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Qubit-qutrit separability-probability ratios

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Paralleling our recent computationally intensive (quasi-Monte Carlo) work for the case $N=4$ (e-print quant-ph/0308037), we undertake the task for $N=6$ of computing to high numerical accuracy, the formulas of Sommers and Życzkowski (e-print 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—and also their analogous formulas (e-print quant-ph/0302197) for the (nonmonotone) flat Hilbert-Schmidt metric. With the same seven 10^9 well-distributed ("low-discrepancy") sample points, we estimate the *unknown* volumes and hyperareas based on five additional (monotone) metrics of interest, including the Kubo-Mori and Wigner-Yanase. Further, we estimate all of these seven volume and seven hyperarea (unknown) quantities when restricted to the *separable* density matrices. The ratios of separable volumes (hyperareas) to separable *plus* nonseparable volumes (hyperareas) yield estimates of the *separability probabilities* of generically rank-6 (rank-5) density matrices. The (rank-6) separability probabilities obtained based on the 35-dimensional volumes appear to be—*independently* of the metric (each of the seven inducing Haar measure) employed—*twice* as large as those (rank-5 ones) based on the 34-dimensional hyperareas. (An additional estimate—33.9982—of the ratio of the rank-6 Hilbert-Schmidt separability probability to the rank-4 one is quite clearly close to integral too.) The doubling relationship also appears to hold for the $N=4$ case for the Hilbert-Schmidt metric, but not the others. We fit simple *exact* formulas to our estimates of the Hilbert-Schmidt *separable* volumes and hyperareas in both the $N=4$ and $N=6$ cases.

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I. INTRODUCTION

In part I of their paper [1,2], Życzkowski *et al.* considered the "question of how many entangled or, respectively, separable states are there in the set of all quantum states." They cited philosophical, practical, and physical reasons for doing so. They gave a qualitative argument ([1], Sec. III B)—contrary to their initial supposition—that the measure of separable states could not be strictly zero. There has since been considerable work [3–14], using various forms of measures, to determine or estimate the "volume of separable states," as well as the volume of separable *and* nonseparable states [15,16], and hence probabilities of separability. One somewhat surprising development has been the (principally numerical) indication—two independent estimates being 0.137 884 [3] and 0.138 119 (Sec. VI C 2 below) that the volume of separable states itself can take on a notably elegant form, in particular, $(\sqrt{2}-1)/3\approx 0.138\,071$, for the case of qubit-qubit pairs endowed with the *statistical distinguishability* metric (4 times the Bures metric). (However, there seems to be a paucity of ideas on how to *formally* prove or disprove such a conjecture.) The research reported below was undertaken initially with the specific purpose of finding whether a putative comparably elegant formula for the volume of separable qubit-qutrit pairs might exist. We will report below (Sec. VI D) the obtaining of certain possible formulas that fit our numerical results well, but none of such striking simplicity (nor none that extends it, in any natural apparent fashion). But we also obtain some new type results of substantial independent interest.

In a recent highly comprehensive analysis [15] (cf. [17]), 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

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

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 hyperhemisphere 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 $N-1$" [15]. The Bures metric on various spaces of density matrices (ρ) has been widely studied [18–21]. In a broader context, it serves as the *minimal* monotone metric [22].

In part II of [1,2], Życzkowski put forth a certain proposition. It was that "the link between the purity of the mixed states and the probability of entanglement is not sensitive to the measure [on the space of $N\times N$ density matrices] used." His assertion was based on comparisons between a unitary product measure and an orthogonal product measure for the (qubit-qubit) case $N=4$ [[2], Fig. 2(b)]. The *participation ratio*—$1/\mathrm{Tr}(\rho^2)$—was used as the measure of purity.

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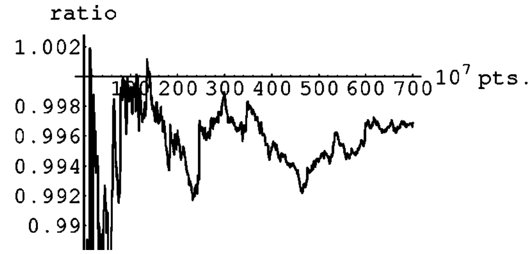

FIG. 1. Ratios of the cumulative estimates of the 35-dimensional volume $S_{6,0}^{(2,Bures)}$ to its *known* value (8). For each addtional point shown—as in all the subsequent plots—10×10^6 (10^7) values of the particular (7×10^9)-point Tezuka-Faure sequence have been generated.

II. SEPARABILITY-PROBABILITY RATIOS

In this study, we present (Sec. VI C) numerical evidence—limited largely to the specific (qubit-qutrit) case $N=6$—for a somewhat related proposition (which appears to be possibly topological in nature [23]). It is that a certain "ratio of ratios"

$$\Omega^{metric} \equiv \frac{R^{metric}_{sep+nonsep}}{R^{metric}_{sep}} \tag{2}$$

is equal to 2, *independently* of the measure used—where the possible measures (including the just-discussed Bures) are comprised of *volume elements* (all incorporating the *Haar* measure as a factor) of certain *metrics* defined on the $N\times N$ density matrices. Here by

$$R^{metric}_{sep+nonsep} \equiv \frac{S_{N,1}^{(2,metric)}}{S_{N,0}^{(2,metric)}} \tag{3}$$

is indicated the ratio of the hyperarea of the (N^2-2)-dimensional boundary of the (N^2-1)-dimensional convex set (C_N) of $N\times N$ density matrices to the total volume of C_N. Further,

$$R^{metric}_{sep} \equiv \frac{\sum_{N,1}^{(2,metric)}}{\sum_{N,0}^{(2,metric)}} \tag{4}$$

is the same type of hyperarea-volume ratio, but now restricted to the (classical and nonquantum) subset of C_N composed of the *separable* states [24] (which we designate using Σ rather than S). A simple algebraic rearrangement of quotients then reveals that Ω^{metric}, Eq. (2), is also interpretable as the ratio

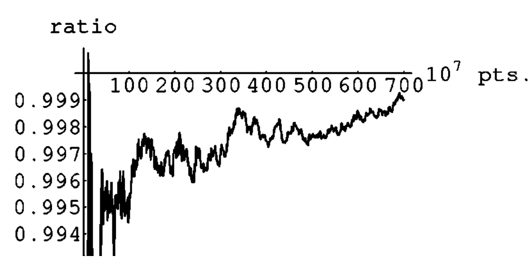

FIG. 2. Ratios of the cumulative estimates of the 34-dimensional hyperarea $S_{6,1}^{(2,Bures)}$ to its known value (9).

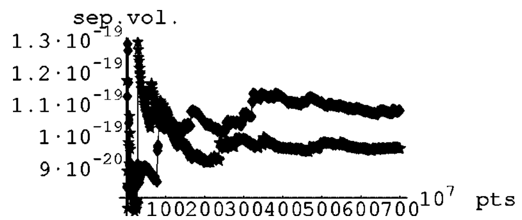

FIG. 3. A *pair* of cumulative estimates of the 35-dimensional Bures volume of *separable* qubit-qutrit states based on the *two* distinct forms of partial transposition.

$$\Omega^{metric} \equiv \frac{P_N^{[metric,rank\text{-}N]}}{P_N^{[metric,rank\text{-}(N-1)]}} \tag{5}$$

of the *separability probability* of the totality of (generically rank-N) states in C_N,

$$P_N^{[metric,rank\text{-}N]} \equiv \frac{\sum_{N,0}^{(2,metric)}}{S_{N,0}^{(2,metric)}}, \tag{6}$$

to the separability probability

$$P_N^{[metric,rank\text{-}(N-1)]} \equiv \frac{\sum_{N,1}^{(2,metric)}}{S_{N,1}^{(2,metric)}} \tag{7}$$

of the [generically rank-$(N-1)$] states that lie on the boundary of C_N.

III. METRICS OF INTEREST

Let us apply the Życzkowski-Sommers Bures formula (1) to the two cases that will be 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* 6×6 density matrices. (It would, of course, also be of interest to study the *real* case $\beta=1$, though we have not undertaken any work in that direction.) We then have that

$$S_{6,0}^{(2,Bures)} = \frac{\pi^{18}}{122213269701653723873280000} \approx 7.27075\times10^{-17} \tag{8}$$

and

$$S_{6,1}^{(2,Bures)} = \frac{\pi^{17}}{1383390657634380595200000} \approx 2.04457\times10^{-15}. \tag{9}$$

Here, we are able (somewhat paralleling our recent work for the qubit-qubit case $N=4$ [3], but in a rather more systematic manner *ab initio* than there), through advanced numerical (quasi–Monte Carlo and quasirandom) methods, to reproduce both of these values (8) and (9), to a considerable accuracy. At the same time, we compute numerical values—it would seem reasonable to presume, at least initially, with

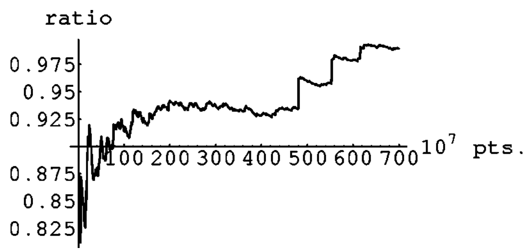

FIG. 4. Ratios of the cumulative estimates of the 35-dimensional volume $S_{6,0}^{(2,KM)}$ to its conjectured value of $32\,768 S_{6,0}^{(2,Bures)}$.

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 [25–28], (arithmetic) average [3], Wigner-Yanase [29–32], Grosse-Krattenthaler-Slater (GKS) [33] (or "quasi-Bures" [34]), and (geometric) average monotone metrics—the two "averages" being formed from the minimal (Bures) and *maximal* (Yuen-Lax [35]) monotone metrics, following the suggested procedure in [36] [Eq. (20)]. No proven formulas, such as Eq. (1), are presently available for these other various quantities, although our research in [3] had suggested that the Kubo-Mori volume of the $N\times N$ density matrices is expressible as

$$S_{N,0}^{(2,KM)} = 2^{N(N-1)/2} S_{N,0}^{(2,Bures)}, \tag{10}$$

which for our case of $N=6$ would give

$$S_{6,0}^{(2,KM)} = 32768 S_{6,0}^{(2,Bures)}. \tag{11}$$

In light of the considerable attention recently devoted to the (Riemannian, but *nonmonotone* [37]) Hilbert-Schmidt metric [16,17,38], including the availability of exact volume and hypersurface formulas [16], we include it in supplementary analyses too. Further, we estimate for all these seven (six monotone and one nonmonotone) metrics the (unknown) 35-dimensional volumes and 34-dimensional hyperareas restricted to the *separable* 2×3 and 3×2 systems. Then, we can, obviously, by taking ratios of separable quantities to their separable *plus* nonseparable counterparts, obtain "probabilities of separability"—a topic which was first investigated in [1] and studied further, using the Bures metric, in [3–6].

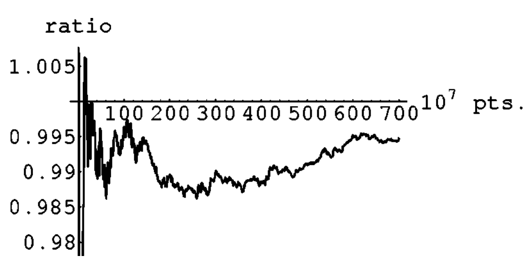

FIG. 5. Ratios of the cumulative estimates of the 35-dimensional Hilbert-Schmidt (Euclidean) volume $S_{6,0}^{(2,HS)}$ to its *known* value (23).

IV. TWO FORMS OF PARTIAL TRANSPOSITION

We will employ the convenient Peres-Horodecki necessary *and* sufficient positive partial transposition criterion for separability [39,40]—asserting that a 4×4 or 6×6 density matrix is separable if and only if all the eigenvalues of its partial transpose are non-negative. (In the 4×4 [qubit-qubit] case, it simply suffices to test the determinant of the partial transpose for nonnegativity [41,42].) But in the 6×6 case, we have the qualitative difference that partial transposes can be determined in (at least) *two* inequivalent ways, either by transposing in place, in the natural blockwise manner, the *nine* 2×2 submatrices or the *four* 3×3 submatrices [[40] Eq. (20)]. (Obviously, such a nonuniqueness arises in a bipartite system only if the dimensions of the two parts are unequal.) We will throughout this study—as in [6]—at the expense of added computation, analyze results using *both* forms of partial transpose.

It is our anticipation—although yet without a formal demonstration—that in the limit of large sample size, the two sets of (separable volume and separable hyperarea) results of interest here should converge to true *common* values. Now, the author must admit that he initially thought that it made no difference at all in which of the two ways the partial transpose was taken; that is, a 6×6 density matrix would either pass or fail *both* tests. Also, this seems to be a common attitude in the quantum information community (as judged by a number of personal reactions (cf. [1], footnote 2). Therefore, we present below a specific example of a 6×6 density matrix (ρ_1) that remains a density matrix if its four 3×3 blocks are transposed, but not its nine 2×2 blocks, since the latter result has a *negative* eigenvalue $(-0.001\,298\,36)$:

$$\begin{pmatrix} \frac{2}{9} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{7} & 0 & 0 & 0 & -\frac{1}{24}+\frac{\imath}{38} \\ 0 & 0 & \frac{1}{5} & \frac{\imath}{23} & \frac{-\imath}{41} & -\frac{1}{10}-\frac{\imath}{21} \\ 0 & 0 & \frac{-\imath}{23} & \frac{1}{7} & 0 & \frac{\imath}{13} \\ 0 & 0 & \frac{\imath}{41} & 0 & \frac{1}{6} & 0 \\ 0 & -\frac{1}{24}-\frac{\imath}{38} & -\frac{1}{10}+\frac{\imath}{21} & \frac{-\imath}{13} & 0 & \frac{79}{630} \end{pmatrix}. \tag{12}$$

Życzkowski has pointed out that the question of whether a given state ρ is entangled or not depends crucially upon the decomposition of the composite Hilbert space $H_A \otimes H_B$ (cf. [43,44]). For instance, for the simplest 2×2 case, the maximally entangled Bell state becomes "separable," he points out, if one considers entanglement with respect to another division of the space—e.g., $A'=\{\Phi_+,\Phi_-\}$, $B'=\{\Psi_+,\Psi_-\}$. So it should not be surprising, at least in retrospect, that some states are separable with respect to one form of partial transposition and not the other. In the course of examining this issue, we found that if one starts with an arbitrary 6×6 matrix (M) and alternates the two forms of partial transposition on it, after 12 $(=2\times 6)$ iterations of this process, one arrives back at the *original* 6×6 matrix. So, in group-theoretic terms, if we denote the three-by-three operation by a_3 and the two-by-two operation by a_2, we have idempotency, $a_2^2=a_3^2=I$ and $(a_2a_3)^6=(a_3a_2)^6=I$. Further, one can go from the partial transpose $a_3(M)$ to the partial transpose $a_2(M)$ via the matrix corresponding to the permutation $\{1,4,2,5,3,6\}$.

Further, we constructed the related density matrix (ρ_2)

$$\begin{pmatrix} \frac{2}{9} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{7} & 0 & 0 & \frac{\imath}{23} & \frac{-\imath}{41} \\ 0 & 0 & \frac{1}{5} & 0 & -\frac{1}{24}+\frac{\imath}{38} & 0 \\ 0 & 0 & 0 & \frac{1}{7} & -\frac{1}{10}-\frac{\imath}{21} & \frac{-\imath}{13} \\ 0 & \frac{-\imath}{23} & -\frac{1}{24}-\frac{\imath}{38} & -\frac{1}{10}+\frac{\imath}{21} & \frac{1}{6} & 0 \\ 0 & \frac{\imath}{41} & 0 & \frac{\imath}{13} & 0 & \frac{79}{630} \end{pmatrix}. \tag{13}$$

Now, if ρ_2 is partially transposed using its nine 2×2 blocks, it gives the identical matrix as when ρ_1 is partially transposed using four 3×3 blocks. But the six eigenvalues of ρ_1—that is, $\{0.322\,635,\ 0.222\,222,\ 0.1721,\ 0.149\,677,\ 0.119\,158,\ 0.014\,207\,6\}$—are *not* the same as the six eigenvalues of ρ_2—that is, $\{0.300\,489,\ 0.222\,222,\ 0.204\,982,\ 0.168\,304,\ 0.099\,276\,3,\ 0.004\,726\,44\}$. So there can be no unitary transformation taking ρ_1 to ρ_2. [The possibility that ρ_1 and ρ_2 might have the same total measure(s) attached to them cannot formally be ruled out, however.]

TABLE I. Scaled estimates based on the Tezuka-Faure sequence of 7×10^9 points of the 35-dimensional volumes and 34-dimensional hyperareas of the 6×6 density matrices, using several monotone metrics. The scaling factors are the *known* values of the volume and hyperarea for the Bures metric, given by Eq. (1), and more specifically for the cases $N=6$, $n=0$, 1, and $\beta=2$ by Eqs. (8) and (9).

Metric	$\tilde{S}_{6,0}^{(2,metric)}/S_{6,0}^{(2,Bures)}$	$\tilde{S}_{6,1}^{(2,metric)}/S_{6,1}^{(2,Bures)}$
Bures	0.996899	0.999022
KM	32419.4	45.4577
Arith	621.714	31.291
WY	131.711	9.76835
GKS	12.4001	3.55929
Geom	2.80011×10^{44}	1.44011×10^{14}

TABLE II. Scaled estimates based on the Tezuka-Faure sequence of 7×10^9 points of the 35-dimensional volumes and 34-dimensional hyperareas of the 6×6 density matrices, using several monotone metrics. The scaling factors are the *estimated* values $(\tilde{S}_{6,0}^{(2,Bures)}=7.2482\times 10^{-17}$ and $\tilde{S}_{6,1}^{(2,Bures)}=2.04257\times 10^{-15})$ of the volume and hyperarea for the Bures metric.

Metric	$\tilde{S}_{6,0}^{(2,metric)}/\tilde{S}_{6,0}^{(2,Bures)}$	$\tilde{S}_{6,1}^{(2,metric)}/\tilde{S}_{6,1}^{(2,Bures)}$
KM	32520.3	45.5022
Arith	623.648	31.3216
WY	132.121	9.77791
GKS	12.4387	3.56278
Geom	2.80882×10^{44}	1.44152×10^{14}

V. RESEARCH DESIGN

Our main analysis will take the form of a quasi–Monte Carlo (Tezuka-Faure [45,46]) numerical integration over the 35-dimensional hypercube $([0,1]^{35})$ and a 34-dimensional subhypercube of it. In doing so, we implement a parametrization of the 6×6 density matrices in terms of 30 Euler angles (parametrizing 6×6 unitary matrices) and *five* hyperspherical angles (parametrizing the *six* eigenvalues—constrained to sum to 1) [47,48]. We hold a single one of the five hyperspherical angles fixed in the 34-dimensional analysis, so that one of the six eigenvalues is always zero—and the density matrix is generically of rank 5. The parameters are linearly transformed so that they each lie in the unit interval [0,1] and, thus, collectively in the unit hypercube. The computations consumed approximately 5 months using six PowerMacs in parallel, each generating a different segment of the Tezuka-Faure sequence.

A. Silver mean $(\sqrt{2}-1)$ conjectures for $N=4$

We have previously pursued a similar numerical analysis in investigating the separable and nonseparable volumes and

TABLE III. Scaled estimates based on the Tezuka-Faure sequence of 7×10^9 points of the 35-dimensional volumes and 34-dimensional hyperareas of the *separable* 6×6 density matrices, using several monotone metrics. The scaling factors are the *estimated* values $(\tilde{\Sigma}_{6,0}^{(2,Bures)}=1.0739\times 10^{-19}$ and $\tilde{\Sigma}_{6,1}^{(2,Bures)}=1.53932\times 10^{-18})$—the true values being unknown—of the separable volume and hyperarea for the Bures metric. To implement the Peres-Horodecki positive partial transposition criterion, we compute the partial transposes of the four 3×3 submatrices (blocks) of the density matrix.

Metric	Bures-scaled separable volume	Bures-scaled separable (rank-5) hyperarea
KM	8694.79	9.43481
Arith	220.75	10.6415
WY	55.3839	4.13924
GKS	7.97798	2.28649
Geom	3.33872×10^{32}	3.61411×10^{8}

TABLE IV. Scaled estimates based on the Tezuka-Faure sequence of 7×10^9 points of the 35-dimensional volumes and 34-dimensional hyperareas of the *separable* 6×6 density matrices, using several monotone metrics. The scaling factors are the *estimated* values ($\tilde{\Sigma}_{6,0}^{(2,Bures)}=9.54508\times10^{-20}$ and $\tilde{\Sigma}_{6,1}^{(2,Bures)}=1.40208\times10^{-18}$)—the true values being unknown—of the separable volume and hyperarea for the Bures metric. To implement the Peres-Horodecki positive partial transposition criterion, we compute the partial transposes of the *nine* 2×2 submatrices (blocks) of the density matrix.

Metric	Bures-scaled separable volume	Bures-scaled separable (rank-5) hyperarea
KM	6465.86	9.0409
Arith	218.602	10.3248
WY	55.5199	4.05201
GKS	7.92729	2.26136
Geom	5.4299×10^{35}	4.35667×10^{9}

hyperareas of the 4×4 density matrices [3]. Highly accurate results (as gauged in terms of *known* Bures quantities [15])—based on two 10^9 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 known Bures volume. [The exponent 6 is expressible—in terms of our general conjecture (10), relating the Bures and Kubo-Mori volumes—as $N(N-1)/2$, with $N=4$.] Most prominently, though, it was conjectured that the statistical distinguishability (SD) volume of separable states is $\sigma_{Ag}/3$ and $10\sigma_{Ag}$ in terms of (4 times) the Kubo-Mori metric. Here, $\sigma_{Ag}=\sqrt{2}-1\approx0.414\,214$ is the "silver mean" [49–52] (cf. [53]). The SD metric is identically 4 times the Bures metric [54]. [Consequently, the SD 15-dimensional volume of the 4×4 complex density matrices is 2^{15} times that of the Bures volume—given by formula (1) for $N=4$, $n=0$, $\beta=2$—thus equaling the volume of a 15-dimensional hyperhemisphere with radius 1, rather than $\frac{1}{2}$ as in the Bures case itself [15].]

TABLE V. Scaled estimates based on the Tezuka-Faure sequence of 7×10^9 points of the 35-dimensional volumes and 34-dimensional hyperareas of the *separable* 6×6 density matrices, using several monotone metrics. The scaling factors are the *estimated* values (1.99772×10^{-19} and 2.90956×10^{-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 separable volume	Bures-scaled separable (rank-5) hyperarea
KM	7735.7	9.30446
Arith	221.689	10.5467
WY	55.8928	4.11453
GKS	7.99075	2.28089
Geom	2.59619×10^{35}	2.29051×10^{9}

TABLE VI. Scaled estimates based on the Tezuka-Faure sequence of 7×10^9 points of the 35-dimensional volumes and 34-dimensional hyperareas of the *separable* 6×6 density matrices, using several monotone metrics. The scaling factors are the *estimated* values (3.06807×10^{-21} and 3.78991×10^{-32})—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 separable volume	Bures-scaled separable (rank-5) hyperarea
KM	1800.19	3.99932
Arith	92.7744	5.3548
WY	26.4785	2.55592
GKS	5.56969	1.77049
Geom	3.96779×10^{27}	1.09937×10^{7}

Unfortunately, there appears to be little in the way of indications in the literature, as to how one might *formally* prove or disprove these conjectures—"brute force" *symbolic* integration seeming to be well beyond present technical and conceptual capabilities (cf. [47], Sec. V). [Certainly, Sommers and Życzkowski [15] did not directly employ symbolic integration methodologies in deriving the Bures volume, hyperarea, etc., for N-level (separable *and* non-separable) systems, but rather, principally, used concepts of random matrix theory.] One approach we have considered in this regard [7] is to parametrize the 15-dimensional convex set of bipartite qubit states in terms of the weights used in the expansion of the state in some basis of 16 extreme separable 4×4 density matrices (cf. [55]). For a certain basis composed of SU (4) generators [56–58], the associated 15×15 Bures metric tensor [20] is *diagonal* in form (having all entries equal) at the fully mixed state ([7], Sec. II)F). (Also, we have speculated that perhaps there is some way of "bypassing" the formidable computation of the Bures metric tensor and yet being able to arrive at the required volume element.) Perhaps, though, at least in the Bures and *minimal* monotone case, a proof might be based on the concept of "minimal volume" [59–61].

B. Formulas for monotone metrics

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

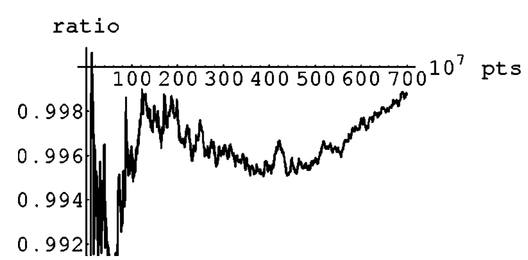

FIG. 6. Ratios of the cumulative estimates of the 34-dimensional Hilbert-Schmidt hyperarea $S_{6,1}^{(2,HS)}$ to its *known* value (24).

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 $\tilde{\Sigma}_{6,0}^{(2,Bures)} = 1.0142 \times 10^{-19}$ and $\tilde{\Sigma}_{6,1}^{(2,Bures)} = 1.4707 \times 10^{-18}$.

Metric	Bures-scaled separable volume	Bures-scaled separable (rank-5) hyperarea
KM	7645.92	9.24704
Arith	219.739	10.4905
WY	55.4479	4.09766
GKS	7.95413	2.27537
Geom	2.55692×10^{35}	2.26584×10^{9}

$$g_\rho(X',X) = \frac{1}{4}\sum_{\alpha,\beta} |\langle\alpha|X|\beta\rangle|^2 c_{monotone}(\lambda_\alpha,\lambda_\beta) \qquad (14)$$

(cf. [18,19]). Here X, X' lie in the tangent space of all Hermitian $N \times N$ density matrices ρ and $|\alpha\rangle$, $\alpha = 1, 2, \ldots$ are the eigenvectors of ρ with eigenvalues λ_α. Now, $c_{monotone}(\lambda_\alpha,\lambda_\beta)$ represents the specific *Morozova-Chentsov* function for the monotone metric in question [36]. This function takes the form for (1) the Bures metric

$$c_{Bures}(\lambda_\alpha,\lambda_\beta) = \frac{2}{\lambda_\alpha + \lambda_\beta}, \qquad (15)$$

(2) the Kubo-Mori (KM) metric (which, up to a scale factor, is the unique monotone Riemannian metric with respect to which the *exponential* and *mixture* connections are dual [28])

$$c_{KM}(\lambda_\alpha,\lambda_\beta) = \frac{\log \lambda_\alpha - \log \lambda_\beta}{\lambda_\alpha - \lambda_\beta}, \qquad (16)$$

(3) the (arithmetic) average metric (first discussed in [3])

$$c_{arith}(\lambda_\alpha,\lambda_\beta) = \frac{4(\lambda_\alpha + \lambda_\beta)}{\lambda_\alpha^2 + 6\lambda_\alpha\lambda_\beta + \lambda_\beta^2}, \qquad (17)$$

(4) the Wigner-Yanase metric (which corresponds to a space of *constant curvature* [29])

$$c_{WY}(\lambda_\alpha,\lambda_\beta) = \frac{4}{(\sqrt{\lambda_\alpha} + \sqrt{\lambda_\beta})^2}, \qquad (18)$$

(5) the GKS–quasi-Bures metric (which yields the asymptotic redundancy for universal quantum data compression [33])

$$c_{GKS}(\lambda_\alpha,\lambda_\beta) = \frac{\left(\frac{\lambda_\alpha}{\lambda_\beta}\right)^{\lambda_\alpha/(\lambda_\beta - \lambda_\alpha)}}{\lambda_\beta} e, \qquad (19)$$

and (6) the (geometric) average metric (apparently previously unanalyzed)

$$c_{geom}(\lambda_\alpha,\lambda_\beta) = \frac{1}{\sqrt{\lambda_\alpha\lambda_\beta}}. \qquad (20)$$

[The results obtained below for the geometric average monotone metric seem, in retrospect, to be of little interest, other than indicating that—like the maximal monotone (Yuen-Lax) metric itself [3]—volumes and hyperareas appear to be simply *infinite* in magnitude.]

VI. ANALYSES

A. Volumes and hyperareas based on certain monotone metrics

Using the first 7×10^9 points of a Tezuka-Faure sequence, we obtained the results reported in Tables I–IX and Figs. 1–12. We followed the Bures formulas in [15] (Secs. III C and III D), substituting for Eq. (15) the Morozova-Chentsov functions given above, Eqs. (16)–(20), to obtain the non-Bures counterparts.

In Fig. 1 we show the ratios of the cumulative estimates of the 35-dimensional volume $S_{6,0}^{(2,Bures)}$ to its *known* value (8). Each successive point is based on 10×10^6 (10^7) more systematically sampled values in the 35-dimensional hypercube than the previous point in the computational sequence. In Fig. 2 we show the ratios of the cumulative estimates of the 34-dimensional hyperarea $S_{6,1}^{(2,Bures)}$ to its known value (9). Each successive point is based on 10×10^6 more sampled values in the 34-dimensional hypercube than the previous point in the computational sequence. The single Tezuka-Faure sequence we employ for all our purposes,

TABLE VIII. Sample estimates of the ratio ($R_{sep+nonsep}^{metric} = S_{6,1}^{(2,metric)}/S_{6,0}^{(2,metric)}$) of the 34-dimensional hyperarea to the 35-dimensional volume for the seven metrics under study and the corresponding ratios for a 35-dimensional *Euclidean* ball having (1) the same volume as for the metric and (2) the same hyperarea.

Metric	Known ratio	Sample ratio ($R_{sep+nonsep}^{metric}$)	Isovolumetric ratio	Isohyperarea ratio
Bures	28.1205	28.1804	2.34553	2.40508
KM	—	0.0394299	1245.79	1536.34
Arith	—	1.41531	38.858	43.2743
WY	—	2.08556	27.5655	30.39
GKS	—	8.07163	7.61987	8.08886
Geom	—	1.44625×10^{-29}	2.45463×10^{29}	1.79638×10^{30}
HS	191.703	192.468	0.543466	0.533806

TABLE IX. Sample estimates of the ratio (R_{sep}^{metric}) of the 34-dimensional hyperarea consisting only of rank-5 6×6 *separable* density matrices to the 35-dimensional separable volume for the seven metrics under study. In the last column there are given the ratios of ratios (Ω^{metric}) of the middle (third) column of Table VIII to these values.

Metric	R_{sep}^{metric}	$\Omega^{metric}\equiv R_{sep+nonsep}^{metric}/R_{sep}^{metric}=P_6^{[metric,6]}/P_6^{[metric,5]}$
Bures	14.501	1.94334
KM	0.0175377	2.24829
Arith	0.692291	2.04439
WY	1.07164	1.94613
GKS	4.14819	1.94582
Geom	1.28502×10^{-25}	0.000112547
HS	94.9063	2.0279

however, is specifically designed as a *35*-dimensional one—of which we take an essentially arbitrary 34-dimensional *projection*. This is arguably a suboptimal strategy for generating well-distributed points in the 34-dimensional hypercube (cf. [62], Sec. VII), but it is certainly highly computationally convenient for us (since we avoid having to generate a totally new 34-dimensional sequence—which would, we believe, increase our computation time roughly 50%) and seems to perform rather well. [In fact, as discussed below, the *bias* of our estimates seems to be—contrary to expectations—markedly less for the known (Bures and Hilbert-Schmidt) 34-dimensional hyperareas than for the 35-dimensional volumes.]

We also present a joint plot (Fig. 3) of the two sets of cumulative estimates of the Bures volume of *separable* qubit-qutrit states based on *both* forms of partial transposition. The estimates obtained using the four blocks of 3×3 submatrices, in general, dominate those using nine blocks of 2×2 submatrices.

In Table I, we scale the estimates (which we denote using $\tilde{S}$) of the volumes and hyperareas by the *known* values (8) and (9) of $S_{6,0}^{(2,Bures)}$ and $S_{6,1}^{(2,Bures)}$, while in Table II we scale these estimates by the *estimated* values ($7.229\,04\times 10^{-17}$ and $2.039\,91\times 10^{-15}$) of these two quantities. (We use *both* approaches because we are uncertain as to which may be more revealing as to possible exact formulas—an approach suggested by our work in [3].) The results for the geometric average monotone metric in Table I appear to be divergent. We might speculate that the middle four scaled hyperareas in the last column of Table I correspond to the actual values $7\times 13/2=45.5$, $2^2\times 5^2/3\approx 31.333$, $3\times 13/4=9.75$, and $7/2=3.5$ and for the second column that we have $132=12\times 11$ and 12, as actual values.

In Tables III and IV, we report our estimates (scaled by the values obtained for the Bures metric) of the volumes and hyperareas of the 6×6 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 6×6 density matrices of *full* rank, the partial transposes of which have a zero eigenvalue, with all other eigenvalues being nonnegative [63]. (We do not compute this additional contribution here—as we undertook to do in our lower-dimensional analysis [3]—as it would slow quite considerably the overall process in which we are engaged, since high-degree polynomials would need to be solved at each iteration.)

In [3], we had been led to conjecture that that part of the 14-dimensional boundary of separable 4×4 density matrices consisting generically of rank-4 density matrices had SD hyperarea $55\sigma_{Ag}/39$ and that part composed of rank-3 density matrices, $43\sigma_{Ag}/39$, for a total 14-dimensional boundary SD hyperarea of $98\sigma_{Ag}/39$. We then sought to apply the "Levy-Gromov isoperimetric inequality" [64] to the relation between the known and estimated SD volumes and hyperareas of the separable and separable plus nonseparable states ([3], Sec. VII C).

Restricting ourselves now to considering only the separable density matrices, for Table III we computed the partial transposes of the 6×6 density matrices by transposing in place the *four* 3×3 submatrices, while in Table IV we transposed in place the nine 2×2 submatrices.

In Table V, we only require the density matrix in question

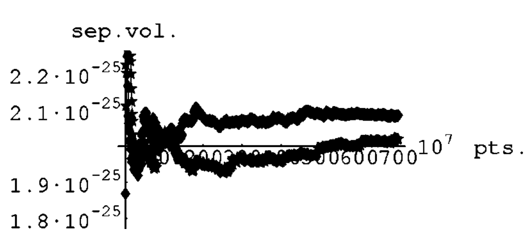

FIG. 7. Cumulative estimates of the 35-dimensional Hilbert-Schmidt volume of *separable* qubit-qutrit states (for the two possible forms of partial transposition).

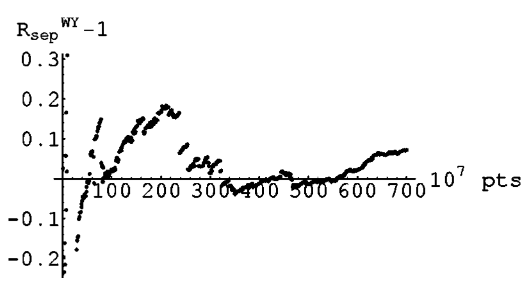

FIG. 8. Deviations of the cumulative estimates of R_{WY}^{sep} from 1.

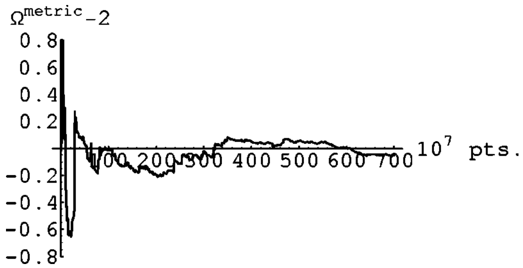

FIG. 9. Deviations from the conjectured value of 2 of the cumulative estimates of R_{GKS}, the ratio of hyperarea-to-volume ratios for the Grosse-Krattenthaler-Slater (GKS or "quasi-Bures") monotone metric.

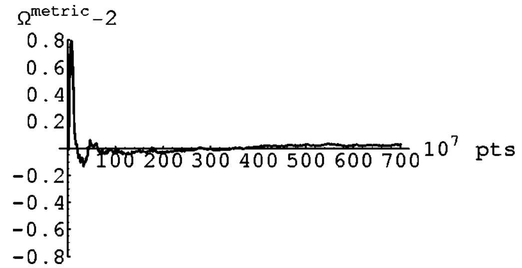

FIG. 11. Deviations from the conjectured value of 2 of the cumulative estimates of R_{HS}, the ratio of hyperarea-to-volume ratios for the Hilbert-Schmidt metric. This plot is particularly flat in character.

to pass *either* of the two tests, while in Table VI, we require it to pass *both* tests for separability. (Of the 7×10^9 points of the Tezuka-Faure 35-dimensional sequence so far generated, approximately 2.91% yielded density matrices passing the test for Table I, 2.84% for Table II, 4% for Table III, and 1.75% for Table IV. Życzkowski commented that "it is not reasonable to ask about the probability that *both* partial transpositions are simultaneously positive, since one should not mix two different physical problems together".)

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.

In Fig. 4 we show the ratios of $\tilde{S}_{6,0}^{(2,KM)}$ to its conjectured value (11) of $32\,768 S_{6,0}^{(2,Bures)}$.

B. Volumes and hyperareas based on the Hilbert-Schmidt metric

Along with the computations based on six distinct monotone metrics, reported above in Sec. VI A, we have at the same time carried out fully parallel analyses of the (Riemannian, but nonmonotone) Hilbert-Schmidt metric [37]. These have only been conducted *after* an earlier less-extensive form of this analysis [8], reporting initial numerical estimates for the same six monotone metrics based on 600×10^6 points of a Tezuka-Faure sequence, was posted. At that stage of our research, we had—with certainly some regrets—decided to *fully* redo the computations reported there. This was done to avoid a (somewhat inadvertent) programming limitation (which seemed of minor importance at the time)—a consequence essentially only of our, in time, having understood how to greatly speed up the computations—of not being able to sample *more* than 2×10^9 Tezuka-Faure points. This fresh beginning (incorporating a much larger limitation, of which we here take advantage) allowed us then, as well, to additionally fully include the Hilbert-Schmidt (HS) metric. [It is somewhat unfortunate, however, at this point, that we had not conducted analyses based on the HS metric for the $N=4$ qubit-qubit case, having restricted our earlier attention to monotone metrics only [3] (cf. Sec. VI C 2).]

Prior to Sommers and Życzkowski reporting their exact formula (1) 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, they had obtained fully analogous formulas for the Hilbert-Schmidt metric, which for the specific volume ($n=0$) case gives [16], Eq. (4.5)]

$$S_{N,0}^{(2,HS)} = \sqrt{N}(2\pi)^{N(N-1)/2}\frac{\Gamma(1)\cdots\Gamma(N)}{\Gamma(N^2)} \tag{21}$$

and the hyperarea ($n=1$) case [16], Eq. (5.2)] gives

$$S_{6,1}^{(2,HS)} = \sqrt{N-1}(2\pi)^{N(N-1)/2}\frac{\Gamma(1)\cdots\Gamma(N+1)}{\Gamma(N)\Gamma(N^2-1)}. \tag{22}$$

For the (qubit-qutrit) case $N=6$ under study in this paper, these give us, for the 35-dimensional HS volume,

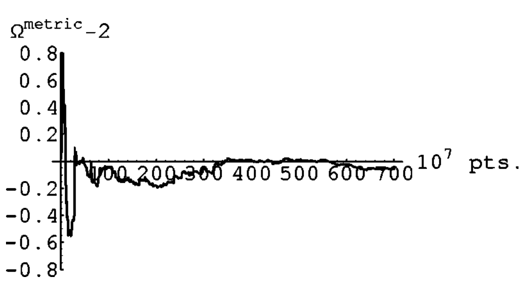

FIG. 10. Deviations from the conjectured value of 2 of the cumulative estimates of R_{Bures}, the ratio of hyperarea-to-volume ratios for the Bures monotone metric.

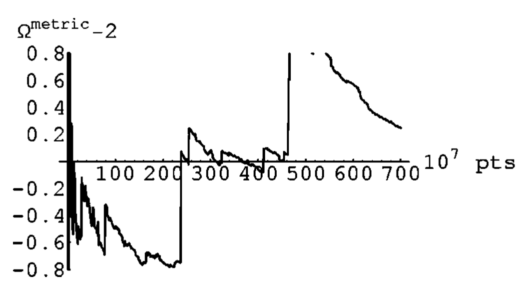

FIG. 12. Deviations from the conjectured value of 2 of the cumulative estimates of R_{KM}, the ratio of hyperarea-to-volume ratios for the KM (Kubo-Mori) monotone metric.

$$S_{6,0}^{(2,HS)} = \frac{\pi^{15}}{1520749664069126407256340000000\sqrt{6}} \approx 7.69334 \times 10^{-24} \quad (23)$$

and for the 34-dimensional HS hyperarea

$$S_{6,1}^{(2,HS)} = \frac{\pi^{15}}{8689998080395008041464800000\sqrt{5}} \approx 1.47483 \times 10^{-21}. \quad (24)$$

So, as above, using the Bures metric, we can further gauge the accuracy of the Tezuka-Faure numerical integration in terms of these *known* volumes and hyperareas. (This somewhat alleviates the shortcoming of the Tezuka-Faure procedure in not lending itself to statistical testing in any straightforward manner.)

The estimated probability of separability is *greater* for the HS metric than for any monotone one. (The minimal monotone or Bures metric appears to give the greatest probability in the nondenumerable class of monotone metrics. Also, the *maximal* monotone metric seems to give a *zero* probability [3].) Therefore, one might surmise that the much-discussed estimates of the sizes of the separable neighborhoods [9–11]—which usually appear to be based on the HS or Frobenius metric—surrounding the fully mixed state are on the rather generous side (cf. [12]), relatively speaking.

In Fig. 5 we show—paralleling Fig. 1—the ratios of our cumulative estimates of $S_{6,0}^{(2,HS)}$ to its known value (23). In Fig. 6 we show—paralleling Fig. 2—the ratios of the cumulative estimates of $S_{6,1}^{(2,HS)}$ to its known value (24).

A plot (Fig. 7) of the cumulative estimates of the Hilbert-Schmidt volume of separable qubit-qutrit states (for the two forms of partial transposition) is also presented. [The ratio of the two cumulative estimates at the final (7×10^9) mark is 1.032 36, while the comparable ratio is 1.125 08 in the analogous Bures plot (Fig. 3).]

In their two studies [15,16], deriving exact formulas for the Bures and Hilbert-Schmidt volumes and hyperareas of the $N\times N$ density matrices, Sommers and Życzkowski also explicitly derived expressions for the *ratios* of (N^2-2)-dimensional hyperareas to (N^2-1)-dimensional volumes. These were [[15], Eq. (4.20)]

$$\gamma_{Bures,N} = \frac{S_{N,1}^{(2,Bures)}}{S_{N,0}^{(2,Bures)}} = \frac{2}{\sqrt{\pi}}\frac{\Gamma(N^2/2)}{\Gamma(N^2/2-1/2)}N \quad (25)$$

and [16], Eq. (6.5)]

$$\gamma_{HS,N} = \frac{S_{N,1}^{(2,HS)}}{S_{N,0}^{(2,HS)}} = \sqrt{N(N-1)}(N^2-1). \quad (26)$$

In the $N=6$ Bures case, this ratio (equivalently what we have earlier denoted $R_{sep+nonsep}^{Bures}$) is

$$\gamma_{Bures,6} \equiv \frac{S_{6,1}^{(2,Bures)}}{S_{6,0}^{(2,Bures)}} = \frac{2^{34}}{3^2\times5\times11\times19\times23\times29\times31\pi} = \frac{17179869184}{194467185\pi} \approx 28.1205 \quad (27)$$

and in the Hilbert-Schmidt case (equivalently $R_{sep+nonsep}^{HS}$),

$$\gamma_{HS,6} \equiv \frac{S_{6,1}^{(2,HS)}}{S_{6,0}^{(2,HS)}} = 35\sqrt{30} \approx 191.703. \quad (28)$$

(The Bures ratio grows proportionally with the dimensionality $(D=N^2-1)$ of the $N\times N$ density matrices as D (for large N) ([15], Sec. IV C) and as $D^{3/2}$ for the Hilbert-Schmidt ratio ([16], Sec. VI).**)** Our sample estimates for these two quantities are 28.1804 and 192.468, respectively. In Table VIII, we report these estimates, as well as the sample estimates for the other five metrics under study here. We also list the two known values and also give the corresponding ratios of hyperarea to volume for a 35-dimensional *Euclidean* ball having (1) the same volume as for the metric in question and (2) the same hyperarea. *Only* for the (flat) HS metric are these last two ratios *less* than unity (cf. [16], Sec. VI).

C. Separability-probability ratios

1. N=6 qubit-qutrit case

In Table IX we list for the seven metrics the estimated ratios, which we denote R_{sep}^{metric}, of the hyperarea (consisting of only the rank-5 but not the rank-6 6×6 density matrices constituting the boundary of the *separable* density matrices [63]) to the volume of all the separable states themselves. We see that R_{WY}^{sep} is quite close to 1. (The Wigner-Yanase metric is one of constant curvature [29].) In Fig. 8 we show the deviations of the cumulative estimates of R_{WY}^{sep} from 1. In the last column of Table IX there are given the ratios of ratios $\Omega^{metric} \equiv R_{sep+nonsep}^{metric}/R_{sep}^{metric}$. [The exceptional (geometric average) case might possibly simply be dismissed for serious consideration on the basis of numerical instabilities, with the associated volumes for this metric appearing to be actually *infinite* in nature. Also, as we will see below, Ω^{KM} is subject to particular severe jumps, perhaps decreasing the reliability of the estimates. The other five are rather close to 2—but it is also somewhat intriguing that three of the estimated monotone metric ratios are quite close to one another ($\approx$1.945) and therefore perhaps a common value *unequal* to 2.] This ratio of ratios can easily be rewritten—as explicated in the Introduction—to take the form of a ratio of separability probabilities. That is, Ω^{metric} is equivalently the ratio of the probability of separability $(P_6^{[(metric,6]})$ for all qubit-qutrit states to the conditional probability of separability $(P_6^{[metric,5]})$ for those states on the (rank-five) boundary of the 35-dimensional convex set.

An interesting conjecture now would be that this ratio (Ω^{metric}) is equal to the integral value 2, *independently* of the (monotone or HS) metric used to measure the volumes and hyperareas. If, in fact, valid, then there is presumably a *topological* explanation [23] for this. (We were able to quite readily reject the speculation that this phenomenon might be in some way an *artifact* of our particular experimental design, in that we employ, as previously discussed, only for simple computational convenience, a 34-dimensional subsequence of the 35-dimensional Tezuka-Faure sequence—rather than an *ab initio* independent 34-dimensional Tezuka-Faure sequence for the calculation of the hyperareas.)

We must observe, however, that all the seven metrics specifically studied here induce the *same* (Haar) measure over 30 of the 35 variables—that is, the 30 Euler angles parametrizing the unitary matrices [47,48]—but not over the five independent eigenvalues of the 6×6 density matrix. Therefore, it is certainly valid to point out that we have not considered *all* types of possible metrics over the 35-dimensional space, but have restricted attention only to certain of those that are *not* inconsistent with quantum mechanical principles. **(**Stolz has pointed out, in a personal communication that, in general, one could modify a metric in the interior away from the boundary *and* outside the separable states, without affecting the metric on the separable states, thus changing $R^{metric}_{sep+nonsep}$ without changing R^{metric}_{sep}, but obviously then also altering the ratio of ratios (*proportio proportionum* [65]) Ω^{metric}. But presumably such a modification would lead, in our context, to the volume element of the so-modified metric *not* respecting Haar measure (cf. [66], Appendix A).**)**

The *topology* of the (N^2-1)-dimensional convex set of $N\times N$ density matrices has been laid out by Życzkowski and Słomczynski ([67], Sec. 2.1). The topological structure is expressible as

$$[U(N)/T^N]\times G_N, \tag{29}$$

where the group of unitary matrices of size N is denoted by $U(N)$ and the unit circle [one-dimensional torus $\approx U(1)$] by T, while G_N represents an $(N-1)$-dimensional *asymmetric* simplex. It would appear, however, that the set of separable states lacks such a product topological structure (thus, rendering integrations over the set—and hence the computation of corresponding volumes—quite problematical).

In Fig. 9 is plotted the deviations from the conjectured integral value of 2 of the cumulative estimates of the ratio (Ω^{GKS})—given in Table IX—of the two hyperarea-to-volume ratios for the GKS monotone metric, the numerator $(R^{sep+nonsep}_{GKS})$ of Ω^{GKS} being based on the entirety of qubit-qutrit states and the denominator (R^{sep}_{GKS}) being based on the boundary qubit-qutrit states only. (All the succeeding plots of deviations from the conjectured integral value of 2 will be drawn to the *same* scale.) In Figs. 10–12, we show the corresponding plots based on the Bures, Hilbert-Schmidt, and Kubo-Mori metrics, respectively. We note that the cumulative estimates in this last plot were relatively close to 2, before a sudden spike in the curve drove it upward. The values for the (quite unrelated) Bures and HS metrics are rather close to 2, which is the main factor in our advancing the conjecture in question.

It would, of course, be of interest to study comparable ratios involving 6×6 density matrices of generic rank less than 5. We did not originally incorporate these into our Mathematica Tezuka-Faure calculations (in particular, since we did not anticipate the apparent metric-independent phenomenon, we have observed here). In Sec. VI C 4 below, we have, however, subsequently pursued such analyses.

TABLE X. Counterparts for the qubit-*qubit* case $N=4$ of the ratios of separability probabilities, based on 400×10^6 points of a Tezuka-Faure sequence

Metric	$r^{metric}_{sep+nonsep}$	r^{metric}_{sep}	ω^{metric}
Bures	12.1563	6.58246	1.84676
KM	0.506688	0.348945	1.45206
Arith	2.19634	1.2269	1.79015
WY	2.93791	1.73028	1.69794
GKS	6.03321	3.3661	1.79234
Geom	4.02853×10^{-16}	7.1263×10^{-16}	0.565304
HS	51.9626	25.9596	2.00167

2. The $N=4$ qubit-qubit case

We adapted our Mathematica routine used so far for the scenario $N=6$, so that it would yield analogous results for $N=4$. Based on 400×10^6 points of a new independent 15-dimensional Tezuka-Faure sequence, we obtained the results reported in Table X. (We now use the lowercase counterparts of the symbols R and Ω to differentiate the $N=4$ case from the $N=6$ one.) Here, once more, the ratios of ratios (ω^{metric}) tend to show rather similar values, with the two exceptional cases again being the geometric average metric [which we suspect—like the maximal (Yuen-Lax) monotone metric, from which it is partially formed—simply gives infinite volumes and hyperareas] and the somewhat unstable KM monotone metric (which now gives an atypically *low* value). We were somewhat surprised that the Hilbert-Schmidt metric again gives, as for $N=6$, a value quite close to 2. In Fig. 13 we show (on a comparatively very fine scale) the deviations from 2 of the cumulative estimates of the ratio of the Hilbert-Schmidt separability probability for the rank-4 states to that for the rank-3 states.

However, it now seems fairly certain that if there is a true common value for ω^{metric} across the metrics, then it is not an integral one (and thus possibly not a *topological* explanation). The theoretical values predicted by Eqs. (25) and (26) for $r^{Bures}_{sep+nonsep}$ and $r^{HS}_{sep+nonsep}$ are $16384/(429\pi)\approx 12.1566$ and $30\sqrt{3}\approx 51.9615$, respectively. Also, consulting Table 6 of our earlier study [3], we find that using the conjectured and known values for the qubit-*qubit* case $(N=4)$ presented there

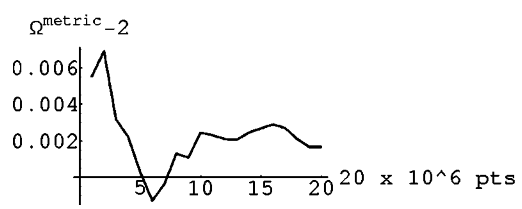

FIG. 13. Deviations from the possible true value of 2 of the cumulative estimates of the ratio of the rank-4 Hilbert-Schmidt separability probability to the rank-3 separability probability in the $N=4$ qubit-qubit case. Note the greatly reduced scale of the y axis.

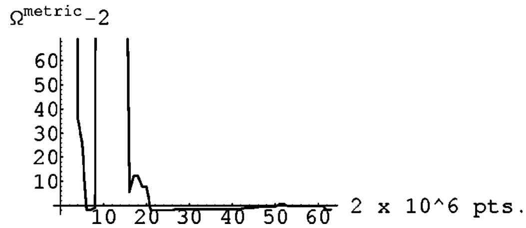

FIG. 14. Deviations from the value of 2 of the cumulative estimates of the ratio of the Hilbert- Schmidt probability of having a positive partial transpose for the 9×9 density matrices of rank 9 to the probability in the rank-8 case.

gives us $\omega^{Bures}=8192/(1419\pi)\approx 1.837\,63$ and a somewhat similar numerical value $\omega^{arith}=408\,260\,608/7\,315\,3125\pi \approx 1.776\,46$.

Let us also indicate in passing that this new independent Tezuka-Faure sequence yields estimates that are quite close to previously known and conjectured values. For example, the ratios of the estimates of $S_{4,0}^{(2,Bures)}$ and $S_{4,1}^{(2,Bures)}$ to their respective known values are 1.0001 and 0.9999. Further, the ratios of the estimates of $\Sigma_{4,0}^{(2,Bures)}$ and $\Sigma_{4,1}^{(2,Bures)}$ (our estimate being 0.138 119) to their respective conjectured values are 1.0001 and 0.999 99.

Let us take this opportunity to note that our analyses here indicate that the conjectures given in Table 6 of [3] for the 14-dimensional hyperareas—denoted B^s and B^{s+n} there—pertaining to the arithmetic average monotone metric, appear to have been too large by a factor of 8.

3. *N*=9 *rank-9 and-8 cases*

Życzkowski has indicated to us that he has an argument, if not yet fully rigorous, to the effect that the ratio of the probability of rank-N states having positive partial transposes to the probability of such rank-$(N-1)$ states should be 2 *independently* of N. Some early analyses of our—based on a so-far relatively short Tezuka-Faure sequence of 126×10^6 points in the extraordinarily high (80)-dimensional hypercube—gave us a Hilbert-Schmidt rank-9/rank-8 probability ratio of 1.89125. [The analogous ratios for the monotone metrics were largely on the order of 0.15. In these same analyses we also—for our first time—implemented, as well, the computable cross-norm criterion for separability [68] and found that *many* more density matrices could not be ruled out as possibly separable than with the (apparently much more discriminating) positive partial transposition criterion. The Hilbert-Schmidt probability ratio based on the cross-norm criterion was 0.223 149.] In Fig. 14 we show the deviations from 2 of the cumulative estimates of the Hilbert-Schmidt rank-9/rank-8 ratio based on the positivity of the partial transpose. However, this plot seems so far very unstable, so we must be quite cautious (pending a much more extended analysis) in its interpretation. (In fact, at some points, the value also seems close to 0.2, as well, similar to the other measures. So we remain very uncertain as to whether there is evidence indicating a true ratio of 2 or possibly some lower common value.)

4. *N*=6 *rank-4 and rank-3 cases*

The principal analyses above have been concerned with the full rank (rank-6) and rank-5 6×6 density matrices. We adapted our Mathematica procedure so that it would analyze the rank-4 and rank-3 cases, in a similar fashion. Now, we are dealing with 31-dimensional and 26-dimensional scenarios, in relation to the original 35- and 34-dimensional ones.

TABLE XI. Estimated ratios of both rank-6 and rank-5 qubit-qutrit separability probabilities to rank-4 separability probabilities.

Metric	Rank-6/rank-4 ratio	Rank-5/rank-4 ratio
Bures	20.9605	10.7858
KM	12.2764	5.4603
arith	17.4245	8.52308
WY	15.5015	7.96527
GKS	18.3778	9.44474
Geom	1.30244×10^{-7}	0.00115724
HS	33.9982	16.7652

In a preliminary run, based on 35×10^6 points of corresponding Tezuka-Faure sequences, not a single rank-3 separable 6×6 density matrix was generated. [The general results of Lockhart [69]—based on Sard's theorem—tells us that the measures of rank-2 and rank-1 6×6 separable density matrices must be zero, but not rank-3, as it appears we have observed (or near to it).] At that stage, we decided to concentrate further in our calculations on the rank-4 case alone.

In Table XI we report results based on 1×10^9 points of a (new and independent) 31-dimensional Tezuka-Faure sequence, coupled with our estimates obtained on the basis of our principal analysis, using the before-mentioned 7×10^9 points. We note that for the Hilbert-Schmidt metric, 33.9982 (2×16.9991) is quite close to integral. In Fig. 15 we show the cumulative estimates of the ratio from the value 34. [Of course, if the ratio of the rank-6 HS separability probability to the rank-5 HS separability probability is exactly, in theory, equal to 2, and the rank-6/rank-4 separability probability exactly 34, then the rank-5/rank-4 ratio should be 17. Since it is based on greater numbers of sampled separable density matrices, we suspect the sample estimate of the rank-6/rank-4 HS separability probability may perhaps be superior to the (less closely integral in value—that is, 16.7652) rank-5/rank-4 estimate.]

Though the convergence to the predicted Hilbert-Schmidt volume was quite good **(**99.9654% of that given by the Życzkowski-Sommers formula [[16], Eq. (5.3)], for $N=6$, n

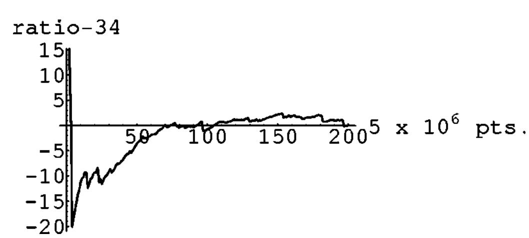

FIG. 15. Deviations from 34 of the cumulative estimates of the ratio of the rank-6 separability probability for the HS metric to the rank-4 separability probability.

=2**)**, we were rather disappointed and surprised that the predicted value of the Bures volume was inaccurate by some 25%. This indicated to us that either the numerics were much more difficult for the Bures computation or there was a possible error in our programming (which we were unable to locate) or even the possibility that something was incorrect with the *specific* Sommers-Życzkowski formula [[17], Eq. (4.19)] we were using,

$$S_{N,n}^{(2,Bures)} = 2^{-d_n}\frac{\pi^{(d_n+1)/2}}{\Gamma((d_n+1)/2)}\binom{N+n-1}{n}. \qquad (30)$$

This last possibility, in fact, proved to be the case, as we found that their formula (4.19) did not agree (for cases other than $n=0$, 1, $N-1$) with the more general formula (5.15)—reproduced above as Eq. (1)—and that using the correct formulation (5.15) (which we found also agrees with (4.18) of [17]) with $\beta=2$, $n=2$, $N=6$, our numerical deviation was reduced from 25% to a more acceptable and less surprising 0.1%. A rectified version of their formula (4.19),

$$S_{N,n}^{(2,Bures)} = 2^{-d_n}\frac{\pi^{(d_n+1)/2}}{\Gamma((d_n+1)/2)}\Pi_{j=0}^{N-n-1}\frac{j\,!\,(j+2n)!}{[(j+n)\,!\,]^2}, \qquad (31)$$

has since been posted by Sommers and Życzkowski [72] after this matter was brought to their attention.

D. Well-fitting formulas for the Bures and Hilbert-Schmidt separable volumes and hyperareas

1. Bures case

Proceeding under the assumption of the validity of our conjecture above (regarding the integral value of 2 for Ω^{metric}), computational experimentation indicates that the Tezuka–Faure quasi-Monte Carlo separable Bures results can be quite well fitted by taking for the *separable* Bures 35-dimensional volume

$$\sum\nolimits_{6,0}^{(2,Bures)} = \frac{3c_{Bures}}{2^{77}} \approx 1.03447\times10^{-19} \qquad (32)$$

and for the *separable* (rank-five) 34-dimensional hyperarea

$$\sum\nolimits_{6,1}^{(2,Bures)} = (2^{43}\times3\times5c_{Bures})^{-1} \approx 1.45449\times10^{-18}, \qquad (33)$$

where by Σ we denote volumes and hyperareas of *separable* states and

$$c_{Bures} = \sqrt{8642986\pi} = \sqrt{\pi\times2\times11\times19\times23\times29\times31} \approx 5210.83. \qquad (34)$$

The pooled *sample* estimates $\tilde{\Sigma}_{6,0}^{(2,Bures)}$ and $\tilde{\Sigma}_{6,1}^{(2,Bures)}$, as indicated in the caption to Table VII, are 1.0142×10^{-19} and 1.4707×10^{-18}.

Then, we would have the Bures probability of separability of the (generically rank-6) qubit-qutrit states as

$$P_6^{[Bures,rank\text{-}6]} = \frac{3^7\times5^3\times7^2\times11\times13\times17c_{Bures}}{2^{27}\pi^{18}} \approx 0.00142278, \qquad (35)$$

and the Bures probability of separability of the generically rank-5 qubit-qutrit states, exactly (by our integral conjecture) one-half of this. (However, there appears to be no obvious way in which the formulas immediately above extend the analogous ones in the qubit-qubit separable case [3], which were hypothesized to involve the "silver mean" $\sigma_{Ag}=\sqrt{2}-1$. Thus, it does not seem readily possible to use the results here to, in any way, support our earlier conjectures.)

We have also devised another set of exact Bures formulas that fit our data roughly as well as Eqs. (32) and (33). These are

$$\sum\nolimits_{6,0}^{(2,Bures)} = \frac{3^2\times11\times19\times23\times29\times31\pi}{2^{76}\times5^6} \approx 1.03497\times10^{-19} \qquad (36)$$

and for the *separable* (rank-5) 34-dimensional hyperarea

$$\sum\nolimits_{6,1}^{(2,Bures)} = (2^{43}\times5^7)^{-1} \approx 1.45519\times10^{-18}. \qquad (37)$$

2. Hilbert-Schmidt case

Additionally, we can achieve *excellent* fits to our Hilbert-Schmidt estimates by taking for the *separable* (rank-6) 35-dimensional volume

$$\sum\nolimits_{6,0}^{(2,HS)} = (2^{45}\times3\times5^{13}\times7\sqrt{30})^{-1} \approx 2.02423\times10^{-25} \qquad (38)$$

(the sample estimate being $2.053\,28\times10^{-25}$) and for the *separable* (rank-5) 34-dimensional hyperarea

$$\sum\nolimits_{6,1}^{(2,HS)} = (2^{46}\times3\times5^{12})^{-1} \approx 1.94026\times10^{-23} \qquad (39)$$

(the sample estimate being $1.948\,69\times10^{-23}$). This gives us a Hilbert-Schmidt probability of separability of the generically rank-6 states of

$$P_6^{[HS,rank\text{-}6]} = \frac{3^{10}\times7^4\times11^3\times13^2\times17^2\times19\times23\times29\times31\sqrt{5}}{2^{37}\times5^7\pi^{15}} \approx 0.0263115, \qquad (40)$$

approximately 18.5 times the predicted Bures probability (35). (As we have noted, the Bures separability probability appears to be the *greatest* among the monotone metrics.) An *upper* bound of $0.166\,083 \approx (0.95)^{35}$ on $P_6^{[HS,rank\text{-}6]}$ is given in Appendix G of [12].

Our simple excellent Hilbert-Schmidt fits here led us to investigate whether the same could be achieved in the qubit-qubit ($N=4$) case, using the same (400×10^6)-point Tezuka-Faure sequence employed in Sec. VI C 2. This, in fact, seemed definitely doable, by taking

$$\Sigma_{4,0}^{(2,HS)} = (3^3 5^7 \sqrt{3})^{-1} \approx 2.73707 \times 10^{-7} \qquad (41)$$

(the sample estimate being $2.739\,28\times 10^{-7}$) and

$$\Sigma_{4,1}^{(2,HS)} = (3^2 5^6)^{-1} \approx 7.11111 \times 10^{-6} \qquad (42)$$

(the sample estimate being $7.111\,09\times 10^{-6}$). The *exact* Hilbert-Schmidt probability of separability of the generically rank-4 qubit-qubit states would then be

$$P_4^{[HS,rank\text{-}4]} = \frac{2^2 \times 3 \times 7^2 \times 11 \times 13\sqrt{3}}{5^3 \pi^6} \approx 0.242379. \qquad (43)$$

[A *lower* bound for $\Sigma_{4,0}^{(2,HS)}$ of $256\pi^7/29\,805\,593\,211\,675 \approx 2.658\,34\times 10^{-8}$—that is, the volume of a 15-dimensional ball of radius $\frac{1}{3}$—appears obtainable from the results of [11], although it is not fully clear to this reader whether the argument there applies to the *two*-qubit case ($m=2$), since the exponent $m/2-1$ appears.] Of course, one would now like to try to extend these Hilbert-Schmidt results to cases $N>6$. Also, let us propose the formula

$$\Sigma_{6,2}^{(2,HS)} = \frac{7\cdot 11}{2^{41} 5^{11} \sqrt{5}\pi} \approx 1.02084 \times 10^{-19} \qquad (44)$$

[the sample estimate (Sec. VI C 4) being 1.04058×10^{-19}].

VII. DISCUSSION

In the main numerical analysis of this study (Secs. VI A and VI B), we have directly estimated 28 quantities of interest—seven total volumes of the 35-dimensional space of qubit-qutrit states, seven 34-dimensional hyperareas of the boundary of those states, and the same quantities when restricted to the separable qubit-qutrit states. Of these 28 quantities, 4 (that is, $S_{6,0}^{(2,Bures)}, S_{6,1}^{(2,Bures)}, S_{6,0}^{(2,HS)}$, and $S_{6,1}^{(2,HS)}$) were precisely known from previous analyses of Sommers and Życzkowski [15,16]. It is interesting to observe that the Tezuka-Faure quasi–Monte Carlo numerical integration procedure has, in all four of these cases, as shown in the corresponding table and figures (Table I and Figs. 1, 2, 5, and 6), slightly but consistently *underestimated* the known values—more so, it seems, with the 35-dimensional volumes, as opposed to the 34-dimensional hyperareas. (So, in statistical terminology, we appear to have *biased* estimators. The very same form of bias—in terms of the Bures metric—was observed in the precursor analysis [8] to this one, based on an independent, shorter Tezuka-Faure sequence. *Randomizing* deterministic algorithms—such as the Tezuka-Faure—can remove such bias [70].) This suggests that we might possibly improve the accuracy of the estimates of the 24 unknown quantities by scaling them in accordance with the magnitude of known underestimation. Also, we have in our several tables only reported the results at the $(7\times 10^9$ point) end of the Tezuka-Faure procedure. We might also report results at intermediate stages at which the estimates of the 4 known quantities are closest to their true values, since estimates of the 24 unknown quantities might arguably also be most accurate at those stages.

Of course, as we have done, taking the *ratios* of estimates of the volumes and hyperareas of separable states to the estimates of the volumes and hyperareas of separable plus nonseparable states, one, in turn, obtains estimates of the probabilities of separability [1] for the various monotone metrics studied. (*Scaling* the estimated volumes and hyperareas by the corresponding estimates for the Bures metric, as we have done in certain of the tables above for numerical convenience and possible insightfulness, would be inappropriate in such a process.) Among the metrics studied, the Hilbert-Schmidt metric gives the *largest* qubit-qutrit probability of separability ($\approx 0.026\,828\,3$), while the Bures metric—the *minimal* monotone one—gives the (considerably smaller) largest separability probability ($\approx 0.001\,399\,25$) among the monotone metrics studied (and presumably among all monotone metrics). The (Yuen-Lax) *maximal* monotone metric appears to give a null separability probability.

In [6], we had attempted a somewhat similar quasi–Monte Carlo qubit-qutrit analysis (but restricted simply to the Bures metric) to that reported above, but based on many fewer points (70×10^6 vs the 7×10^9 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 entirely superseded by the one here. **(**Our pooled estimate of the Bures volume of the separable qubit-qutrit systems here (Table VII) is 1.0142×10^{-19}, while in [6], following our earlier work for $N=4$ [13], we formulated a conjecture [[6], 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 $2^{-35}\times(2.190\,53\times 10^{-9})\approx 6.375\,28\times 10^{-20}$.**)** We also anticipate revisiting—as in Sec. VI C 2—the $N=4$ (qubit-qubit) case [3] with our newly accelerated programming methods, in a similarly systematic manner.

Perhaps, in the future, subject to research priorities, we will add to the 7×10^9 points of the Tezuka-Faure sequence employed above and hope to report considerably more accurate results in the future (based on which, possibly, we can further appraise the hypotheses offered above as to the values of the various volumes and hyperareas). Also, we may seek to estimate the hyperarea of that part of the boundary of the separable qubit-qutrit states consisting of generically rank-6 6×6 density matrices [3,63], though this involves a much greater amount of computation per point. [This would entail first finding the values, if any, of the undetermined (35th) parameter that would set the determinants of the two forms of partial transpose equal to zero and then—using these values—ascertaining whether or not all the six eigenvalues of the resultant partial transposes were non-negative.]

In this study, we have utilized additional computer power recently available to us, together with an advanced quasi–Monte Carlo procedure (scrambled Faure-Tezuka sequences [45,46]—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 frame-work of Neiderreiter." [$A^{(i)}$ is an arbitrary nonsingular lower triangular (NLT) matrix, P is the Pascal matrix [71], 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 [45,46]. "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" ([70], p. 107).

It would be interesting to conduct analogous investigations to those reported here ($N=6$) and in [3] for the case $N=4$, using quasirandom sequences *other* than Tezuka-Faure ones [45,46], particularly those for which it is possible to do *statistical* testing on the results (such as constructing confidence intervals) [70]. It is, of course, possible to conduct statistical testing using simple Monte Carlo methods, but their convergence is much weaker than that of the quasi–Monte Carlo procedures. Since we have been dealing with extraordinarily high-dimensional spaces, good convergence has been a dominant consideration in the selection of numerical integration methodologies to employ.

"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" ([70], p. 95). G. Ökten is presently developing a new Mathematica version of scrambled Faure-Tezuka sequences in which there will be a random generating matrix for each dimension—rather than one for all the dimensions together—which will then be susceptible to *statistical* testing [70].

At the strong urging of K. Zyczkowski, we disaggregated the pooled result in the last column of Table IX into the part based on partial transposition of four three-by-three blocks and obtained {1.966, 2.53505, 2.04826, 1.94679, 1.96481, 9.32089×10^{-7}, 1.99954} and into the part based on nine two-by-two blocks and obtained {1.91846, 1.91976, 2.04, 1.94539, 1.92476, 0.0001227, 2.05803}. We bring the attention of the reader to the particular closeness to 2 of the first (Hilbert-Schmidt) ratio.

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