Two-Qubit Hilbert-Schmidt Separability Functions and
Probabilities for Full-Dimensional Even-Dyson-Index Scenarios

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Abstract

We extend the findings and analyses of our two recent studies (Phys. Rev. A 75, 032326 [2007] and arXiv:0704.3723) by, first, obtaining numerical estimates of the separability function based on the (Euclidean, flat) Hilbert-Schmidt (HS) metric for the 27-dimensional convex set of quaternionic two-qubit systems. The estimated function appears to be strongly consistent with our previously-formulated Dyson-index ($\beta = 1, 2, 4$) ansatz, dictating that the quaternionic ($\beta = 4$) separability function should be exactly proportional to the square of the separability function for the 15-dimensional convex set of two-qubit complex ($\beta = 2$) systems, as well as the fourth power of the separability function for the 9-dimensional convex set of two-qubit real ($\beta = 1$) systems. In particular, we conclude that $S_{\text{quat}}(\mu) = \left(\frac{6}{71}\right)^2 \left(\frac{3}{7} - \mu^2\right)^4 = (S_{\text{complex}}(\mu))^2$, $0 \leq \mu \leq 1$. Here, $\mu = \sqrt{\frac{\rho_{11}\rho_{22}}{\rho_{22}\rho_{33}}}$, where $\rho$ is a 4 x 4 two-qubit density matrix. We can, thus, supplement (and fortify) our previous assertion that the HS separability probability of the two-qubit complex states is $\frac{8}{33} \approx 0.242424$, by claiming that its quaternionic counterpart is $\frac{7244244}{936259725} \approx 0.0773765$. We also comment on and analyze the odd $\beta = 1$ and 3 cases.

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For several years now, elaborating upon an idea proposed in [1], we have been pursuing the problem of deriving (hypothetically exact) formulas for the proportion of states of qubit-qubit and qubit-qutrit systems that are separable (classically-correlated) in nature [2, 3, 4, 5, 6, 7, 8, 9]. Of course, any such proportions will critically depend upon the measure that is placed upon the quantum systems. In particular, we have—in analogy to Bayesian analyses, in which the volume element of the Fisher information metric for a parameterized family of probability distributions is utilized as a measure (“Jeffreys’ prior”) [10]—principally employed the volume elements of the well-studied (Euclidean, flat) Hilbert-Schmidt (HS) and Bures (minimal monotone) metrics (as well as a number of other [non-minimal] monotone metrics [6]).

Zyczkowski and Sommers [11, 12] have, using methods of random matrix theory [13] (in particular, the Laguerre ensemble), obtained formulas, general for all $n$, for the HS and Bures total volumes (and hyperareas) of $n \times n$ (real and complex) quantum systems. Up to normalization factors, the HS total volume formulas were also found by Andai [14], in a rather different analytical framework, using a number of (spherical and beta) integral identities and positivity (Sylvester) conditions. (He also obtained formulas—general for any monotone metric [including the Bures]—for the volume of one-qubit [$n = 2$] states [14, sec. 4].)

Additionally, Andai did specifically study the HS quaternionic case. He derived the HS total volume for $n \times n$ quaternionic systems [14, p. 13646],

$$V_{\text{quat}}^{\text{HS}} = \frac{(2n - 2)!\pi^{n^2-n}}{(2n^2-n-1)!}\Pi_{i=1}^{n-2}(2i)!,$$

(1)

giving us for the two-qubit ($n = 4$) case of specific interest here, the 27-dimensional volume,

$$\frac{\pi^{12}}{315071454005160652800000} \approx 2.93352 \cdot 10^{-18}.$$

(2)

(In the analytical setting employed by Zyczkowski and Sommers [11], this volume would appear as $2^{13}$ times as large [14, p. 13647].) If one then possessed a companion volume formula for the separable subset, one could immediately compute the HS two-qubit quaternionic separability probability by taking the ratio of the two volumes.

One analytical approach to the separable volume/probability question that has recently proved to be productive [15]—particularly, in the case of the Hilbert-Schmidt (HS) metric (cf. [16])—makes fundamental use of a form of density matrix parameterization first proposed.
by Bloore [17]. (This methodology can be seen to be strongly related to the very common and long-standing use of correlation matrices in statistics and its many fields of application [18, 19, 20].)

In the Bloore parameterization, one simply represents an off-diagonal $ij$-entry of a density matrix $\rho$, as $\rho_{ij} = \sqrt{\rho_{ii}\rho_{jj}} w_{ij}$, where $w_{ij}$ might be real, complex or quaternionic [21, 22, 23] in nature. The particular attraction of the Bloore scheme, in terms of the separability problem in which we are interested, is that one can (in the two-qubit case) implement the well-known Peres-Horodecki separability (positive-partial-transpose) test [24, 25] using only the ratio $\mu = \sqrt{\frac{\rho_{11}\rho_{44}}{\rho_{22}\rho_{33}}}$, rather than the four (three independent) diagonal entries of $\rho$ individually [9, eq. (7)] [15, eq. (5)].

Utilizing the Bloore parameterization, we have, accordingly, been able to reduce the problem of computing the desired HS volumes of two-qubit separable states to the computations of one-dimensional integrals over $\mu \in [0, \infty]$. The associated integrands are the products of two functions, one a readily determined jacobian function $J(\mu)$ (corresponding, first, to the transformation to the Bloore variables $w_{ij}$ and, then, to $\mu$) and the other, the more problematical (what we have termed) separability function $S_{HS}(\mu)$ [9, eqs. (8), (9)]. (In the qubit-qutrit case, two ratios, $\mu_1$ and $\mu_2$, are required to express the separability conditions, but analytically the corresponding separability functions also appear to be univariate in nature, being simply functions of $\mu_1$ or $\mu_2$, or the product $\mu_1\mu_2$ [15, sec. III].)

In our extensive numerical (quasi-Monte Carlo integration) investigation [9] of the 9-dimensional and 15-dimensional convex sets of real and complex $4 \times 4$ density matrices, we had formulated ansätze for the two associated separability functions ($S_{\text{real}}^{HS}(\mu)$ and $S_{\text{complex}}^{HS}(\mu)$), proposing that they were proportional to certain (independent) incomplete beta functions [26],

$$B_{\mu_2}(a, b) = \int_0^{\mu_2} \omega^{a-1}(1 - \omega)^{b-1} d\omega,$$

for particular values of $a$ and $b$. However, in the subsequent study [15], we were led to somewhat modify these ansätze, in light of multitudinous exact lower-dimensional results. Since these further results clearly manifested patterns fully consistent with the Dyson index (“repulsion exponent”) pattern ($\beta = 1, 2, 4$) of random matrix theory [27], we proposed that, in the (full 9-dimensional) real case, the separability function was proportional to a specific
incomplete beta function \((a = \frac{1}{2}, b = 2)\),
\[
S_{\text{real}}^{HS}(\mu) \propto B_{\mu^2}(\mu^2, \frac{1}{2}, 2) \equiv \frac{3}{4}(3 - \mu^2)\mu \tag{4}
\]
and in the complex case, proportional, not to an independent function, but simply to the square of \(S_{\text{real}}^{HS}(\mu)\). (These proposals are strongly consistent \cite{15, Fig. 4} with the numerical results generated in \cite{9}.) This chain of reasoning, then, immediately compels one to the further proposition that the separability function in the quaternionic case is exactly proportional to the fourth power of that for the real case (and, obviously, the square of that for the complex case). It is that specific proposition we will, first, seek to evaluate here.

We, thus, hope thereby to further test the validity of our Dyson-index ansatz, first advanced in \cite{15}, as well as possibly develop an enlarged perspective on the still not yet fully resolved problem of the HS separability probabilities in all three (real, complex and quaternionic) cases. (In \cite{15}, we proposed, combining numerical and theoretical arguments, that in the real two-qubit case, the HS separability probability is \(\frac{8}{17}\), and in the complex two-qubit case, \(\frac{8}{33}\). The arguments, thusly, employed in \cite{15}, however, do not yet rise to the level of a formal demonstration.)

Due to the “curse of dimensionality” \cite{28, 29}, we must anticipate that for the same number of sample (“low-discrepancy” Tezuka-Faure \cite{30, 31}) points generated in the quasi-Monte Carlo integration procedure employed in \cite{9} and here, our numerical estimates of the quaternionic separability function will be less precise than the estimates were for the complex, and \textit{a fortiori}, real cases. (An interesting, sophisticated alternative approach to computing the volume of convex bodies involves a variant of \textit{simulated annealing} \cite{32} (cf. \cite{33}), and allows one—unlike the Tezuka-Faure approach, we have so far employed—to establish confidence intervals for estimates.)

Our first extensive numerical analysis here involved the generation of sixty-four million 24-dimensional Tezuka-Faure points, all situated in the 24-dimensional unit hypercube \([0, 1]^{24}\). (The three independent diagonal entries of the density matrix \(\rho\)—being incorporated into the jacobian \(J(\mu)\)—are irrelevant at this stage of the calculations of \(S_{\text{quat}}^{HS}(\mu)\). The 24 [off-diagonal] Bloore variables had been transformed so that each ranged over the unit interval \([0,1]\). The computations were done over several weeks, using compiled Mathematica code, on a MacMini workstation.)

Of the sixty-four million sample points generated, 7,583,161, approximately 12%, corre-
sponded to possible $4 \times 4$ quaternionic density matrices—satisfying nonnegativity require-
ments. For each of these feasible points, we evaluated whether or not the Peres-Horodecki
positive-partial-transpose separability test was satisfied for 2,001 equally-spaced values of
$\mu \in [0, 1]$.

Here, we encounter another computational “curse”, in addition to that already mentioned
pertaining to the high-dimensionality of our problem, and also the infeasibility of most (88%)
of the sampled Tezuka-Faure points. In the standard manner [13, eq. (5.1.4)] [22, p. 495]
[34, eq. (17)] [35, sec. II], making use of the Pauli matrices, we transform the $4 \times 4$
quaternionic density matrices—and their partial transposes—into $8 \times 8$ density matrices
with [only] complex entries. Therefore, given a feasible 24-dimensional point, we have to
check for each of the 2,001 values of $\mu$, an $8 \times 8$ matrix for nonnegativity, rather than a
$4 \times 4$ one, as was done in both the real and complex two-qubit cases. In all three of these
cases, we found that it would be incorrect to simply assume—which would, of course, speed
computations—that if the separability test is passed for a certain $\mu_0$, it will also be passed
for all $\mu$ lying between $\mu_0$ and 1. This phenomenon reflects the intricate (quartic both in $\mu$
and in the Bloore variables $w_{ij}$’s, in the real and complex cases) nature of the polynomial
separability constraints [9, eq. (7)] [15, eq. (5)].

In Fig. 1 we show the estimate we, thus, were able to obtain of the two-qubit quaternionic
separability function $S_{quat}^{HS}(\mu)$, in its normalized form. (Around $\mu = 1$, one must have the
evident symmetrical relation $S^{HS}(\mu) = S^{HS}(1/\mu)$.) Accompanying our estimate in the plot
is the (well-fitting) hypothetical true form (according with our Dyson-index ansatz [13]) of
the HS two-qubit separability function, that is, the fourth power, $(\frac{1}{2}(3 - \mu^2)\mu)^4$, of the
normalized form of $S_{real}^{HS}(\mu)$.

For the specific, important value of $\mu = 1$, the ratio ($R_1$) of the 24-dimensional HS
measure ($m_{sep} = R_1^{numner}$) assigned in our estimation procedure to separable density matrices
to the total 24-dimensional HS measure ($m_{tot} = R_1^{denom}$) allotted to all (separable and
nonseparable) density matrices is $R_1 = 0.123328$. The exact value of $m_{sep}$ is, of course, to
begin here, unknown, being a principal desideratum of our investigation. On the other hand,
we can directly deduce that $m_{tot} = R_1^{denom} = \frac{\pi^{12}}{776000} \approx 0.118862$—our sample estimate being
FIG. 1: Estimate—based on 64,000,000 sampled 24-dimensional points—of the normalized form of the two-qubit quaternionic separability function, along with its (well-fitting) hypothetical true form, the fourth power of the normalized form of $S_{\text{real}}^{HS}(\mu)$, that is, $\left(\frac{1}{2}(3-\mu^2)\mu\right)^4$

0.115845—by dividing the two-qubit HS quaternionic 27-dimensional volume (2) by $R_{\text{denom}} = 2 \int_0^1 J_{\text{quat}}(\mu)d\mu = \frac{\Gamma\left(\frac{3\beta}{2} + 1\right)^4}{\Gamma(6\beta + 4)} = \frac{1}{40518448303132800} \approx 2.46801 \cdot 10^{-17}$, $\beta = 4$.

(5)

Here, $J_{\text{quat}}(\mu)$ is the quaternionic jacobian function (Fig. 2), obtained by transforming the quaternionic Bloore jacobian $\left(\rho_{11}\rho_{22}\rho_{33}(1 - \rho_{11} - \rho_{22} - \rho_{33})\right)^{\frac{3\beta}{2}}$, $\beta = 4$, to the $\mu$ variable by replacing, say $\rho_{33}$ by $\mu$, and integrating out $\rho_{11}$ and $\rho_{22}$. (We had presented plots of $J_{\text{real}}(\mu)$ and $J_{\text{complex}}(\mu)$ in [9, Figs. 1, 2], and observed apparently highly oscillatory behavior in both functions in the vicinity of $\mu = 1$. However, a referee of [15] informed us that this was simply an artifact of using standard machine precision, and that with sufficiently enhanced precision, the oscillations could be seen to be, in fact, illusory.) We can obtain an estimate of the two-qubit quaternionic separability probability $P_{\text{sep/quat}}^{HS}$ by multiplying the ratio $R_1$ by a second ratio $R_2$. The denominator of $R_2$ has already been given (5). The numerator of $R_2$ is the specific value

\[ R_{\text{numer}}^2 = 2 \int_0^1 J_{\text{quat}}(\mu)\left(\frac{1}{2}(3-\mu^2)\mu\right)^4 d\mu = \frac{5989}{35834708624282568000} \approx 1.67128 \cdot 10^{-17}, \]

(6)

where, to obtain the integrand, we have multiplied (in line with our basic [Bloore-parameterization] approach to the separability probability question) the quaternionic jacobian function by the (normalized) putative form of the two-qubit quaternionic separability function. (Note the use of the $\beta = 4$ exponent.)
The counterpart of $R_2^{\text{numer}}$ in the 9-dimensional real case is $\frac{1}{151200}$ and in the 15-dimensional complex case, $\frac{71}{99891792000}$. We now note that

$$99891792000 = \binom{11}{2}\frac{\Gamma(16)}{\Gamma(7)}$$

is the coefficient of $\mu^2$ in $11!L_{11}^4(\mu)$ and $\frac{151200}{2} = 75600$ plays the exact same role in $6!L_6^4(\mu)$, where $L_m^a(\mu)$ is a generalized $(a = 4)$ Laguerre polynomial (see sequences A062260 and A062140 in the The On-Line Encyclopaedia of Integer Sequences). (Also, as regards the denominator of (6), $\frac{358347086242825680000}{3587352665} = 99891792000$.) Życzkowski and Sommers had made use of the Laguerre ensemble in deriving the HS and Bures volumes and hyperareas of $n$-level quantum systems [11, 12]. Generalized (associated/Sonine) Laguerre polynomials (“Laguerre functions”) have been employed in, in another important quantum-information context, in proofs of Page’s conjecture on the average entropy of a subsystem [36, 37].

We, thus, have, for our two-qubit quaternionic case, that

$$R_2 = \frac{R_2^{\text{numer}}}{R_2^{\text{denom}}} = \frac{125769}{185725} \approx 0.677179.$$ 

(8)
(The real counterpart of $R_2$ is $\frac{1024}{135\pi^2} \approx 0.76854$, and the complex one, $\frac{71}{99} \approx 0.717172$. Additionally, we computed that the corresponding “truncated” quaternionic ratio—when one of the four quaternionic parameters is set to zero, that is the Dyson-index case $\beta = 3$—is $\frac{769923214848}{1056376241975\pi^2} \approx 0.692379$. Thus, we see that these four important ratios monotonically decrease as $\beta$ increases, and also, significantly, that the two ratios for odd values of $\beta$ differ qualitatively—both having $\pi^2$ in their denominators—from those two for even $\beta$.)

Our quasi-Monte Carlo (preliminary) estimate of the two-qubit quaternionic separability probability is, then,

$$P_{sep/quat}^{HS} \approx R_1 R_2 = 0.0813594. \quad (9)$$

Multiplying the total volume of the 27-dimensional convex set of two-qubit quaternionic states, given in the framework of Andai [14] by (2), by this result (9), we obtain the two-qubit quaternionic separable volume estimate $V_{sep/quat}^{HS} \approx 2.38777 \cdot 10^{-19}$.

Our 24-dimensional quasi-Monte Carlo integration procedure leads to a derived estimate of (the total 27-dimensional volume) $V_{quat}^{HS}$, that was somewhat smaller, $2.85906 \cdot 10^{-18}$, than the $2.93352 \cdot 10^{-18}$ given by (2). Although rather satisfying, this was sufficiently imprecise to discourage us from attempting to “guestimate” the (all-important) constant ($R_1$) by which to multiply the putative normalized form, $(\frac{1}{2}(3 - \mu^2)\mu)^4$, of the quaternionic separability function in (9) in order to yield the true separable volume. In our previous study [15, sec. IX.A], we presented certain plausibility arguments to the effect that the corresponding constant in the 9-dimensional real case might be $\frac{135\pi^2}{2176} = (\frac{204}{17})/(\frac{512\pi^2}{27})$, and $\frac{24}{71} = (\frac{256\pi^6}{639})/(\frac{32\pi^6}{27})$ in the 15-dimensional complex case. (This leads—multiplying by the corresponding $R_2$’s, $\frac{1024}{135\pi^2}$ and $\frac{71}{99}$—to separability probabilities of $\frac{8}{17}$ and $\frac{8}{33}$, respectively.)

In light of such imprecision, we undertook a supplementary analysis, in which, instead of examining each feasible 24-dimensional point for 2,001 possible values of $\mu$, with respect to separability or not, we simply used $\mu = 1$. This, of course, allows us to significantly increase the number of 24-dimensional Tezuka-Faure points generated from the 64,000,000 so far employed.

We, thusly, generated 1,360,000,000 points, finding that we obtained a remarkably good fit to the important ratio $R_1$ of the 24-dimensional measure, at $\mu = 1$, assigned to the separable two-qubit quaternionic density matrices to the measure (known to be $\frac{\pi^{12}}{1776000}$) by setting $R_1 = (\frac{24}{71})^2 \approx 0.114263$ (our sample estimate of this quantity being 0.114262). This is exactly the square of the corresponding ratio $\frac{24}{71}$ we had conjectured (based on extensive

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numerical and theoretical evidence) for the full (15-dimensional) complex two-qubit case in [15].

Under this hypothesis on $R_1$, we have the ensuing string of relationships

$$S_{\text{quat}}^{HS}(\mu) = \left( \frac{24}{71} \right)^2 \frac{1}{2} (3 - \mu^2) \mu \right)^4 = \left( \frac{6}{71} \right)^2 \left( (3 - \mu^2) \mu \right)^4 = \left( S_{\text{complex}}^{HS}(\mu) \right)^2,$$  \hspace{1cm} (10)

with (as already advanced in [15])

$$S_{\text{complex}}^{HS}(\mu) = \frac{24}{71} \left( \frac{1}{2} (3 - \mu^2) \mu \right)^2 = \frac{6}{71} \left( (3 - \mu^2) \mu \right)^2.$$  \hspace{1cm} (11)

Then, using our knowledge of the complementary ratio $R_2$, given in (8), we obtain

$$P_{\text{sep/quat}}^{HS} = \frac{R_1 R_2}{936239725} \approx 0.0773765,$$  \hspace{1cm} (12)

as well as—in the framework of Andai [14]—that

$$V_{\text{sep/quat}}^{HS} = \frac{5989 \pi^{12}}{2438677343362613741388000000000} \approx 2.26986 \cdot 10^{-19}.$$  \hspace{1cm} (13)

For possible further insight into the HS two-qubit separability probability question, we undertook a parallel quasi-Monte Carlo (Tezuka-Faure) integration (setting $\mu = 1$) for the truncated quaternionic case ($\beta = 3$), in which one of the four quaternionic parameters is set to zero. Although there was no corresponding formula for the HS total volume for this scenario given in [14], upon request, A. Andai kindly derived the result

$$V_{\text{trunc}}^{HS} = \frac{\pi^{10}}{38445858946432000} \approx 2.43584 \cdot 10^{-13}.$$  \hspace{1cm} (14)

(In fact, Andai was able to derive one simple overall comprehensive formula—which we leave for him to publish—yielding the total HS volumes for all $n \times n$ systems and Dyson indices $\beta$.) Let us, further, note that Andai obtains the result (14) as the product of three factors,

$$V_{\text{trunc}}^{HS} = \pi_1 \pi_2 \pi_3,$$

where

$$\pi_1 = \frac{128 \pi^8}{105}; \quad \pi_2 = \frac{128}{893025}; \quad \pi_3 = \frac{189 \pi^2}{1269635648386416}.$$  \hspace{1cm} (15)

Now, we will simply assume—in line with our basic Dyson-index ansatz, substantially supported in [15] and above—that the corresponding separability function is of the form

$$S_{\text{trunc}}^{HS}(\mu) \propto \left( (3 - \mu^2) \mu \right)^{\beta}, \quad \beta = 3.$$  \hspace{1cm} (16)

(Of course, one should ideally test this specific application of the ansatz too, perhaps in the manner we have examined the $\beta = 4$ instance above [Fig. 1].)
We were somewhat perplexed, however, by the results of our quasi-Monte Carlo integration procedure, conducted in the 18-dimensional space of off-diagonal entries of the truncated quaternionic density matrix \( \rho \). Though, we anticipated (from our previous extensive numerical experience here and elsewhere) that our estimate of the associated 18-dimensional volume would be, at least, within a few percentage points of \( \pi_1 \pi_2 \approx 1.65793 \), the estimate was, in fact, close to 0.967 (1, thus, falling within the possible margin of error). Assuming the correctness of the analysis of Andai, which we have no other reason to doubt, the only possible explanations seemed to be that we had committed some programming error (which we were unable to discern) or that we had some conceptual misunderstanding regarding the analysis of truncated quaternions. (Let us note that we do convert the \( 4 \times 4 \) density matrix to \( 8 \times 8 \) [complex] form \([22\text{, p. 495]} \) \([34\text{, eq. (17)}] \) \([35\text{, sec. II]} \), while it appears that Andai does not directly employ such a transformation in his derivations.)

In any case, we did devote considerable computing time to the \( \beta = 3 \) problem (generating 1,180,000,000 18-dimensional Tezuka-Faure points), with the hope being that if we were in some way in error, the error would be an unbiased one, and that the all-important ratio of volumes would be unaffected.

Proceeding thusly, our best estimate (not making use of the Andai result \([14] \) for the present) of the HS separability probability was 0.193006. One interesting possible candidate exact value is, then, \( \frac{128}{633} = \frac{2^7}{3 \cdot 13 \cdot 17} \approx 0.193062 \). (Note the presence of 128 in the numerators, also, of both factors \( \pi_1 \) and \( \pi_2 \).) This would give us a counterpart \([\beta = 3] \) value for the ratio \( R_2 \) of \( \frac{160446825 \pi^2}{5679087616} \approx 0.278838 \). In \([15] \), we had asserted that, in the other odd \( \beta = 1 \) case, the counterpart of \( R_2 \) was \( \frac{135 \pi^2}{2176} \approx 0.612315 \). (Multiplying this by \( \frac{1024}{135 \pi^2} \) gave us the conjectured HS real two-qubit separability probability of \( \frac{8}{17} \).)

So, let us say in conclusion, that although we believe we have successfully resolved—though still far from having formal proofs—the two-qubit Hilbert-Schmidt separability probability question for the \( \beta = 2 \) and 4 (complex and quaternionic) cases, the odd \( \beta = 1, 3 \) cases, in particular \( \beta = 3 \), appear still to be somewhat more problematical.
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