Volumes and Hyperareas of the Spaces of Separable and Nonseparable Qubit-Qutrit Systems: Initial Numerical Analyses

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Abstract

Paralleling our recent computationally-intensive work for the case \( N = 4 \) (quant-ph/0308037), we undertake the task for \( N = 6 \) of computing to high numerical accuracy, the formulas of Sommers and Życzkowski (quant-ph/0304041) for the \((N^2 - 1)\)-dimensional volume and \((N^2 - 2)\)-dimensional hyperarea of the (separable and nonseparable) \( N \times N \) density matrices, based on the Bures (minimal monotone) metric. At the same time, we estimate the unknown volumes and hyperareas based on a number of other monotone metrics of interest. Additionally, we estimate — but with perhaps unavoidably diminished accuracy — all these volume and hyperarea quantities, when restricted to the “small” subset of \( 6 \times 6 \) density matrices that are separable (classically correlated) in nature. The ratios of separable to separable plus nonseparable volumes, then, yield corresponding estimates of the “probabilities of separability”. We are particularly interested in exploring the possibility that a number of the various 35-dimensional volumes and 34-dimensional hyperareas, possess exact values — which we had, in fact, conjectured to be the case for the qubit-qubit systems \( (N = 4) \), with the “silver mean”, \( \sqrt{2} - 1 \), appearing to play a fundamental role as regards the separable states.

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I. INTRODUCTION

In a recent highly comprehensive analysis [1] (cf. [2]), Sommers and Życzkowski obtained “a fairly general expression for the Bures volume of the submanifold of the states of rank \(N - n\) of the set of complex \((\beta = 2)\) or real \((\beta = 1)\) \(N \times N\) density matrices

\[
S_{N,n}^{(\beta)} = 2^{-d_n} \frac{\pi^{(d_n+1)/2}}{\Gamma((d_n + 1)/2)} \prod_{j=1}^{N-n} \frac{\Gamma(j\beta/2)\Gamma[1 + (2n + j - 1)\beta/2]}{\Gamma[(n + j)\beta/2]\Gamma[1 + (n + j - 1)\beta/2]},
\]

(1)

where \(d_n = (N - n)[1 + (N + n - 1)\beta/2] - 1\) represents the dimensionality of the manifold . . . for \(n = 0\) the last factor simply equals unity and (1) gives the Bures volume of the entire space of density matrices, equal to that of a \(d_0\)-dimensional hyper-hemisphere with radius 1/2. In the case \(n = 1\) we obtain the volume of the surface of this set, while for \(n = N - 1\) we get the volume of the set of pure states . . . which for \(\beta = 1(2)\) gives correctly the volume of the real (complex) projective space of dimensions \(N - 1\)” [1].

The Bures metric on various spaces of density matrices has been widely studied [3, 4, 5, 6]. In a broader context, it serves as the minimal monotone metric [4].

Let us apply (1) to the cases of specific interest in this study, \(N = 6, n = 0, \beta = 2\) and \(N = 6, n = 1, \beta = 2\) — that is, the Bures 35-dimensional volume and 34-dimensional hyperarea of the complex \(6 \times 6\) density matrices. We then have that

\[
S_{6,0}^{(2)} = \frac{\pi^{18}}{12221326970165372387328000} \approx 7.27075 \cdot 10^{-17}
\]

(2)

and

\[
S_{6,1}^{(2)} = \frac{\pi^{17}}{13833906576343805952000} \approx 2.04457 \cdot 10^{-15}
\]

(3)

Here, we are able (somewhat paralleling our recent work for \(N = 4\) [8], but in a rather more systematic manner than there) through numerical (quasi-Monte Carlo/quasi-random) methods to reproduce both of these values (2), (3), to a considerable accuracy. At the same time, we compute numerical values — it would seem reasonable to assume, with roughly the same level of accuracy — of these two quantities, but for the replacement of the Bures metric by five other monotone metrics of interest. These are the Kubo-Mori [9, 10, 11, 12], (arithmetic) average [8], Wigner-Yanase [13, 14, 15, 16], Grosse-Krattenthaler-Slater (GKS) [17, 18] and (geometric) average monotone metrics — the two “averages” being formed from the minimal and maximal monotone metrics, following the suggested procedure in [19, eq. (20)]. No proven formulas, such as (1), are presently available for these various quantities,
although our research here and in [8] strongly suggests that the Kubo-Mori volume of the $N \times N$ density matrices is equal to simply $2^{N(N-1)/2}S^{(2)}_{N,0}$, which for our case of $N = 6$ would be $32768S^{(2)}_{6,0}$ (cf. Tables I and II). (In light of the considerable attention recently devoted to the (Riemannian, but non-monotone) Hilbert-Schmidt metric [2, 20, 21] — it would certainly seem appropriate to include it as well in any further analyses along the lines here and in [8].)

Further, we compute for all these six metrics the 35-dimensional volumes and 34-dimensional hyperareas restricted to the separable $2 \times 3$ and $3 \times 2$ systems. (Then, we can, obviously, by taking ratios obtain “probabilities of separability” — a topic which was first investigated in [22], and studied further, using the Bures metric, in [23, 24, 25]). For this purpose, we employ the convenient Peres-Horodecki necessary and sufficient positive partial transposition criterion for separability [26, 27] — asserting that a $4 \times 4$ or $6 \times 6$ density matrix is separable if and only if all the eigenvalues of its partial transpose are positive. (But in the $6 \times 6$ case, we have the qualitative difference that partial transposes can be determined in two inequivalent ways, either by transposing in place, in the natural manner, the nine $2 \times 2$ submatrices or the four $3 \times 3$ submatrices. We will throughout this study — as in [28] — analyze results using both forms of partial transpose. It is our anticipation — although without a formal demonstration — that in the limit of large sample size, the two sets of results will converge to true common values.)

Our main analysis takes the form of a quasi-Monte Carlo (Tezuka-Faure [29]) numerical integration over the 35-dimensional hypercube ($[0,1]^{35}$) and a 34-dimensional subhypercube of it. In doing so, we implement a parameterization of the $6 \times 6$ density matrices in terms of thirty Euler angles (parameterizing $6 \times 6$ unitary matrices) and five hyperspherical angles (parameterizing the six eigenvalues — constrained to sum to 1 [30, 31]). We hold a single one of the five hyperspherical angles fixed in the 34-dimensional analysis. (The parameters are linearly transformed so that they all lie in the interval [0,1].)

We have previously pursued a similar numerical analysis in investigating the separable and nonseparable volumes and hyperareas of the $4 \times 4$ density matrices [8]. Highly accurate results (as gauged in terms of known Bures quantities [1]) — based on two billion points of a Tezuka-Faure (“low discrepancy”) sequence lying in the 15-dimensional hypercube — led us to advance several strikingly simple conjectures. For example, it was indicated that the Kubo-Mori volume of separable and nonseparable states was exactly $64 = 2^6$ times...
the Bures volume. (The exponent 6 is expressible — in terms of our general conjecture, mentioned above, relating the Bures and Kubo-Mori volumes — as \(N(N - 1)/2, N = 4\).)

Most prominently, though, it appeared that the statistical distinguishability (SD) volume was simply expressible as \(\frac{\sigma_{Ag}}{3}\), where the “silver mean” \(\sigma_{Ag} = \sqrt{2} - 1 \approx 0.414214\), and \(10\sigma_{Ag}\) in terms of (four times) the Kubo-Mori metric. (The SD metric is identically four times the Bures metric \(\text{for } N = 4, n = 0, \beta = 2\) — thus equalling the volume of a 15-dimensional hyper-hemisphere with radius 1, rather than \(\frac{1}{2}\) as in the Bures case itself.) Unfortunately, there appears to be little in the way of “clues” in the literature, as to how one might formally prove or disprove these conjectures — “brute force” symbolic integration appearing to be well beyond present technical/conceptual capabilities — although the author “suspects” that at least in the Bures/minimal monotone case, a proof might conceivably be based on the concept of “minimal volume” \(\text{for } N\)-level [separable and nonseparable] systems, but rather, principally, used concepts of random matrix theory.

The monotone metrics (of which we study five, in addition to the Bures) can all be expressed in the form

\[
g_{\rho}(X', X) = \frac{1}{4} \Sigma_{\alpha, \beta} |\langle \alpha | X | \beta \rangle|^2 c_{\text{monotone}}(\lambda_\alpha, \lambda_\beta)
\]

(cf. \(\text{for } N = 4, n = 0, \beta = 2\)). Here \(X, X'\) lie in the tangent space of all Hermitian \(N \times N\) density matrices \(\rho\) and \(|\alpha\rangle, \alpha = 1, 2 \ldots\) are eigenvectors of \(\rho\) with eigenvalues \(\lambda_\alpha\). Now, \(c_{\text{monotone}}(\lambda_\alpha, \lambda_\beta)\) represents the specific Morozova-Chentsov function for the monotone metric in question \(\text{for } N\)-level [separable and nonseparable] systems, but rather, principally, used concepts of random matrix theory.)

This function takes the form for the Bures metric,

\[
c_{\text{Bures}}(\lambda_\alpha, \lambda_\beta) = \frac{2}{\lambda_\alpha + \lambda_\beta},
\]

for the Kubo-Mori metric (which, up up to a scale factor, is the unique monotone Riemannian metric with respect to which the exponential and mixture connections are dual \(\text{for } N\)-level [separable and nonseparable] systems, but rather, principally, used concepts of random matrix theory.)

\[
c_{\text{KM}}(\lambda_\alpha, \lambda_\beta) = \log \frac{\lambda_\alpha - \lambda_\beta}{\lambda_\alpha - \lambda_\beta},
\]

for the (arithmetic) average metric (first discussed in \(\text{for } N\)-level [separable and nonseparable] systems, but rather, principally, used concepts of random matrix theory.)
for the Wigner-Yanase metric (which corresponds to a space of constant curvature $^{13}$),
\[ c_{WY}(\lambda_\alpha, \lambda_\beta) = \frac{4}{(\sqrt{\lambda_\alpha} + \sqrt{\lambda_\beta})^2}, \tag{8} \]
for the GKS/quasi-Bures metric (which yields the asymptotic redundancy for universal quantum data compression $^{17}$),
\[ c_{GKS}(\lambda_\alpha, \lambda_\beta) = \frac{\lambda_\alpha^{\lambda_\beta/(\lambda_\beta-\lambda_\alpha)}}{\lambda_\beta} \tag{9} \]
and for the (geometric) average metric (apparently previously unanalyzed),
\[ c_{geom}(\lambda_\alpha, \lambda_\beta) = \frac{1}{2\sqrt{\lambda_\alpha \lambda_\beta}}. \tag{10} \]

II. ANALYSES

Based on the first 600 million points of a Tezuka-Faure sequence, to which we are continuing to copiously add, we obtained the results reported in Tables I -VII. (We followed the Bures formulas in [1, secs. III.C, III.D], substituting the Morozova-Chentsov functions given above (6)-(10), in the appropriate manner, to obtain their counterparts for the various non-Bures monotone metrics.)

In Table I, we scale the estimates of the volumes and hyperareas by the known values (2), (3) of $S^{(2)}_{6,0}$ and $S^{(2)}_{6,1}$, while in Table II we scale these estimates by the estimated values ($7.21259 \cdot 10^{-17}$ and $2.04607 \cdot 10^{-15}$) of these two quantities. (We use both approaches because we are uncertain as to which may be more revealing as to possible exact ratios — the possibility of which is suggested by our work in [8]. It is interesting to observe that the convergence to the true values of $S^{(2)}_{6,0}$ and $S^{(2)}_{6,1}$ appears to be more pronounced in the 34-dimensional case than in the 35-dimensional one, although the Tezuka-Faure sequence we employ is specifically designed as a 35-dimensional one — of which we take an essentially arbitrary 34-dimensional projection (cf. [40, sec. 7]).)

In Tables III and Tables IV we report our estimates (scaled by the values obtained for the Bures metric) of the volumes and hyperareas of the $6 \times 6$ separable complex density matrices. Let us note, however, that to compute the hyperarea of the complete boundary of the separable states, one must also include those $6 \times 6$ density matrices of full rank, the partial transposes of which have a zero eigenvalue, and all other eigenvalues nonnegative.
TABLE I: Scaled estimates based on the Tezuka-Faure sequence of 600 million points of the 35-dimensional volumes and 34-dimensional hyperareas of the $6 \times 6$ density matrices, using several monotone metrics. The scaling factors are the known values of the volume and hyperarea for the Bures metric, given by [1], and more specifically for the cases $N = 6$, $n = 0, 1$, $\beta = 2$ by [2] and [3].

| metric | volume/$S^{(2)}_{6,0}$ | hyperarea/$S^{(2)}_{6,1}$ |
|--------|-----------------|-----------------|
| Bures  | 0.992001        | 1.00073         |
| KM     | 31046.8         | 45.5328         |
| arith  | 614.789         | 31.3225         |
| WY     | 130.323         | 9.78041         |
| GKS    | 12.2984         | 3.56433         |
| geom   | $6.53456 \cdot 10^{38}$ | $2.1581 \cdot 10^9$ |

TABLE II: Scaled estimates based on the Tezuka-Faure sequence of 600 million points of the 35-dimensional volumes and 34-dimensional hyperareas of the $6 \times 6$ density matrices, using several monotone metrics. The scaling factors ($\tilde{S}$) are the estimated values ($7.21259 \cdot 10^{-17}$ and $2.04606 \cdot 10^{-15}$) of the volume and hyperarea for the Bures metric.

| metric | volume/$\tilde{S}^{(2)}_{6,0}$ | hyperarea/$\tilde{S}^{(2)}_{6,1}$ |
|--------|-----------------|-----------------|
| KM     | 31297.2         | 45.4995         |
| arith  | 619.747         | 31.2995         |
| WY     | 131.374         | 9.77326         |
| GKS    | 12.3976         | 3.56172         |
| geom   | $6.58726 \cdot 10^{38}$ | $2.15652 \cdot 10^9$ |

[41]. (We do not compute this contribution here, as it would slow considerably the overall process in which we are engaged, since high-degree polynomials would need to be solved at each step.) In [8], we had been led to conjecture that that part of the 14-dimensional boundary of separable $4 \times 4$ density matrices consisting generically of rank-four density matrices had SD hyperarea $\frac{554\sigma_{Ag}}{39}$ and that part composed of rank-three density matrices, $\frac{433\sigma_{Ag}}{39}$, for a total 14-dimensional boundary SD hyperarea of $\frac{984\sigma_{Ag}}{39}$. We, then, sought to
TABLE III: Scaled estimates based on the Tezuka-Faure sequence of 600 million points of the 35-dimensional volumes and 34-dimensional hyperareas of the separable $6 \times 6$ density matrices, using several monotone metrics. The scaling factors are the estimated values ($1.58803 \cdot 10^{-19}$ and $1.86401 \cdot 10^{-18}$) — the true values being unknown — of the volume and hyperarea for the Bures metric. To implement the Peres-Horodecki positive partial transposition criterion, we compute the partial transposes of the four $3 \times 3$ submatrices (blocks) of the density matrix.

| metric | Bures-scaled volume | Bures-scaled hyperarea |
|--------|---------------------|------------------------|
| KM     | 2491.77             | 9.83988                |
| arith  | 226.332             | 11.3251                |
| WY     | 49.7186             | 4.30152                |
| GKS    | 8.05581             | 2.35047                |
| geom   | $3.66418 \cdot 10^{23}$ | 52086.9               |

apply the “Levy-Gromov isoperimetric inequality” to the relation between the known and estimated SD volumes and hyperareas of the separable and separable plus nonseparable states [8, sec. VII.C].

In Table III we compute the partial transposes of the $6 \times 6$ density matrices by transposing in place the four $3 \times 3$ submatrices, while in Table IV we transpose in place the nine $2 \times 2$ submatrices. In Table V we only require the density matrix in question to pass either of the two tests, while in Table VII we require it to pass both tests for separability. (Of the 600 million points of the Tezuka-Faure 35-dimensional sequence so far generated, approximately 2.91 percent yielded density matrices passing the test for Table I, 2.84 percent for Table II, 4 percent for Table III and 1.74 percent for Table IV.)

In Table VII, we “pool” (average) the results for the separable volumes and hyperareas reported in Tables III and IV, based on the two distinct forms of partial transposition, to obtain possibly superior estimates of these quantities, which presumably are actually one and the same independent of the particular form of partial transposition.
TABLE IV: Scaled estimates based on the Tezuka-Faure sequence of 600 million points of the 35-dimensional volumes and 34-dimensional hyperareas of the *separable* $6 \times 6$ density matrices, using several monotone metrics. The scaling factors are the estimated values ($1.03484 \cdot 10^{-19}$ and $1.46223 \cdot 10^{-18}$) — the true values being unknown — of the volume and hyperarea for the Bures metric. To implement the Peres-Horodecki positive partial transposition criterion, we compute the partial transposes of the nine $2 \times 2$ submatrices (blocks) of the density matrix.

| metric | Bures-scaled volume | Bures-scaled hyperarea |
|--------|---------------------|------------------------|
| KM     | 2563.64             | 8.41556                |
| arith  | 198.163             | 10.3172                |
| WY     | 46.5238             | 3.98471                |
| GKS    | 7.59133             | 2.25601                |
| geom   | $7.61764 \cdot 10^{23}$ | 12275.1               |

TABLE V: Scaled estimates based on the Tezuka-Faure sequence of 600 million points of the 35-dimensional volumes and 34-dimensional hyperareas of the *separable* $6 \times 6$ density matrices, using several monotone metrics. The scaling factors are the estimated values ($2.59687 \cdot 10^{-19}$ and $3.30035 \cdot 10^{-18}$) — the true values being unknown — for the Bures metric. A density matrix is included here if it passes *either* form of the positive partial transposition test.

| metric | Bures-scaled volume | Bures-scaled hyperarea |
|--------|---------------------|------------------------|
| KM     | 2534.46             | 9.25073                |
| arith  | 216.379             | 10.9214                |
| WY     | 48.6732             | 4.17378                |
| GKS    | 7.89451             | 2.31228                |
| geom   | $4.63187 \cdot 10^{23}$ | 34855.9               |

III. DISCUSSION

Of course, by taking the ratios of estimates of the volumes/hyperareas of separable states to the estimates of the volumes/hyperareas of separable plus nonseparable states, one would, in turn, obtain estimates of the probabilities of separability [22] for the various monotone
TABLE VI: Scaled estimates based on the Tezuka-Faure sequence of 600 million points of the 35-dimensional volumes and 34-dimensional hyperareas of the separable $6 \times 6$ density matrices, using several monotone metrics. The scaling factors are the estimated values ($2.59945 \cdot 10^{-21}$ and $3.59687 \cdot 10^{-31}$) — the true values being unknown — for the Bures metric. A density matrix is included here only if it passes both forms of the positive partial transposition test.

| metric | Bures-scaled volume | Bures-scaled hyperarea |
|--------|---------------------|------------------------|
| KM     | 1087.9              | 4.50082                |
| arith  | 98.6297             | 5.85995                |
| WY     | 26.9706             | 2.69208                |
| GKS    | 5.67912             | 1.80686                |
| geom   | $6.43785 \cdot 10^{24}$ | 117.375                |

TABLE VII: Scaled estimates obtained by pooling the results from Tables III and IV — based on the two forms of partial transposition — for the separable volumes and hyperareas. The Bures scaling factors (pooled volume and hyperarea) are $1.31143 \cdot 10^{-19}$ and $1.66312 \cdot 10^{-18}$.

| metric | Bures-scaled volume | Bures-scaled hyperarea |
|--------|---------------------|------------------------|
| Bures  | 2520.12             | 9.21374                |
| arith  | 215.212             | 10.882                 |
| WY     | 48.4581             | 4.16225                |
| GKS    | 7.87255             | 2.30894                |
| geom   | $5.224 \cdot 10^{23}$ | 34585.5                |

metrics studied. (Obviously, scaling the estimated volumes and hyperareas by the corresponding estimates for the Bures metric, as we have done in the tables above for numerical convenience and possible insightfulness, would be inappropriate in such a process.) The Bures metric gives the largest probability of separability.

In [28], we attempted a somewhat similar quasi-Monte Carlo qubit-qutrit analysis (but restricted to the Bures metric) to that reported above, but based on many fewer points (70 million vs. the 600 million so far used here) of a (Halton) sequence. At this stage, having made use of considerably increased computer power (and streamlined MATHEMATICA
programming — in particular employing the Compile command, which enables the program to proceed under the condition that certain variables will enter a calculation only as machine numbers, and not as lists, algebraic objects or any other kind of expression), we must regard this earlier study as superseded by the one here. (Our pooled estimate of the Bures volume of the separable qubit-qutrit systems here [Table VII] is $1.31143 \cdot 10^{-19}$, while in [28], following our earlier work for $N = 4$ [42], we formulated a conjecture ([28, eq. (5)]) — in which we can now have but very little confidence — that would give [converting from the SD metric to the Bures] a value of $2.19053 \cdot 10^{-9} \cdot 2^{-35} \approx 6.37528 \cdot 10^{-20}$.) We also anticipate revisiting the $N = 4$ (qubit-qubit) case [8] with our newly accelerated programming methods.

We continue to add to the 600 million points of the Tezuka-Faure sequence employed above, and hope to report considerably more accurate results in the future (based on which, hopefully, we can advance plausible hypotheses as to the true underlying values of the 35-dimensional volumes and 34-dimensional hyperareas). In fact, at the time of submission of this paper, we have already generated an additional 110 million points, using several independent processors. Since the additional points are not numbered 600,000,001 to 710,000,000 in the sequence — with the gaps remaining to be filled in — it seems inappropriate to report the results fully now. Let us only indicate that if we were to do so, the first line of Table I (that is, $0.992001=1/1.00806$ and $1.00073=1/0.999269$) would be replaced by $0.9985$ and $0.999644$, so certainly the prognosis for considerably greater accuracy, as we extend the length of the sequence, is good.

It would be interesting to conduct analogous investigations to those reported here and in [8] for the case $N = 4$, using quasi-random sequences other than Tezuka-Faure ones [29], particularly those for which it is possible to do statistical testing on the results (such as constructing confidence intervals) [43]. (It is, of course, possible to conduct statistical testing using simple Monte Carlo methods, but their convergence is much slower than that of the quasi-Monte Carlo procedures. Since we are dealing with quite high-dimensional spaces, good convergence has been our dominant consideration in the selection of numerical integration methodologies to employ.)
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