Analytic Fits to Separable Volumes and Probabilities for Qubit-Qubit and Qubit-Qutrit Systems

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Abstract

We investigate the possibility of deriving analytical formulas for the 15-dimensional separable volumes, in terms of any of a number of metrics of interest (Hilbert-Schmidt [HS], Bures,...), of the two-qubit (four-level) systems. This would appear to require 15-fold symbolic integrations over a complicated convex body (defined by both separability and feasibility constraints). The associated 15-dimensional integrands — in terms of the Tilma-Byrd-Sudarshan Euler-angle-based parameterization of the $4 \times 4$ density matrices $\rho$ ($J. \ Phys. \ A$ 35 [2002], 10445) — would be the products of 12-dimensional Haar measure $\mu_{Haar}$ (common to each metric) and 3-dimensional measures $\mu_{\text{metric}}$ (specific to each metric) over the 3d-simplex formed by the four eigenvalues of $\rho$. We attempt here to estimate/determine the 3-dimensional integrands (the products of the various [known] $\mu_{\text{metric}}$’s and an unknown symmetric weighting function $W$) remaining after the (putative) 12-fold integration of $\mu_{Haar}$ over the twelve Euler angles. We do this by first fitting $W$, so that the conjectured HS separable volumes and hyperareas ($Phys. \ Rev. \ A$ 71 [2005], 052319; cf. quant-ph/0609006) are reproduced. We further evaluate a number of possible such choices of $W$ by seeing how well they also yield the conjectured separable volumes for the Bures, Kubo-Mori, Wigner-Yanase and (arithmetic) average monotone metrics and the conjectured separable Bures hyperarea ($J. \ Geom. \ Phys.$ 53 [2005], 74, Table VI). We, in fact, find two such exact (rather similar) choices for $W$ that give these five conjectured (non-HS) values all within 5%. In addition to the above-mentioned Euler angle parameterization of $\rho$, we make extensive use of the Bloore parameterization ($J. \ Phys. \ A$ 9 [1976], 2059) in a companion set of two-qubit separability analyses.

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I. INTRODUCTION

In a pair of major, skillful papers, making use of the theory of random matrices \[1\], Sommers and \(\dot{Z}\)yczkowski were able to derive explicit formulas for the volumes occupied by the \(d = (n^2 - 1)\)-dimensional convex set of \(n \times n\) (complex) density matrices (as well as the \(d = \frac{(n-1)(n+1)}{2}\)-dimensional convex set of real \(n \times n\) density matrices), both in terms of the Hilbert-Schmidt (HS) metric \[2\] — inducing the flat, Euclidean geometry — and the Bures metric \[3\] (cf. \(4\)). (These results are also more lately discussed in the highly comprehensive new text of Bengtsson and \(\dot{Z}\)yczkowski \[5,\ chap. 14\].) Of course, it would be of obvious considerable quantum-information-theoretic interest in the cases that \(n\) is a composite number, to also obtain HS and Bures volume formulas restricted to those states that are separable — the sum of product states — in terms of some factorization of \(n\) \[6\]. Then, by taking ratios — employing these Sommers-\(\dot{Z}\)yczkowski results — one would obtain corresponding separability probabilities.

In particular, again for the 15-dimensional complex case, \(n = 4 = 2 \times 2\), numerical evidence has been adduced that the Bures volume of separable states is (quite elegantly) \(2^{-15}(\sqrt{2} - 1) \approx 4.2136 \cdot 10^{-6}\) [7, Table VI] and the HS volume \((5\sqrt{3})^{-7} \approx 2.73707 \cdot 10^{-7}\) [8, eq. (41)]. Then, taking ratios (using the Sommers-\(\dot{Z}\)yczkowski results \[2, 3\]), we have the derived conjectures that the Bures separability probability is \(\frac{1680(\sqrt{2} - 1)}{\pi^8} \approx 0.0733389\) and the HS one, considerably larger, \(\frac{2^2 \cdot 3^2 \cdot 11 \cdot 13 \cdot \sqrt{3}}{5^8 \cdot \pi^6} \approx 0.242379\) [8, eq. (43), but misprinted as \(5^3\) not \(5^4\) there]. (Szarek, Bengtsson and \(\dot{Z}\)yczkowski — motivated by the numerical findings of \[8, 9\] — have recently formally demonstrated “that the probability to find a random state to be separable equals 2 times the probability to find a random boundary state to be separable, provided the random states are generated uniformly with respect to the Hilbert-Schmidt (Euclidean) distance. An analogous property holds for the set of positive-partial-transpose states for an arbitrary bipartite system” \[10\] (cf. \[11\]). (“Since our reasoning hinges directly on the Euclidean geometry, it does not allow to predict any values of analogous ratios computed with respect to Bures measure, nor other measures” \[10,\ p. L125\].) These three authors also noted \[10,\ p. L125\] that “one could try to obtain similar results for a general class of multipartite systems”. In this latter vein, numerical analyses of ours give some [but certainly not yet conclusive] indication that for the three-qubit triseparable states, there is an analogous probability ratio of 6 — rather than 2.)
However, the analytical derivation of (conjecturally) exact formulas for these HS and Bures (as well as other, such as the Kubo-Mori [12] and Wigner-Yanase [8, 13]) separable volumes still appears to be quite remote (cf. [14]) — the only such progress to report so far being certain exact formulas when the number of dimensions of the 15-dimensional space of $4 \times 4$ density matrices has been severely curtailed (nullifying or holding constant most of the 15 parameters) to $d \leq 3$ [15, 16] (cf. [17]). Most notably, in this research direction, in [16, Fig. 11], we were able to find a highly interesting/intricate (one-dimensional) continuum ($-\infty < \beta < \infty$) of two-dimensional (the associated parameters being $b_1$, the mean, and $\sigma_q^2$, the variance of the Bell-CHSH observable) HS separability probabilities, in which the golden ratio [18] was featured, among other items. (The associated HS volume element $\frac{1}{32\beta(1+\beta)}d\beta db_1d\sigma_q^2$ is independent of $b_1$ and $\sigma_q^2$ in this three-dimensional scenario. Extensions to higher-dimensional scenarios $d > 3$ appear problematical, though.) Further, in [15], building upon work of Jakóbczyk and Siennicki [19], we obtained a remarkably wide-ranging variety of exact HS separability ($n = 4, 6$) and PPT (positive partial transpose) ($n = 8, 9, 10$) probabilities based on two-dimensional sections of sets of (generalized) Bloch vectors corresponding to $n \times n$ density matrices.

In this paper we are able to report some additional progress in these directions. We obtain exact formulas for certain $d = 4$, $n = 4$ scenarios and upper bounds for $d = 7$ and $d = 9$ instances. (Nevertheless, the full $d = 9$ and/or $d = 15$, $n = 4$ real and complex scenarios still appear quite daunting — due to the numerous separability constraints at work, some being active [binding] in certain regions and in complementary regions, inactive [nonbinding]. “The geometry of the 15-dimensional set of separable states of two qubits is not easy to describe” [10, p. L125].)

To proceed initially (secs. III, IV, V), we employ the (quite simple) form of parameterization of the density matrices put forth by Bloore [20] some thirty years ago. (Of course, there are several other possible parametrizations [21, 22, 23, 24, 25, 26, 27], a number of which we have also utilized in various studies [28, 29] to estimate volumes of separable states. Our greatest progress at this stage, in terms of increasing dimensionality, has been achieved with the Bloore parameterization — due to a certain computationally attractive feature of it, allowing us to decouple diagonal and non-diagonal parameters — as detailed shortly below.)

In our final (quite differently structured) series of analyses (sec. V), though, we employ not the Bloore parameterization, but the Euler-angle-based one of Tilma, Byrd and
Sudarshan [23]. Our motivation here is to bypass/circumvent the necessity of the putative-achievability, but computationally daunting first twelve steps (over the twelve Euler angles) of a 15-fold integration. (“we would like to derive a subset of the ranges of the Euler angle parameters...dividing the 15-parameter space into entangled and separable subsets. Unfortunately, due to the complicated nature of the parameterization, both numerical and symbolic calculations of the eigenvalues of the partial transpose...have become computationally intractable using standard mathematical software” [23, p. 10453].) We seek to find the three-dimensional (weighting) function $W(\lambda_1, \lambda_2, \lambda_3, \lambda_4)$ of the four eigenvalues ($\lambda_4 = 1 - \lambda_1 - \lambda_2 - \lambda_3$) which would yield our various conjectured 15-dimensional separable volumes and 14-dimensional separable hyperareas for the two-qubit systems. In sec. VI, we also apply this approach exploratorily to the $n=6, d=35$ case of qubit-qutrit pairs, seeking to find a suitable 5-dimensional weighting function $W_{n=6}(\lambda_1, \lambda_2, \lambda_3, \lambda_4, \lambda_5, \lambda_6)$.

Let us also point out to the reader, our even more recent companion-type study [30], in which solely for the (relatively simple) Hilbert-Schmidt (non-monotone) metric, are we able (making use of the Bloore parameterization) to reduce the two-qubit (both real and complex) separable volume determination problems to those of finding one-dimensional weighting functions (which turned out to be well-approximated by certain incomplete beta functions — functions of the ratio $\frac{\rho_{11}\rho_{44}}{\rho_{22}\rho_{33}}$ of diagonal entries of the $4 \times 4$ density matrices $\rho$).

II. BLOORE PARAMETERIZATION OF THE DENSITY MATRICES

The main presentation of Bloore [20] was made in terms of the $3 \times 3$ ($n = 3$) density matrices. It is clearly easily extendible to cases $n > 3$. The fundamental idea is to scale the off-diagonal elements ($\rho_{ij}, i \neq j$) of the density matrix in terms of the square roots of the diagonal entries ($\rho_{ii}$). That is, we set (introducing the new [Bloore] variables $z_{ij}$),

$$\rho_{ij} = \sqrt{\rho_{ii}\rho_{jj}} z_{ij}. \quad (1)$$

This allows the determinant of $\rho$ (and analogously all its principal minors) to be expressible as the product ($|\rho| = AB$) of two factors, one ($A$) of which is itself simply the product of (positive) diagonal entries ($\rho_{ii}$) and the other — in the $n = 4$ case under investigation here (easily extendible from the case of real density matrices to complex ones) —

$$B = (z_{34}^2 - 1) z_{12}^2 + 2 (z_{14} (z_{24} - z_{23} z_{34}) + z_{13} (z_{23} - z_{24} z_{34})) z_{12} - z_{23}^2 - z_{24}^2 - z_{34}^2 + \quad (2)$$
\[ z_{14}^2 (z_{23}^2 - 1) + z_{13}^2 (z_{24}^2 - 1) + 2z_{23}z_{24}z_{34} + 2z_{13}z_{14}z_{34} - z_{12}z_{13}z_{24} + 1, \]

involving (only) the \( z_{ij} \)'s \((i \neq j)\) [20, eqs. (15), (17)]. Since, clearly, the factor \( A \) is positive in all nondegenerate cases \((\rho_{ii} \geq 0)\), one can — by only analyzing \( B \) — essentially ignore the diagonal entries (and thus reduce by \((n - 1)\)) the dimensionality of the problem of finding nonnegativity conditions to impose on \( \rho \). This is the feature we will seek to maximally exploit here.

It is, of course, necessary and sufficient for \( \rho \) to serve as a density matrix (that is, an Hermitian, nonnegative definite, trace one matrix) that all its principal minors be nonnegative [31]. The condition — quite natural in the Bloore parameterization — that all the principal \( 2 \times 2 \) minors be nonnegative requires simply that \(-1 \leq z_{ij} \leq 1, i \neq j \). The joint conditions that all the principal minors be nonnegative are not as readily apparent. But for the 9-dimensional real case \( n = 4 \) — that is, \( \Re(\rho_{ij}) = 0 \) — we have been able to obtain one such set, using the Mathematica implementation of the cylindrical algorithm decomposition [32]. (The set of solutions of any system of real algebraic equations and inequalities can be decomposed into a finite number of “cylindrical” parts [33].) Applying it, we were able to express the conditions that an arbitrary 9-dimensional \( 4 \times 4 \) real density matrix \( \rho \) must fulfill. These took the form, \( z_{12}, z_{13}, z_{14} \in [-1, 1] \) and

\[
 \begin{align*}
 z_{23} & \in [Z_{23}, Z_{23}^+], \\
 z_{24} & \in [Z_{24}, Z_{24}^+], \\
 z_{34} & \in [Z_{34}, Z_{34}^+],
\end{align*}
\]

(3)

where

\[
\begin{align*}
 Z_{23}^+ = z_{12}z_{13} & \pm \sqrt{1 - z_{12}^2} \sqrt{1 - z_{13}^2} , \\
 Z_{24}^+ = z_{12}z_{14} & \pm \sqrt{1 - z_{12}^2} \sqrt{1 - z_{14}^2}, \\
 Z_{34}^\pm = z_{13}z_{14} - z_{12}z_{14}z_{23} & - z_{12}z_{13}z_{24} + z_{23}z_{24} \pm s, \\
 s = \sqrt{1 + z_{12}^2 + z_{13}^2 - 2z_{12}z_{13}z_{23} + z_{23}^2} \sqrt{1 + z_{12}^2 + z_{14}^2 - 2z_{12}z_{14}z_{24} + z_{24}^2}.
\end{align*}
\]

(4)

Making use of these results, we were able to confirm via exact symbolic integrations, the (formally demonstrated) result of \( \acute{Z} \)yczkowski and Sommers [2] that the HS volume of the real two-qubit \((n = 4)\) states is \( \frac{\pi^4}{60480} \approx 0.0016106 \). (This result was also achievable through a somewhat different Mathematica computation, using the implicit integration feature first introduced in version 5.1. That is, the only integration limits employed were that \( z_{ij} \in \)
[-1, 1], i ≠ j — broader than those in (3) — while the Boolean constraints were imposed that the determinant of ρ and one [all that is needed to ensure nonnegativity] of its principal 3 × 3 minors be nonnegative.

However, when we tried to combine these integration limits (3) with the (Peres-Horodecki [34, 35, 36] n = 4) separability constraint that the determinant (C = |ρPT|) of the partial transpose of ρ be nonnegative [37, Thm. 5], we exceeded the memory availabilities of our workstations. In general, the term C — unlike the earlier term B — unavoidably involves the diagonal entries (ρii), so the dimension of the accompanying integration problems must increase — in the 9-dimensional real n = 4 case from 6 to 9.

A. Restricting diagonal entries

Nevertheless, we found that by imposing the condition that the four diagonal entries (ρii, i = 1, . . . , 4) fall into two equal pairs (say, ρ11 = ρ22 and ρ33 = ρ44, so that ρ33 = (1−2ρ11)/2), the determinant (C) of the partial transpose could now be expressed as the product

\[ C = |ρ_{PT}| = \frac{1}{4} (1 - 2ρ_{11})^2 ρ_{11}^2 D, \quad 0 ≤ ρ_{11} ≤ \frac{1}{2}, \quad (6) \]

where

\[ D = \left( z_{24}^2 - 1 \right) z_{13}^2 + 2z_{23} (z_{34} - z_{14}z_{24}) z_{13} - z_{24}^2 - z_{34}^2 + \]

\[ (z_{14} - 1) (z_{14} + 1) (z_{23} - 1) (z_{23} + 1) + 2z_{14}z_{24}z_{34} + \]

\[ (z_{34}^2 - 1) z_{12}^2 + 2 (z_{13}z_{14} + z_{23}z_{24} - (z_{14}z_{23} + z_{13}z_{24}) z_{34}) z_{12}. \quad (7) \]

Thus, the term D (like B in (2)) is itself independent of the diagonal entries of ρ (in particular, the specific value of ρ11) — allowing us to proceed, as indicated, with integrations in a lower-dimensional (d ≤ 7) setting. (This same form of factorizability takes place, as well, for all the [four] 3 × 3 and [six] 2 × 2 minors of ρPT.) If we can further guarantee the nonnegativity of D — in addition to that of B — we can ensure separability of ρ. Let us also note that

\[ B - D = 2(z_{14} - z_{23})(z_{13} - z_{24})(z_{12} - z_{34}). \quad (8) \]

(So, if any of the three factors in (8) are zero, the associated state must be separable.)

We will now proceed to some specific analyses within this more restrictive framework (7-dimensional in nature, since we started with the 9-dimensional real setting and have essentially only one free diagonal parameter [ρ11] left).
III. 7-DIMENSIONAL REAL SETTING \((\rho_{11} = \rho_{22}, \rho_{33} = \rho_{44})\)

A. 7-dimensional analysis

The associated 7-dimensional HS volume of all these states (separable and nonseparable) is \(\frac{\pi^2}{15120} \approx 0.000652752\). The six principal \(2 \times 2\) minors of the partial transpose simply yield the (Bloore) conditions that \(z_{ij} \in [-1,1]\), so nothing can be gained — in terms of obtaining upper bounds on the separable volume — by using the nonnegativity of these six minors as further constraints in our integrations. However, if we require that one of the \(3 \times 3\) principal minors of the partial transpose be nonnegative, we do succeed in obtaining a nontrivial upper bound of \(\frac{\pi^4}{172032} \approx 0.000566227\) on the 7-dimensional volume of separable states. So, we have a derived upper bound (probably rather weak, we surmise) on the HS separability probability for our 7-dimensional real set of \(4 \times 4\) density matrices of \(\frac{45\pi^2}{312} \approx 0.867446\).

B. 4-dimensional analyses

1. \(z_{12} = z_{23} = z_{24} = 0\)

Here, we set the three indicated Bloore parameters to zero. (So, the four free parameters of the initial seven are \(\rho_{11}, z_{13}, z_{14}\) and \(z_{34}\).) Then, using the implicit integration feature of Mathematica (rather than the limits \(\overline{3}\)), we were able to obtain for the total HS volume \(\frac{\pi^2}{384} \approx 0.0257021\) and (further adding the separability constraint that \(D\), given by \(\overline{7}\), be greater than 0) the separable volume of \(\frac{4+\pi^2}{1536} \approx 0.00902969\). Taking the appropriate quotient, we find for the HS separability probability for this scenario (quite elegantly), \(\frac{4+\pi^2}{4\pi^2} \approx 0.351321\).

2. \(z_{23} = 0, z_{24} = 0, z_{34} = 0\)

Now, \(HS^{tot}_{vol} = \frac{\pi}{144} \approx 0.0218166\) and \(HS^{sep}_{vol} = \frac{4+\pi^2}{1536} \approx 0.00902969\), so
\[
HS_{sepprob} = \frac{HS^{sep}_{vol}}{HS^{tot}_{vol}} = \frac{3(4+\pi^2)}{32\pi} \approx 0.413891.
\]

There are twenty possible 4-dimensional scenarios. Of these four each have one of these two nontrivial HS separability probabilities \(\frac{4+\pi^2}{4\pi^2}\) or \(\frac{3(4+\pi^2)}{32\pi}\). For the remaining twelve cases, the HS separability probabilities are simply 1.
C. 3-dimensional analyses

We also observe that for the fifteen possible 3-dimensional scenarios, all the HS separability probabilities are (trivially) 1. (Eight of these scenarios have HS total volume equal to $\frac{\pi^2}{128}$, four, $\frac{\pi}{48}$ and three $\frac{1}{12}$.)

D. 5-dimensional analyses

For all twelve possible scenarios, setting two $z_{ij}$'s to zero, the total HS volume of states is $\frac{\pi^2}{1440} \approx 0.00685389$.

1. $z_{23} = z_{24} = 0$

To compute the separable HS volume we had to resort to numerical means, obtaining 0.00532303, for a separability probability of 0.776643. (This is also the probability for the 5-dimensional scenario $z_{12} = z_{13} = 0$ — and [at least] five others.)

2. $z_{14} = 0 = z_{23} = 0$

Here, as indicated, the total HS volume is $\frac{\pi^2}{1440} \approx 0.00685389$. This is also the separable volume — since $B = D$ in this case. (This is also the situation with the scenarios $z_{13} = z_{24} = 0$ and $z_{12} = z_{34} = 0$.)

IV. 9-DIMENSIONAL REAL CASE

As previously mentioned, we know from the Sommers-Życzkowski analyses \[2\] that the HS volume of the 9-dimensional convex set of real $4 \times 4$ density matrices is $\frac{\pi^4}{60480} \approx 0.0016106$. (In this section — to fully accord with their results \[2\] — we have to adjust by an overall scaling factor of $2^4 = 16$ the results of our usual integration procedure employed previously in this study, in which we simply employed 1 as our integrand, rather than some other constant. This scaling, of course, does not have any impact on separability probabilities.) We can also computationally verify the Sommers-Życzkowski HS volume formula in either of two manners: (a) employing the integration limits \[3\] obtained by application of the cylindrical
decomposition algorithm or (b) implementing the implicit integration feature (requiring here that the determinant of \( \rho \) and one of its \( 3 \times 3 \) principal minors be nonnegative) of Mathematica, using for the integration limits simply that \(-1 \leq z_{ij} \leq 1\) for all \( i \neq j \). We investigated how far we could proceed in the full 9-dimensional \( n = 4 \) real case, by imposing increasingly greater requirements (corresponding to the Peres-Horodecki criterion \([34, 35]\)) that would need to be fulfilled for \( \rho_{PT} \) to be nonnegative definite. Now, of the six \( 2 \times 2 \) principal minors of \( \rho_{PT} \), only two are distinct from the six such minors of \( \rho \) itself. If we demand that, in addition, to the feasibility constraints on \( \rho \) that one of these two minors be nonnegative we obtain (to high precision) 0.0014242052589 yielding an upper bound on the HS separability probability of the 9-dimensional real two-qubit states of 0.88426997055. Further (tighter) numerical results — using additional principal minors of \( \rho_{PT} \) (even the remaining \( 2 \times 2 \) nonredundant one) — proved difficult to achieve, however.

V. 3-DIMENSIONAL WEIGHT FOR THE FULL 15-DIMENSIONAL PROBLEM

The direct straightforward (“brute force”) computations by symbolic means of the 15-dimensional separable volumes (for any of a wide variety of metrics) of the (complex) two-qubit states seem to far exceed present workstation capabilities. Nevertheless, we will here try to gain some analytical insight into these formidable problems.

Let us first note that the computation of the separable volumes could be seen to require the evaluation (in which the Peres-Horodecki separability and feasibility criteria are both enforced) of a 15-fold integral. Following the innovative Euler-angle-based parameterization of \( 4 \times 4 \) density matrices of Tilma, Byrd and Sudarshan \([23]\), the first twelve variables over which to integrate can be taken to be the twelve Euler angles \((\alpha_i, i = 1, \ldots, 12)\) and the last three to be the eigenvalues \( \lambda_1, \lambda_2, \lambda_3 \) of the density matrix \( \rho \). (Of course, \( \Sigma_{i=1}^4 \lambda_i = 1. \) Now for any of the metrics of interest, the associated 15-dimensional integrand can be represented as the product of a 12-dimensional Haar measure \((\mu_{Haar})[23, eq. (34)]\) (common to all the metrics of interest) over the twelve Euler angles

\[
\mu_{Haar} = \cos(\alpha_4)^3 \cos(\alpha_6) \cos(\alpha_{10}) \sin(2\alpha_2) \sin(\alpha_4) \sin(\alpha_6)^5 \sin(2\alpha_8) \sin(\alpha_{10})^3 \sin(2\alpha_{12}) d\alpha_1 ... d\alpha_{12}
\]

\((0 \leq \alpha_{even} \leq \frac{\pi}{2}, 0 \leq \alpha_{odd} \leq \pi)[23, eq. (47)]\) and a 3-dimensional metric-specific measure \((\mu_{metric})\) over the eigenvalues (cf. \([38]\)). (So, if the Peres-Horodecki criterion is not enforced,
we simply obtain the [known in the Bures and HS cases] volumes of the separable and nonseparable states, the volumes decomposing into the products of the results of 3-fold and 12-fold integrations \[\text{eq. (3.7)}, \text{eq. (3.17)}\].

Consequently, after the first twelve steps of the (presumptively theoretically achievable, but apparently totally impractical) integrations for the separable volumes, we can imagine obtaining three-dimensional integration problems (over the three-dimensional simplex of eigenvalues). The integrands of the problem would now be the products of \(\mu_{\text{metric}}\) and a common three-dimensional weighting function \(W\), acquired during the course of the 12-fold integration. Certainly, \(W\) should be a symmetric function of the four eigenvalues.

A. First analysis

We will try to fit \(W\) to our various conjectures for the separable volumes, previously obtained by numerical methods. In particular, we have found (after some limited trial and error) that the (symmetric) choice (being neither a convex nor a concave function, we observed — nor even approximately so),

\[
W(\lambda_1, \lambda_2, \lambda_3, \lambda_4) = 6086(\lambda_1\lambda_2\lambda_3 + \lambda_1\lambda_2\lambda_4 + \lambda_1\lambda_3\lambda_4 + \lambda_2\lambda_3\lambda_4)^{\frac{53}{20}}, \tag{10}
\]

reproduces the conjectures for both the Hilbert-Schmidt volumes and hyperareas of the separable two-qubit states to good accuracy (0.01643%). (These conjectured volume and hyperarea are \((5\sqrt{3})^{-7} \approx 2.73707 \cdot 10^{-7}\) and \((3^{256})^{-1} \approx 7.1111 \cdot 10^{-6}\), respectively \[\text{eqs. (41), (42)}\].) For the computation of the 14-dimensional separable hyperarea, the weighting function \(W\) reduces (since we can take \(\lambda_4 = 0\)) to

\[
W(\lambda_1, \lambda_2, \lambda_3) = 6086(\lambda_1\lambda_2\lambda_3)^{\frac{53}{20}}. \tag{11}
\]

Now, the acid test of the legitimacy/validity of our choice of weighting function — and the raison d’être of our exercise — is to see how well (in addition to the separable Hilbert-Schmidt volumes and hyperareas (which we constructed to satisfy the Szarek-Bengtsson-Zyczkowski two-fold ratio \[10\]) it reproduces (our presumptively correct) conjectures for metrics other than the Hilbert-Schmidt one.

For the Bures (minimal monotone) metric, we found that the use of the weighting function \(W\) — coupled with \(\mu_{\text{Bures}}\) — predicted a separable volume 0.938275 times the magnitude of the conjectured value of \(2^{-15}(\frac{\sqrt{3}-1}{3}) \approx 4.2136 \cdot 10^{-6}\). For the Kubo-Mori monotone
metric, we obtained an estimate that is $0.910768 \times$ the magnitude of the conjectured value of $2^{-15}(10(\sqrt{2} - 1)) \approx 0.000126408$, for the (arithmetic) average monotone metric, $0.903281$ times the magnitude of the conjectured value of $2^{-15}(\frac{29}{9}(\sqrt{2} - 1)) \approx 0.0000407314$, and for the Wigner-Yanase monotone metric, $0.919585$ times the conjectured value of $2^{-15}(\frac{7}{4}(\sqrt{2} - 1)) \approx 0.0000221214$. So, our choice of $W$ works rather well, at least for a first simply heuristic effort. (In [7], we also had additional volume conjectures for the GKS (Grosse-Krattenthaler-Slater) (“quasi-Bures”) monotone metric (cf. [41]). However, we encountered numerical difficulties in trying to analyze it here, in the fashion of the other metrics.)

If we try, as well, to predict the 14-dimensional separable hyperarea for the Bures metric using (11), we obtain an estimate of $0.0000262122$, which is $0.940364$ times as large as the conjectured value of $2^{-14}(\frac{43(\sqrt{2} - 1)}{39}) \approx 0.0000278746$ [7, Table VI]. (For the Kubo-Mori metric, we also obtain an estimate of the separable hyperarea of $0.0000399861$ and of the separable probability of a state on the 14-dimensional boundary of $0.0214689$ — but there were no prior conjectures for these quantities in [7, Table VI]. For the arithmetic average metric, our estimate of the separable hyperarea is $0.738784$, while our conjecture in [7, Table VI] [to be corrected by a factor of 8 as noted in [8, p. 1-11]] amounts to $2^{-14}(\frac{255(\sqrt{2} - 1)}{128}) \approx 0.825191$.)

B. Further analyses — exact weighting functions

We, then, altered our analytical strategy somewhat and succeeded (twice) in reproducing our five indicators — the Bures, Kubo-Mori, Wigner-Yanase and (arithmetic) average separable volumes and the Bures hyperarea — all now within $5\%$ of their conjectured values. We accomplished this by exactly fitting (by finding the values for $a$ and $b$) the conjectured HS separable volume and separable hyperarea to weighting functions of the form (and their $\lambda_4 = 0$ reductions),

$$W(\lambda_1, \lambda_2, \lambda_3, \lambda_4) = a(\sum_{i<j}^4 \lambda_i \lambda_j)^{m_1} + b(\sum_{i<j<k}^4 \lambda_i \lambda_j \lambda_k)^{m_2}.$$ (12)

We conducted separate analyses for pairs of low integral values of the exponents ($1 \leq m_1, m_2 \leq 4$). For $m_1 = 3, m_2 = 3$ we had the results

$$a = \frac{325909584\sqrt{3}}{464375\pi^6} \approx 1.26422, \quad b = \frac{5070990172248\sqrt{3}}{464375\pi^6} \approx 19673.7$$ (13)
\( \left( \frac{b}{a} = \frac{31119}{2} \right) \), and for \( m_1 = 4, m_2 = 3 \),
\[
a = \frac{8834477652\sqrt{3}}{3109375\pi^6} \approx 5.11881, b = \frac{33503284082268\sqrt{3}}{3109375\pi^6} \approx 19412.2
\]  
\( \left( \frac{b}{a} = \frac{11377}{3} \right) \). (Numerical tests showed that neither of these two functions was Schur-convex nor Schur-concave \([42]\), nor even approximately so.) As indicated, for both these settings of \([12]\), our five (non-HS) indicators all lay within at most 5\% of their conjectured values \([7]\). (Additionally, the estimated arithmetic average separable hyperarea lay within 5\% of the conjectured value for the \( m_1 = 4, m_2 = 3 \) case, and 10\% for the other. Since the two functions both fit the conjectured separable HS volume and hyperarea, any linear combination of them will also. We have found that by weighting the function associated with \([13]\) by 0.570347, and the other function by 0.429653, there is no deviation in the associated non-HS indicators by more than 3.61\%.) The closeness of our estimates to their conjectured values, certainly it would seem, should lend some further support (beyond the original numerical evidence \([7, 8]\)) for the reasonableness of the associated conjectures.

Of course, it behooves us and possibly other interested researchers, at this stage, to explore the properties (and desirably derive guiding principles) of additional candidates for the presumptive three-dimensional weighting function \( W \). (We are compelled to note, however, that contrary to our construction of \( W \) so far, that it is clear that \( W \) has to be simple flat in some finite neighborhood of the fully mixed state \( \lambda_1 = \lambda_2 = \lambda_3 = \lambda_4 = \frac{1}{4} \) \([43]\) \( \text{sec. 15.5} \). So, it seems that \( W \) needs to be defined in a piecemeal manner over differing domains (cf. \([16]\)).)

VI. 5-DIMENSIONAL QUBIT-QUTRIT WEIGHTING FUNCTION

Proceeding analogously to our (first) analysis in sec. \( VA \) for the two-qubit case \( n = 4 \), we sought to obtain a 5-dimensional weighting function \( W_{n=6} \) for the qubit-qutrit case \( n = 6 \). Using the conjectures — based on extensive numerical results — stated in \([8]\) sec. VI.D.2], in particular, those for the Hilbert-Schmidt separable volume and separable hyperarea of the 35-dimensional convex set of 6 \times 6 density matrices (conjectured to be \((2^{45} \cdot 3 \cdot 5^{13} \cdot 7 \sqrt{30})^{-1} \approx 2.02423 \cdot 10^{-25} \) and \((2^{46} \cdot 3 \cdot 5^{12})^{-1} \approx 1.94026 \cdot 10^{-23} \), respectively), we fitted the weighting function (reproducing the HS separable volume to very high accuracy
and the hyperarea to an accuracy of .7%),

\[ W_{n=6}(\lambda_1, \lambda_2, \lambda_3, \lambda_4, \lambda_5, \lambda_6) = 986304. (\Sigma_{i<j<k<l<m}^6 \lambda_i \lambda_j \lambda_k \lambda_l \lambda_m)^{\frac{2}{n}}. \]  \hspace{1cm} (15)

Now, in applying this to the Bures metric, we derived an estimate of the 35-dimensional Bures volume that was 1.82587 times as large as the conjectured value of \(2^{-77} \cdot 3 \sqrt{8642986} \pi \approx 1.03447 \cdot 10^{-19}\) [7, eq. (32)]. Our estimate of the 34-dimensional Bures hyperarea was 1.91223 times as large as the conjectured value of \(2^{43} \cdot 3 \cdot 5 \sqrt{8462986} \pi \approx 1.45449 \cdot 10^{-18}\) [8, eq. (33)].

Though, somewhat disappointingly large, these two early results are certainly of the same order of magnitude as the conjectures (and the underlying supporting numerical evidence), and suggest additional research.

\section*{VII. REMARKS}

We have sought to determine a certain 3-dimensional weighting function by fitting the conjectured values of the Hilbert-Schmidt separable 15-dimensional volume and 14-dimensional hyperarea [8, eqs. (41), (42)]. It would be of interest to attempt to fit additional conjectured values as well (such as those for the Bures [minimal monotone] metric). (No conjecture is presently available for the HS separable hyperarea of the 11-dimensional space spanned by the rank-2 density matrices. Otherwise it could be incorporated into our further analyses too — if the weighting function did not degenerate with two zero eigenvalues present, and if the corresponding 11-dimensional separable hyperarea is not actually zero [cf. [44] [8, sec. VI.C.4]].)

Let us — as was done in [10] — bring to the reader's attention some other studies, such as [45, 46, 47, 48, 49] pertaining to volumes of sets of separable and/or positive-partial-transpose states, as well as our more recent analysis [30], concerning the Hilbert-Schmidt metric. (It becomes quite clear in this last study, that the separability constraint on two-qubit systems is, in general, \textit{quartic} in nature (cf. [50, 51]), thus, to some extent, explaining the associated difficulties in enforcing it — as well as raising certain interesting topological questions (cf. [52]).)

In conclusion, let us also make reference to a certain capsule review [14] in the database MathSciNet of our previous paper [7] in this journal. In particular, we add emphasis to the final sentence of the review, devising a response to which comment has been the main
motivation of this paper, as well as that of [30].

“The paper concerns properties of the convex set of separable two-qubit states. Although the positive partial transpose criterion gives in this very case a concrete answer to the question of whether a given mixed state is separable, the geometry of the 15-dimensional set $S$ of separable states is still not well understood.

The author analyzes numerically the volume of the set $S$ with respect to measures induced by several monotone metrics. In particular, he studies the one-parameter family of metrics interpolating between the maximal and the minimal (Bures) metrics.

Working with the Bures measure he conjectures that the relative volume of the set of separable states is equal to the silver mean, $\sigma = \sqrt{2} - 1$. In a similar way the volume of the 14-dimensional hyperarea of $S$ is estimated with respect to various measures, and the ratios area/volume are analyzed.

The conjectures of Slater, based on numerical integration, still await analytical confirmation.”

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