a "counterexample" to the proposition (a matter of considerable interest in the theoretical analysis of quantum computation) that for bipartite quantum systems of finite dimension, there *is* a separable neighborhood of the fully mixed state of finite volume [56–59]. (These conclusions were obtained with the use of either the trace or Hilbert–Schmidt metric—the first of which is monotone, but not Riemannian, while the second is Riemannian, but not monotone [14].)

We have conducted a test along these lines. Using a simple *Monte Carlo* (rather than quasi-Monte Carlo) scheme, we generated 10 sets of 10 million points *randomly* distributed over the 15-dimensional hypercube. For each of the 10 sets, we obtained estimates of V_{max}^{s+n}, V_{max}^s and hence P_{max}^s. Based on the 100 million points the (mean) estimate of P_{max}^s was $\mu = 1.77038 \times 10^{-7}$ and the standard deviation across the 10 samples, $\eta = 3.692 \times 10^{-7}$. So, the value 0 lies *less* than one-half (i.e., 0.479510) standard deviations from μ. For a student, t-distribution with $9 = 10 - 1$ degrees of freedom, 40% of the probability lies outside 0.261 standard deviations from the mean and 25% outside 0.703 standard deviations. So there is little evidence here for rejecting a hypothesis that P_{max}^s equals 0. For an independent analysis based on 10 sets of 4 million points, the estimates were roughly comparable, i.e., $\mu = 2.4196 \times 10^{-7}$, $\eta = 5.09683 \times 10^{-7}$. Also, for 10 sets of 5 million points, but setting the interpolation parameter a not to 0 but to 0.05, there were obtained $\mu = 0.00438593$ and $\eta = 0.000229437$, with $\mu/\eta = 19.1611$. So, here one *can* decisively reject a hypothesis that the probability of separability for $a = 0.05$ is 0.

Table 4
Monte Carlo analysis based on $15 \cdot 3^{15} = 215, 233, 605$ density matrices

Metric	Est.	S.D.	cj.-Est./S.D.
$V^s_{\widetilde{\text{metric}}}$			
Bures	0.13800	0.00021	0.3354
GKS	0.32990	0.00057	2.5696
WY	0.72811	0.00152	–
Avg	1.3363	0.00287	−0.5821
KM	4.1574	0.02242	−0.6792
NI	848.05	28.997	–
$V^{s+n}_{\widetilde{\text{metric}}}$			
Bures	1.88295	0.00102	−0.2985
GKS	5.4232	0.00315	−0.3867
WY	14.5084	0.00943	–
Avg	28.0781	0.01769	0.0618
KM	120.256	0.17489	1.3363
NI	48668.2	421.712	–

Estimates (est.) of the volumes, standard deviations (S.D.) of these estimates and the number of standard deviations they are away from their conjectured (cj.) or known values, as given in Table 6, are presented.

6. Further Monte Carlo analyses

We also undertook a series of *Monte Carlo* analyses, incorporating together the GKS, Bures, average, Kubo–Mori, Wigner–Yanase, maximal and Noninformative (NI) [55] monotone metrics. (The operator monotone function $f(t)$ associated with the NI metric is $2(t-1)^2/(1+t)\log^2(t)$.) We subdivide the unit hypercube into $3^{15} = 14, 348, 907$ subhypercubes, pick a *random* point in each one of these, and then repeat the procedure. . . We are now able to report in Table 4 the results of 15 iterations of this process. The *central limit theorem* tells us that for a large enough sample size, the distribution of the sample mean will approach a normal/Gaussian distribution. This is true for a sample of independent random variables from any population distribution, so long as the population has a *finite* standard deviation. The population standard deviation is equal to the standard deviation of the mean times the square root of the sample size N, which in our case is $15 \cdot 3^{15}$. If one were to use *two* standard deviations as a rejection criterion, then the only one of our conjectures that would be rejected would be that for $V^s_{\text{GK}\tilde{\text{S}}}$. (However, the standard deviations in the separable cases would be approximately four times as large if we only used the number of points corresponding to separable states, rather than to *all* states, as we have done here. This would lead, then, to *none* of our conjectures being rejected.) The estimate of $P^s_{\max}$, obtained in the same Monte Carlo procedure, was $4.33981 \times 10^{42}/1.93678 \cdot 10^{52} = 2.24073 \times 10^{-10}$.

7. 14-Dimensional boundaries

7.1. Initial analyses

In the analyses above, we have been concerned with the volume of the 15-dimensional convex set of 4×4 density matrices, as measured in terms of a number of monotone metrics.

We have modified the computer programs involved, so that they would provide estimates of the volume ("hyperarea") of the boundary of this set.

Our numerical integrations were conducted over a 14-dimensional hypercube, now allowing one of the original 15 variables (specifically, the hyperspherical angle designated θ_3 in [4, Eq. (2)]) to be determined not by the quasi-Monte Carlo procedure, but by the requirement that the determinant of the partial transpose equal zero. This considerably increases the computational effort *per* point generated.

Our early estimates, in this regard, were: 0.587532 (SD), 6.25466 (aṽg) and 19.8296 (K̃M), all three based on the first 2,600,000 points of a scrambled Faure–Tezuka sequence; 1.47928 (GǨS), 3.37384 (W̃Y) and 19.9277 (K̃M), all three based on the first 1,500,000 points of a scrambled Halton sequence; and 0.588816 ($a = 1$), 837.072 ($a = 10^{-1}$), 414676 ($a = 10^{-2}$), 1.57088×10^8 ($a = 10^{-3}$), 4.87246×10^{10} ($a = 10^{-4}$), 1.30774×10^{13} ($a = 10^{-5}$), 8.57852×10^{27} ($a = 0$) (all seven based on the first 1,100,000 points of a scrambled Faure sequence).

Let us note that in terms of the Bures metric—identically one-fourth of the statistical distinguishability (SD) metric—the pure state [rank 1] boundary of the 4×4 density matrices, *both* separable and nonseparable, is known to have volume $\pi^3/6 \approx 5.16771$. (This is equal to the volume of a 6-dimensional ball of radius 1 and to the volume of a 3-dimensional complex projective space [14, Section IV.C].) The 14-dimensional [60] submanifold of 4×4 density matrices of rank 3 has Bures volume $\pi^7/4324320 \approx 6.98444 \times 10^{-4}$. Multiplying by 2^{14}, we obtain the SD counterpart to this of

$$B_{\mathrm{SD}}^{s+n} = \frac{512\pi^7}{135135} \approx 11.4433. \tag{23}$$

This is *twice* (a "double-covering") the $(n-1)$-content (surface area or hyperarea) of the unit sphere in $n = 15$ dimensions.

7.2. Further analysis

Subsequently, we joined all the monotone metrics of interest into a single joint analysis, using an independent Faure–Tezuka sequence of points in the 14-dimensional hypercube. Up to this point in time, we have generated 35 million points (Table 5). For each of these points, we sought values of the 15 coordinate—θ_3—for which the partial transpose of the corresponding 4×4 density matrix had zero determinant. For 24,038,658 of the points at least one feasible value of θ_3 was found. The even-numbered solutions strongly dominated the odd-numbered solutions. (This may pertain to the fact that in this series of analyses, we had used—adjusting accordingly—the range $[0, \pi]$, rather than $[0, \pi/2]$, as in our other analyses, for θ_1, θ_2 and θ_3.) There were 74 points with one solution, 30 with three, and 11 with five, while there were 2,553,168 with two, 21,312,933 with four, 172,429 with six and 3 with eight.

In Fig. 9, we show the cumulative approximations (in steps of 100,000 points) to the known value (23) of B_{SD}^{s+n}.

We conjecture (Fig. 10) that the component of B_{SD}^{s+n} consisting of separable states [61], that is B_{SD}^{s}, has the value $43\sigma_{\mathrm{Ag}}/39 \approx 0.456697$.

Table 5
Estimates of 14-dimensional boundary volumes based on (four times) the Bures, Grosse–Krattenthaler–Slater, Wigner–Yanase, average, Kubo–Mori and noninformative metrics, using a scrambled Faure–Tezuka sequence composed of 35 million points

Metric	B^s	B^{s+n}	β
Bures	0.456593	11.4443	0.584072
GKS	–	–	1.45204
WY	3203.81	17576.3	6606.58
Avg	6.60067	246.716	6.20592
KM	–	–	19.6215
NI	–	–	4333.36

The concomitant estimate of the SD/Bures probability of separability of such rank-three states would then be

$$\Pi^s_{\text{SD/Bures}} = \frac{B^s_{\text{SD}}}{B^{s+n}_{\text{SD}}} = \frac{297297\sigma_{\text{Ag}}}{1024\pi^7} \approx 0.0398167. \tag{24}$$

This is considerably less than the general probability of separability [of, generically, rank-*four* states], conjectured in formula (16) to be 0.0733389. The ratio of these two probabilities is $14157\pi/81920 \approx 0.542194$.
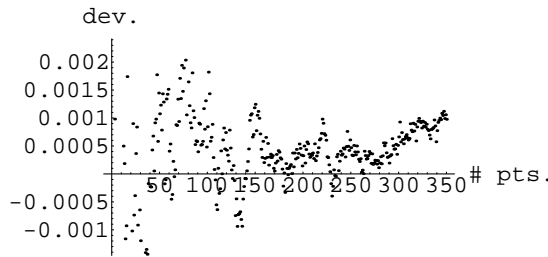

Fig. 9. Deviations of the estimated value of B^{s+n}_{SD} from the *known* value of $512\pi^7/135135 \approx 11.4433$, as the number of points in a certain scrambled Faure–Tezuka sequence increases from 100,000 to 35 million
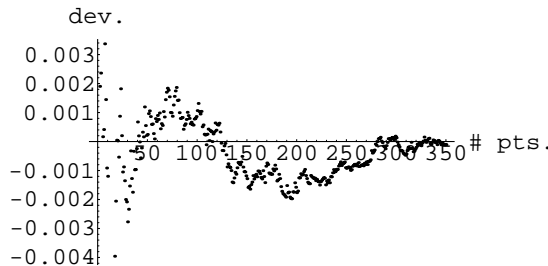

Fig. 10. Deviations of the cumulative estimates of B^s_{SD} from the conjectured value of $43\sigma_{\text{Ag}}/39 \approx 0.456697$. The number of points are recorded in steps of 100,000.

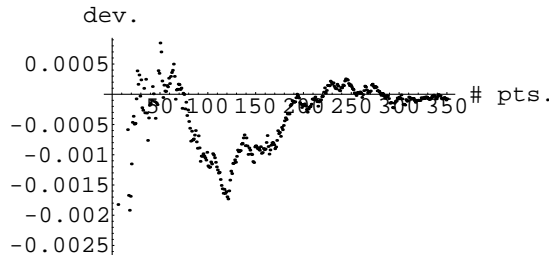Fig. 11. Deviations from the conjectured value of $\beta_{\mathrm{SD}} = 55\sigma_{\mathrm{Ag}}/39 \approx 0.584147$ of the cumulative estimates of the SD volume of that part of the 14-dimensional boundary of the separable states consisting of nondegenerate states. The number of points are recorded in steps of 100,000.

In Fig. 11, we show the cumulative approximations to a conjectured value of $\beta_{\mathrm{SD}} = 55\sigma_{\mathrm{Ag}}/39 \approx 0.584147$ for the 14-dimensional SD boundary of separable two-qubit states composed of generically rank-*four* states. (The test for membership in this class is that the determinant of the partial transpose of the corresponding 4×4 density matrix be zero.) Thus, we have an implied conjecture that the 14-dimensional boundary of separable 4×4 density matrices has *total* SD-volume of $\beta_{\mathrm{SD}} + B_{\mathrm{SD}}^{s} = 98\sigma_{\mathrm{Ag}}/39 \approx 1.04084$. The fit of our cumulative estimates to this conjecture is shown in Fig. 12. Numerical evidence (Fig. 13) also possibly suggests that $B_{\mathrm{avg}}^{s} = 255\sigma_{\mathrm{Ag}}/16 \approx 6.60153$; that (Fig. 14) $B_{\tilde{\mathrm{WY}}}^{s} = 7735\sigma_{\mathrm{Ag}} \approx 3203.94$; that (Fig. 15) $B_{\tilde{\mathrm{WY}}}^{s+n} = 2^{9} \cdot 3 B_{\mathrm{SD}}^{s+n} \approx 17576.9$; that (Fig. 16) $\beta_{\tilde{\mathrm{KM}}} = 616\sigma_{\mathrm{Ag}}/13 \approx 19.6274$; and that (Fig. 17), $\beta_{\mathrm{G\tilde{K}S}} = 270\sigma_{\mathrm{Ag}}/77 \approx 1.45244$ (although, it is intriguing also to consider that $77 \approx 78 = 2 \cdot 39$). So, surprisingly, the probability of separability of a rank-three state appears to be much higher, that is, $348, 423, 075\sigma_{\mathrm{Ag}}/262144\pi^{7} = 3^{2} \cdot 5^{2} \cdot 7^{2} \cdot 11 \cdot 13^{2} \cdot 17\sigma_{\mathrm{Ag}}/2^{18}\pi^{7} \approx 0.182281$ using the Wigner–Yanase metric (but not the average metric, for which we have a sample estimate of 0.0267541 and a conjecture of $10729125\sigma_{\mathrm{Ag}}/54992\pi^{7} \approx 0.0267572$) than with the Bures or SD metric, in strong contrast to the rank-four case examined earlier (Sections 3 and 4).
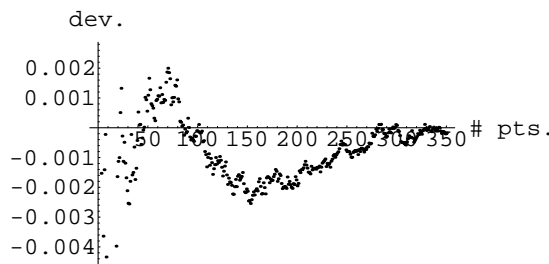

Fig. 12. Deviations from the conjectured value of $B_{\mathrm{SD}}^{s} + \beta_{\mathrm{SD}} = 98\sigma_{\mathrm{Ag}}/39 \approx 1.04084$ of the SD-volume of the *total* boundary of separable states—composed of nondegenerate (rank-four) and degenerate (rank-three) 4×4 density matrices. The number of points of the Faure–Tezuka sequence are recorded in steps of 100,000.
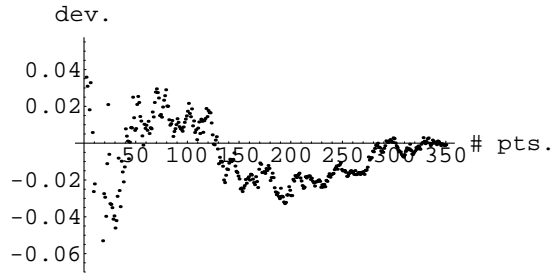
Fig. 13. Deviations from the conjectured value of $255\sigma_{\mathrm{Ag}}/16 \approx 6.60153$ of the cumulative estimates of $B^{s}_{\mathrm{a\bar{v}g}}$.
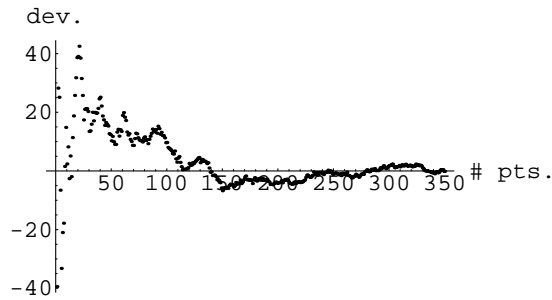

Fig. 14. Deviations from the conjectured value of $7735\sigma_{\mathrm{Ag}} \approx 3203.94$ of the cumulative estimates of B^{s}_{WY}.

7.3. Levy–Gromov isoperimetric inequality

The scalar curvature of the Bures metric for the 4×4 density matrices is bounded below by 570 [27, Corollary 3]. However, application of the Levy–Gromov isoperimetric inequality [62, Appendix C] requires a lower bound of N on $Ricci(Y, Y)$, where $Ricci$ is the Ricci tensor and Y runs over all unit tangent vectors, for closed $(N + 1)$-dimensional manifolds, we did not immediately know if this condition is satisfied or not (given that one cannot apparently "control" the Ricci curvature in terms of the [bounded] scalar curvature),
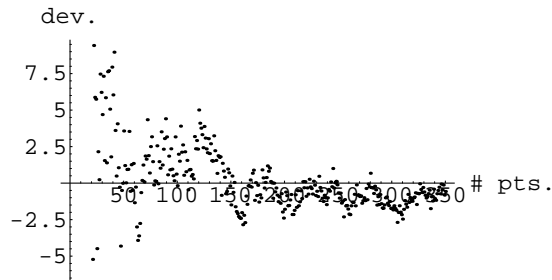

Fig. 15. Deviations from the conjectured value of B^{s+n}_{WY} of $262144\pi^{7}/45045 = 2^{9} \cdot 3B^{s+n}_{\mathrm{SD}} \approx 17576.9$.
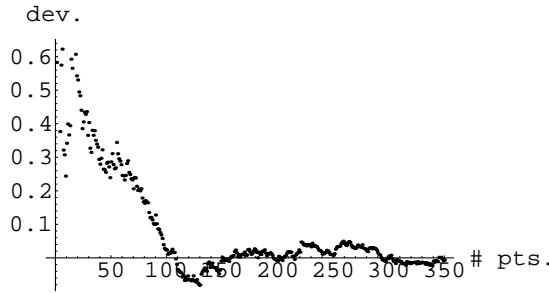
Fig. 16. Deviations from the conjectured value of $\beta_{\mathrm{K\bar{M}}} = 616\sigma_{\mathrm{Ag}}/13 \approx 19.6274$.

but we have found that the inequality is violated, and that the condition is *not* satisfied in the case before us.

To reach this conclusion, we first took the parameter α (strictly following the notation in [62]) to be $P_{\mathrm{SD/Bures}} = V_{\mathrm{SD}}^{s}/V_{\mathrm{SD}}^{s+n} \approx 0.0736881$, according to our conjecture (6) above. Then, the function $s(\alpha)$ is the 14-dimensional volume of the boundary sphere ∂B_{α}, where the volume of the ball B_{α} itself is equal to $\alpha \operatorname{vol}(S^{15})$, and S^{15} is the standard 15-dimensional sphere. Further, the function $Is_{15}(\alpha)$ is the ratio of $s(\alpha) \approx 0.499459$ to $\operatorname{vol}(S^{15}) = 256\pi^{7}/2027025 \approx 0.381443$. The Levy–Gromov inequality then asserts that $Is_{15}(\alpha)$, which here equals 1.30939, must be less than a certain ratio, which in our case would— according to our conjectures and known values—be

$$\frac{B_{\mathrm{Bures}}^{s} + \beta_{\mathrm{Bures}}}{V_{\mathrm{Bures}}^{s+n}} = \frac{2^{-14}(B_{\mathrm{SD}}^{s} + \beta_{\mathrm{SD}})}{2^{-15}(V_{\mathrm{SD}}^{s+n})} \approx 1.10573. \tag{25}$$

So, the indicated inequality is violated.

At this point, we applied formula (7a) of [27], giving the Ricci tensor based on the Bures metric for *diagonal* density matrices,

$$\mathrm{Ricci}(Y, Z) = 3\Sigma_{\mu,\nu,\eta} \frac{Y_{\nu\mu}\rho_{\eta}Z_{\mu\nu}}{(\rho_{\mu} + \rho_{\nu})(\rho_{\mu} + \rho_{\eta})(\rho_{\nu} + \rho_{\eta})} - \frac{3}{2}\Sigma_{\mu,\nu}\frac{Y_{\mu\mu}Z_{\nu\nu}}{(\rho_{\mu} + \rho_{\nu})^{2}}, \tag{26}$$
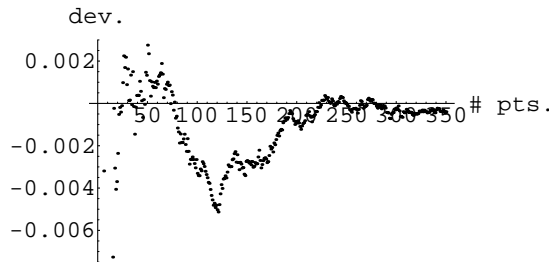

Fig. 17. Deviations from the conjectured value of $\beta_{\mathrm{G\bar{K}S}} = 270\sigma_{\mathrm{Ag}}/77 \approx 1.45244$.

where Y and Z are tangent vectors (traceless Hermitian matrices). We, in fact found, using numerical simulations, violations of the lower bound of N for $(N-1)$-dimensional manifolds on the Ricci tensor required by the Levy–Gromov inequality, with $N = 14$ in our case. The lowest value we were able to achieve in a series of simulations was 3.45666, so no *negative* values were recorded. (The upper value appeared to be unbounded. We also applied the formula (26) to the 8-dimensional convex set of 3×3 density matrices and found, through Monte Carlo simulations, a value of the Ricci curvature as low as 3.00332, so it appears conjecturable that 3 is the actual lower bound.) Thus, our evidence here indicates that the inequality is not satisfied, apparently since all the conditions for its application have not been met. (Using the ansatz elaborated upon earlier in Section 1.3, we also found numerically for the average and WY monotone metrics that the lower bound of $N = 14$ on the Ricci tensor was violated.)

7.3.1. Area/volume ratios

Let us also note here (cf. [16, Section 6]), in terms of the known values [14] and our conjectures, that for the separable *plus* nonseparable states, the ratio of the SD 14-dimensional hyperarea to the SD 15-dimensional volume, is

$$\frac{B_{\mathrm{SD}}^{s+n}}{V_{\mathrm{SD}}^{s+n}} = \frac{8192}{429\pi} \approx 6.07831 \tag{27}$$

while for only the separable states, it is

$$\frac{B_{\mathrm{SD}}^{s} + \beta_{\mathrm{SD}}}{V_{\mathrm{SD}}^{s}} = \frac{98}{13} \approx 7.53846. \tag{28}$$

8. Concluding remarks

Needless to say, to the extent any of the conjectures above are, in fact, valid ones, their remains the apparently formidable task of finding formal/rigorous proofs.

A direct/naive "brute force" strategy of *symbolically* integrating the volume elements of the various monotone metrics over the 15-dimensional convex sets of separable and all two-qubit states —while successful for lower-dimensional scenarios [8]— appears to be quite impractical computationally speaking. It seems that one would have to deal with multiple ranges of integration given by fourth-degree polynomials. One might speculate that the integration of the (product) measures for the volume elements of monotone metrics over the 12 parameterizing Euler angles would yield a result simply proportional to σ_{Ag}, common to all monotone metrics, and that additional distinguishing factors would appear from integrating over the final three variables ($\theta_1, \theta_2, \theta_3$ in the notation of [4]) parameterizing the eigenvalues of the 4×4 density matrices.

Perhaps, in this regard, the work of Sommers and Życzkowski [14]—which they view "as a contribution to the theory of random matrices"—in constructing a general formula for V_{Bures}^{s+n} for N-level systems, is extendible to (monotone) metrics *other* than the Bures. The volume V_{SD}^{s+n} is known, and we have indicated our conjectures that $V_{\mathrm{KM}}^{s+n} = 64 V_{\mathrm{SD}}^{s+n}$, $V_{\mathrm{avg}}^{s+n} = 25\pi^8/8448$, $V_{\mathrm{GKS}}^{s+n} = \pi^8/1750$ and $V_{\mathrm{max}}^{s+n} = \infty$, but we have no similar conjecture, at the

present, for $V_{\mathrm{W\tilde{Y}}}^{s+n}$. (The Wigner–Yanase metric corresponds to a space of *constant curvature* [52].) But there appears to be no "hint" in the literature as to how one might *formally* derive simply the *separable*—as opposed to separable *plus* nonseparable—volumes for any of the monotone metrics.

In this study, we have conjectured that the volumes of separable two-qubit states is, as measured in terms of several monotone metrics of interest, simple multiples of the silver mean (σ_{Ag}). It is interesting to point out, it seems, that in certain ("phyllotactic") models of the arrangements of (rose) petals, the positions of the petals (in fractions of a full turn) are given by the fractional parts of simple multiples of the *golden* ratio [63, p. 113][64, pp. 122–123] (cf. [65, p. 137]). (Of course, it remains possible that we have been somewhat "overeager" here to find multiple roles for σ_{Ag}. In this regard, a sceptically inclined reader might point out that $2000\sigma_{\mathrm{br}} \approx 6605.55$ is quite close to our sample estimate of 6606.58 (Table 5) for $\beta_{\mathrm{W\tilde{Y}}}$ and $2\sigma_{\mathrm{br}} \approx 6.60555$ approximates our sample estimate of 6.60067 for $B_{\mathrm{a\tilde{v}g}}^s$. Here, $\sigma_{\mathrm{br}} = (3 + \sqrt{13})/2$ is the "bronze mean"[42].)

In this and other papers [4–8,16], attention has been focused on the matter of determining the volumes of quantum states in terms of various monotone metrics. An even more considerable body of work concerned with differential geometric properties of the monotone metrics is devoted to issues of the *scalar curvature* of monotone metrics [52,66,67]. For instance, it has been found that the scalar curvature of the $N \times N$ density matrices D_N is, in terms of the Wigner–Yanase metric, $(1/4)(N^2 - 1)(N^2 - 2)$ [52], while for the Bures metric, it is 24 for $N = 2$ and for general N, no less than $(1/2)(5N^2 - 4)(N^2 - 1)$, which value is assumed for the fully mixed state $(1/N)\mathbf{I}$ [67]. (For the *infinite*-dimensional case of thermal squeezed states, Twamley [68, Eq. (30)] has found the scalar curvature to be given by $-(8(\cosh^2 \beta/4 + 12\sinh^4 \beta/4))/(\cosh^2 \beta/2)$, where the "non-unitary" parameter β corresponds to the inverse temperature.) It would certainly be of interest to find linkages between these two interesting areas of investigation. We note that the *scalar curvature* determines the *asymptotic* behavior of the *volume* of a Riemannian manifold [52] [69, p. 55, Corollary 5.5 and Example 3]. Andai [70, Eq. (1)] has recently presented a formula for the relation between the volume of a geodesic ball centered at the fully mixed state and the scalar curvature there (see also [71, Eq. (29)]).

Our earlier conjecture (3)—in its unadjusted form—as to the exact value of V_{SD}^s had suggested a similar-type conjecture for qubit–*qutrit* pairs [12]. Now that we have found compelling numerical evidence to reject (3) (and replace it by (15)), we obviously must be dubious as to the presumed validity of its qubit–qutrit analogue, but presently lack any notion as to how to replace it. Additionally, our numerical experience so far indicates that it would be extraordinarily difficult to "pinpoint" (accurately estimate) the value of the volume of separable qubit–qutrit pairs, since one would then be proceeding in a (more computationally demanding) much higher dimensional (35 dimensional versus 15 dimensional) space, plus the size of the separable domain one would be estimating would be much smaller relatively speaking (i.e., relatively fewer sampled 6×6 density matrices would be separable vis-á-vis the 4×4 case).

We summarize in Table 6 our present state of presumed knowledge in regard to the various monotone metrics studied here. Of course, one would aspire to find the *functionals* that map an operator monotone function $f_{\mathrm{metric}}(t)$ into V_{metric}^s, $V_{\mathrm{metric}}^{s+n}$, B_{metric}^s, $B_{\mathrm{metric}}^{s+n}$ and β_{metric}.

Table 6
Conjectured values (except for V^{s+n}_{Bures} and B^{s+n}_{Bures}, which are *known*) of $V^s_{\widetilde{\text{metric}}}$, V^{s+n}_{metric}, B^{s+n}_{metric}, $B^s_{\widetilde{\text{metric}}}$ and $\beta_{\widetilde{\text{metric}}}$ for (four times) various monotone metrics, listed in order of increasing volume size, together with the corresponding operator monotone functions and Morozova–Chentsov functions

Metric	$f(t)$	$c(\rho_\mu, \rho_\nu)$	V^s	V^{s+n}	B^s	B^{s+n}	β	$B^s + \beta$
Bures	$\dfrac{1+t}{2}$	$\dfrac{2}{\rho_\mu + \rho_\nu}$	$\dfrac{\sigma_{\text{Ag}}}{3}$	$\dfrac{\pi^8}{5040}$	$\dfrac{43\sigma_{\text{Ag}}}{39}$	$\dfrac{512\pi^7}{135135}$	$\dfrac{55\sigma_{\text{Ag}}}{39}$	$\dfrac{98\sigma_{\text{Ag}}}{39}$
GKS	$\dfrac{t^{t/(t-1)}}{e}$	$\dfrac{e(\rho_\mu/\rho_\nu)^{\rho_\mu/(\rho_\nu-\rho_\mu)}}{\rho_\nu}$	$\dfrac{4\sigma_{\text{Ag}}}{5}$	$\dfrac{\pi^8}{1750}$	?	?	$\dfrac{270\sigma_{\text{Ag}}}{77}$	?
WY	$\dfrac{(\sqrt{t}+1)^2}{4}$	$\dfrac{4}{(\sqrt{\rho_\mu}+\sqrt{\rho_\nu})^2}$	$\dfrac{7\sigma_{\text{Ag}}}{4}$	?	$7735\sigma_{\text{Ag}}$	$\dfrac{262144\pi^7}{45045}$	$15950\sigma_{\text{Ag}}$	$23685\sigma_{\text{Ag}}$
Avg	$\dfrac{1+6t+t^2}{4+4t}$	$\dfrac{4(\rho_\mu + \rho_\nu)}{\rho_\mu^2 + 6\rho_\mu\rho_\nu + \rho_\nu^2}$	$\dfrac{29\sigma_{\text{Ag}}}{9}$	$\dfrac{25\pi^8}{8448}$	$\dfrac{255\sigma_{\text{Ag}}}{16}$	$\dfrac{3437\pi^7}{42075}$	$15\sigma_{\text{Ag}}$	$\dfrac{495\sigma_{\text{Ag}}}{16}$
KM	$\dfrac{t-1}{\log t}$	$\dfrac{\log(\rho_\mu/\rho_\nu)}{\rho_\mu - \rho_\nu}$	$10\sigma_{\text{Ag}}$	$\dfrac{4\pi^8}{315}$	?	?	$\dfrac{616\sigma_{\text{Ag}}}{13}$	?
NI	$\dfrac{2(t-1)^2}{(1+t)(\log t)^2}$	$\dfrac{(\rho_\mu + \rho_\nu)\log^2(\rho_\mu/\rho_\nu)}{2(\rho_\mu - \rho_\nu)^2}$	?	?	?	?	?	?
Maximal	$\dfrac{2t}{1+t}$	$\dfrac{\rho_\mu + \rho_\nu}{2\rho_\mu\rho_\nu}$	∞	∞	∞	∞	∞	∞

For the various denominators, we have the interesting prime decompositions: $5040 = 2^4 \cdot 3^2 \cdot 5 \cdot 7$; $1750 = 2 \cdot 5^3 \cdot 7$; $8448 = 2^8 \cdot 3 \cdot 11$; $315 = 3^2 \cdot 5 \cdot 7$; $135135 = 3^3 \cdot 5 \cdot 7 \cdot 11 \cdot 13$; $42075 = 3^2 \cdot 5^2 \cdot 11 \cdot 17$ and $45045 = 3^2 \cdot 5 \cdot 7 \cdot 11 \cdot 13$. As pertains to numerators: $512 = 2^9$; $7735 = 5 \cdot 7 \cdot 13 \cdot 17$; $262144 = 2^{18}$; $15950 = 2 \cdot 5^2 \cdot 11 \cdot 29$; $255 = 3 \cdot 5 \cdot 17$; $495 = 3^3 \cdot 5 \cdot 11$; $270 = 2 \cdot 3^3 \cdot 5$; and $616 = 2^3 \cdot 7 \cdot 11$.

Acknowledgments

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