Qubit-Qubit and Qubit-Qutrit Separability Functions and Probabilities

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Abstract

We list in increasing order — \{ \frac{1}{10}, \frac{1}{3}, \frac{3}{5}, 2, \frac{135\pi}{1024}, \frac{16\pi}{5}, \frac{3\pi}{10}, \frac{5\pi}{312}, 2 - \frac{435\pi}{1024}, \frac{11}{16}, 1 \} — a number of exact two-qubit Hilbert-Schmidt (HS) separability probabilities, we are able to compute. Each probability corresponds to a specific scenario — a class of \( 4 \times 4 \) density matrices (\( \rho \)) with an \( m \)-subset (\( m < 6 \)) of its six off-diagonal pairs of symmetrically located entries set to zero. Initially, we consider only scenarios in which the \((6 - m)\) non-nullified pairs are real, but then permit them to be complex (as well as quaternionic) in nature. The general analytical strategy we implement is based on the Bloore density matrix parameterization (\( J. \ Phys. \ A, \ 9, \ 2059 \ [1976] \)), allowing us to conveniently reduce the dimensionalities of required integrations. For each scenario, we identify a certain univariate “separability function” \( S_{scenario}(\nu) \), where \( \nu = \frac{\rho_{11}\rho_{44}}{\rho_{22}\rho_{33}} \). The integral over \( \nu \in [0, \infty] \) of the product of this function with a scenario-specific (marginal) jacobian function \( J_{scenario}(\nu) \) yields the HS separable volume (\( V_{HS}^{sep} \)). The ratio of \( V_{HS}^{sep} \) to the HS total (entangled and non-entangled) volume gives us the HS scenario-specific separability probability. Among the possible forms that we have so far determined for \( S_{scenario}(\nu) \) are piecewise combinations of \( c \), \( c\sqrt{\nu} \) and \( c\nu \) for \( \nu \in [0, 1] \) and (in a dual manner) \( \frac{c}{\sqrt{\nu}} \) and \( \frac{c}{\nu} \) for \( \nu \in [1, \infty] \). We also obtain bivariate separability functions \( S_{scenario}^{6 \times 6}(\nu_1, \nu_2) \) in the qubit-qutrit case, involving \( 6 \times 6 \) density matrices, having ratio variables, \( \nu_1 = \frac{\rho_{11}\rho_{55}}{\rho_{22}\rho_{44}} \) and \( \nu_2 = \frac{\rho_{22}\rho_{66}}{\rho_{33}\rho_{55}} \). Additionally, we investigate parallel two-qutrit and three-qubit problems. Further still, we find some analytic evidence for the relevance of beta functions to the two-qubit separability function problem, while we previously (\( Phys. \ Rev. \ A [2007] \)) had found numerical evidence of such a nature.

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I. Introduction
   A. Bloore (off-diagonal-scaling) parameterization
   B. Previous analysis
   C. Computational limitations
   D. Research design and objectives

II. Qubit-Qubit Analyses
   A. Five nullified pairs of off-diagonal entries — 6 scenarios
      1. 4-dimensional real case — $P_{sep}^{HS} = \frac{3\pi}{10}$
      2. 5-dimensional complex case — $P_{sep}^{HS} = \frac{1}{3}$
      3. 7-dimensional quaternionic case — $P_{sep}^{HS} = \frac{1}{10}$
   B. Four nullified pairs of off-diagonal entries — 15 scenarios
      1. 5-dimensional real case — $P_{sep}^{HS} = \frac{5}{8}; \frac{16}{3\pi^2}$
      2. 6-dimensional mixed (real and complex) case — $P_{sep}^{HS} = \frac{105\pi}{312}; \frac{135\pi}{1024}; \frac{3}{8}$
      3. 7-dimensional complex case — $P_{sep}^{HS} = \frac{2}{5}$
      4. 8-dimensional mixed (real and quaternionic) case
   C. Three nullified pairs of off-diagonal entries — 20 scenarios
      1. 6-dimensional real case — $P_{sep}^{HS} = 2 - \frac{435\pi}{1024}; \approx \frac{9}{16}$
      2. 7-dimensional mixed (one complex and two real) case — $P_{sep}^{HS} = \frac{11}{16}$
      3. 8-dimensional mixed (two complex and one real) case
      4. 9-dimensional complex case
   D. Two or fewer nullified pairs of off-diagonal entries
      1. 7-dimensional real case
      2. 8-dimensional real case

III. Qubit-Qutrit Analyses
   A. Fourteen nullified pairs of off-diagonal entries — 15 scenarios
      1. 6-dimensional real case — $P_{sep}^{HS} = \frac{3\pi}{16}$
      2. 7-dimensional complex case — $P_{sep}^{HS} = \frac{1}{3}$
   B. Thirteen nullified pairs of off-diagonal entries — 105 scenarios
      1. 7-dimensional real case — $P_{sep}^{HS} = \frac{5}{8}; \frac{5}{16}; \frac{3\pi}{32}; \frac{16}{3\pi^2}$

3
2. 8-dimensional mixed (real and complex) case — \( P_{\text{sep}}^{HS} = \frac{105\pi}{512} \)

3. 9-dimensional complex case — \( P_{\text{sep}}^{HS} = \frac{1}{3}; \frac{2}{3} \)

C. Twelve nullified pairs of off-diagonal entries — 455 scenarios

IV. Qutrit-Qutrit Analyses

A. Thirty-five nullified pairs of off-diagonal entries — 36 scenarios

1. 10-dimensional complex case — \( P_{\text{PPT}}^{HS} = \frac{1}{3}; \frac{1}{6} \)

B. Thirty-four nullified pairs of off-diagonal entries — 630 scenarios

1. 12-dimensional complex case — \( P_{\text{PPT}}^{HS} = \frac{1}{3}; \frac{7}{30} \)

V. Qubit-Qubit-Qubit Analyses, I

A. Twenty-seven nullified pairs of off-diagonal entries — 28 scenarios

1. 9-dimensional complex case — \( P_{\text{PPT}}^{HS} = \frac{1}{3} \)

B. Twenty-six nullified pairs of off-diagonal entries — 378 scenarios

1. 11-dimensional complex case — \( P_{\text{PPT}}^{HS} = \frac{1}{3}; \frac{1}{9} \)

VI. Qubit-Qubit-Qubit Analyses, II

A. Twenty-seven nullified pairs of off-diagonal entries — 28 scenarios

1. 9-dimensional complex case — \( P_{\text{PPT}}^{HS} = \frac{1}{3} \)

2. 11-dimensional complex case — \( P_{\text{PPT}}^{HS} = \frac{17}{60}; \frac{1}{3} \)

VII. Approximate Approaches to 9-Dimensional Real Qubit-Qubit Scenario

A. Analytically-derived beta functions

VIII. Concluding Remarks

Acknowledgments

References

I. INTRODUCTION

In the abstract to their recent comprehensive review, the Horodecki family note that while quantum entanglement is “usually fragile to environment, it is robust against conceptual and
mathematical tools, the task of which is to decipher its rich structure” \[1\]. In the study below, we certainly encounter such robustness and pursue the task of surmounting it — with some successes.

Given a generic class composed of composite quantum systems, the question of the “relative proportion” of entangled and non-entangled states in that class was apparently first raised by Życzkowski, Horodecki, Sanpera and Lewenstein (ZHSL) in a much-cited paper \[2\]. They gave “three main reasons” — “philosophical”, “practical” and “physical” — upon which they elaborated, for pursuing the topic. The present author, motivated by the ZHSL paper, has investigated this issue in a number of settings, using various (monotone and non-monotone) measures on quantum states, and a variety of numerical and analytical methods \[3, 4, 5, 6, 7, 8, 9, 10\] (cf. \[11, 12, 13, 14\]). Though the problems are challenging (high-dimensional) in nature, many of the results obtained in answer to the ZHSL question in these various contexts have been strikingly simple and elegant (and/or conjecturally so). The new results below certainly fit into such an interesting, appealing pattern.

Specifically here, we develop an approach recently presented in \[15\]. This was found to be relatively effective in studying the question posed by ZHSL, in the context of two-qubit systems (the smallest possible example exhibiting entanglement), endowed with the (non-monotone \[16\]) Hilbert-Schmidt (HS) measure \[17\], inducing the flat, Euclidean geometry on the space of $4 \times 4$ density matrices. This approach \[15\] exploits two distinct features of a form of density matrix parameterization first discussed by Bloore \[18\]. These properties allow us to deal with lower-dimensional integrations (more amenable to computation) than would otherwise be possible. We further find that the interesting advantages of the Bloore parameterization do, in fact, carry over — in a somewhat modified fashion — to the qubit-qutrit (sec. \[III\]), qutrit-qutrit (sec. \[IV\]) and qubit-qubit-qubit (secs. \[V\] and \[VI\]) domains.
A. Bloore (off-diagonal-scaling) parameterization

We shall, first, consider the 9-dimensional convex set of (two-qubit) $4 \times 4$ density matrices with real entries, and parameterize them — following Bloore [18] (cf. [19, p. 235]) — as

$$
\rho = \begin{pmatrix}
\rho_{11} & z_{12} \sqrt{\rho_{11}\rho_{22}} & z_{13} \sqrt{\rho_{11}\rho_{33}} & z_{14} \sqrt{\rho_{11}\rho_{44}} \\
\z_{12} \sqrt{\rho_{11}\rho_{22}} & \rho_{22} & z_{23} \sqrt{\rho_{22}\rho_{33}} & z_{24} \sqrt{\rho_{22}\rho_{44}} \\
\z_{13} \sqrt{\rho_{11}\rho_{33}} & z_{23} \sqrt{\rho_{22}\rho_{33}} & \rho_{33} & z_{34} \sqrt{\rho_{33}\rho_{44}} \\
\z_{14} \sqrt{\rho_{11}\rho_{44}} & z_{24} \sqrt{\rho_{22}\rho_{44}} & z_{34} \sqrt{\rho_{33}\rho_{44}} & \rho_{44}
\end{pmatrix}.
$$

(1)

One, of course, has the standard requirements that $\rho_{ii} \geq 0$ and (the unit trace condition)

$$
\Sigma_i \rho_{ii} = 1.
$$

Now, three additional necessary conditions (which can be expressed without using the diagonal entries, due to the $\rho_{ii} \geq 0$ stipulation) that must be fulfilled for $\rho$ to be a density matrix (with all eigenvalues non-negative) are: (1) the non-negativity of the determinant (the principal $4 \times 4$ minor),

$$
(z_{34}^2 - 1) z_{12}^2 + 2 (z_{14} (z_{24} - z_{23} z_{34} + z_{13} (z_{23} - z_{24} z_{34})) z_{12} - z_{23}^2 - z_{24}^2 - z_{34}^2 + (2)
$$

$$
+ z_{14}^2 (z_{23}^2 - 1) + z_{13}^2 (z_{24}^2 - 1) + 2 z_{23} z_{24} z_{34} + 2 z_{13} z_{14} (z_{34} - z_{23} z_{24}) + 1 \geq 0;
$$

(2): the non-negativity of the leading principal $3 \times 3$ minor,

$$
- z_{12}^2 + 2 z_{13} z_{23} z_{12} - z_{13}^2 - z_{23}^2 + 1 \geq 0; 
$$

(3): the non-negativity of the principal $2 \times 2$ minors (although actually only the $i = j = 1$ case is needed, it is natural to impose them all),

$$
1 - z_{ij}^2 \geq 0.
$$

(4)

As noted, the diagonal entries of $\rho$ do not enter into any of these constraints — which taken together are sufficient to guarantee the nonnegativity of $\rho$ itself — as they can be shown to contribute only (cancellable) non-negative factors to the determinant and principal minors. This cancellation property is certainly a principal virtue of the Bloore parameterization, allowing one to proceed analytically in lower dimensions than one might initially surmise. (Let us note that, utilizing this parameterization, we have been able to establish a recent conjecture of Månsson, Porta Mana and Björk regarding Bayesian state assignment for three-level quantum systems, and, in fact, verify our own four-level analogue of their conjecture [20, eq. (52)] [21].)
Additionally, implementing the Peres-Horodecki condition \[22, 23, 24\] requiring the non-negativity of the partial transposition of \(\rho\), we have the necessary and sufficient condition for the separability (non-entanglement) of \(\rho\) that (4):

\[
\nu \left( z_{34}^2 - 1 \right) z_{12}^2 + 2 \sqrt{\nu} \left( \nu z_{13} z_{14} + z_{23} z_{24} - \sqrt{\nu} (z_{14} z_{23} + z_{13} z_{24}) z_{34} \right) z_{12} - z_{23}^2 - \nu z_{34}^2 + \nu + (5)
\]

\[ + \nu \left( \left( z_{34}^2 - 1 \right) z_{13}^2 - 2 z_{14} z_{23} z_{24} z_{13} - z_{24}^2 + z_{14}^2 \left( z_{23}^2 - \nu \right) \right) + 2 \sqrt{\nu} (z_{13} z_{23} + \nu z_{14} z_{24}) z_{34} \geq 0,
\]

where

\[
\nu = \mu^2 = \frac{\rho_{11} \rho_{44}}{\rho_{22} \rho_{33}}, \quad (6)
\]

being the only information needed, at this stage, concerning the diagonal entries of \(\rho\). (It is interesting to contrast the role of our variable \(\nu\), as it pertains to the determination of entanglement, with the rather different roles played by the concurrence and negativity \[25, 26\].) We have vacillated between the use of \(\nu\) and \(\mu\) as our principal variable in our two previous studies \[15, 27\]. In sec. VII we will revert to the use of \(\mu\), as it appears that its use avoids the appearances of square roots which definitely seem to impede certain Mathematica operations.

So, the Bloore parameterization is evidently even further convenient here, in reducing the apparent dimensionality of the separable volume problem. That is, we now have to consider, initially at least, only the separability variable \(\nu\) rather than three independent (variable) diagonal entries. (This supplementary feature had not been commented upon by Bloore, as he discussed only \(2 \times 2\) and \(3 \times 3\) density matrices, and also, obviously, since the Peres-Horodecki separability condition had not yet been formulated.) The (two variable — \(\nu_1, \nu_2\)) analogue of (6) in the \(6 \times 6\) (qubit-qutrit) case will be discussed and implemented in sec. III. Additionally still, we find a four-variable counterpart in the \(9 \times 9\) qutrit-qutrit instance [sec. IV], and three-variable counterparts in two sets of qubit-qubit-qubit analyses (secs. V and VI). (The question of whether any or all of these several ratio variables are themselves observables would appear to be of some interest.)

In \[15, eqs. (3)-(5)\], we expressed the conditions (found through application of the “cylindrical algebraic decomposition” \[28\]) that — in terms of the \(z_{ij}\)’s — an arbitrary 9-dimensional \(4 \times 4\) real density matrix \(\rho\) must fulfill. These took the form,

\[
z_{12}, z_{13}, z_{14} \in [-1, 1], z_{23} \in [Z_{23}^-, Z_{23}^+], z_{24} \in [Z_{24}^-, Z_{24}^+], z_{34} \in [Z_{34}^-, Z_{34}^+], \quad (7)
\]
where

$$Z_{23}^\pm = z_{12}z_{13} \pm \sqrt{1 - z_{12}^2 \sqrt{1 - z_{13}^2}}, \quad Z_{24}^\pm = z_{12}z_{14} \pm \sqrt{1 - z_{12}^2 \sqrt{1 - z_{14}^2}},$$

(8)

$$Z_{34}^\pm = \frac{z_{13}z_{14} - z_{12}z_{14}z_{23} - z_{12}z_{13}z_{24} + z_{23}z_{24}}{1 - z_{12}^2},$$

and

$$s = \sqrt{-1 + z_{12}^2 + z_{13}^2 - 2z_{12}z_{13}z_{23} + z_{12}^2 \sqrt{1 + z_{13}^2 - 2z_{12}z_{14}z_{24} + z_{24}^2}}. \quad (9)$$

In his noteworthy paper, Bloore also presented [18, secs. 6, 7] a quite interesting discussion of the “spheroidal” geometry induced by his parameterization. This strongly suggests that it might prove useful to reparameterize the $z_{ij}$ variables in terms of spheroidal-type coordinates. Closely following the argument of Bloore — that is, performing rotations of the $(z_{13}, z_{23})$ and $(z_{14}, z_{24})$ vectors by $\frac{\pi}{4}$ and recognizing that each pair of so-transformed variables lay in ellipses with axes of length $\sqrt{1 \pm z_{12}}$ — we were able to substantially simplify the forms of these conditions (7)-(9).

Using the set of transformations (having a Jacobian equal to $(1 - z_{12}^2)^{\gamma_1}$)

$$z_{13} \to \left(\sqrt{1 - z_{12} \cos (\theta_1)} + \sin (\theta_1) \sqrt{z_{12} + 1}\right) \sqrt{\gamma_1 \gamma_2 + 1},$$

$$z_{23} \to \left(\sin (\theta_1) \sqrt{z_{12} + 1} - \cos (\theta_1) \sqrt{1 - z_{12}}\right) \sqrt{\gamma_1 \gamma_2 + 1},$$

$$z_{14} \to \left(\sqrt{1 - z_{12} \cos (\theta_2)} + \sin (\theta_2) \sqrt{z_{12} + 1}\right) \sqrt{\gamma_1 + \gamma_2},$$

$$z_{24} \to \left(\sin (\theta_2) \sqrt{z_{12} + 1} - \cos (\theta_2) \sqrt{1 - z_{12}}\right) \sqrt{\gamma_1 + \gamma_2},$$

$$z_{34} \to Z_{34} - \frac{\cos (\theta_1 - \theta_2) \sqrt{\gamma_1 + \gamma_2} \sqrt{\gamma_1 \gamma_2 + 1}}{\sqrt{\gamma_2}},$$

(10)

one is able to replace the conditions (7)-(9) that the real two-qubit density matrix $\rho$ — given by (11) — must fulfill by

$$\gamma_1 \in [0, 1]; \quad \gamma_2 \in [\gamma_1, 1]; \quad Z_{34} \in [-\gamma_1, \gamma_1]; \quad z_{12} \in [-1, 1]; \quad \theta_1, \theta_2 \in [0, 2\pi]. \quad (11)$$

We became aware of this set of transformations at a rather late stage of the research reported here, and have not been able so far — somewhat disappointingly — to exploit it in regards to the HS separability-probability question. So, the results reported below rely essentially upon the conditions (7)-(9) and the parameterization in terms of the $z_{ij}$’s of Bloore..
B. Previous analysis

In [15], we studied the four nonnegativity conditions (as well as their counterparts — having completely parallel cancellation and univariate function properties — in the 15-dimensional case of $4 \times 4$ density matrices with, in general, complex entries) using numerical (primarily quasi-Monte Carlo integration) methods. We found a remarkably close fit to the function [15, Figs. 3, 4],

$$S_{\text{real}}(\nu) \approx \left(4 + \frac{1}{5\sqrt{2}}\right) B\left(\frac{1}{2}, \sqrt{3}\right)^8 B\nu\left(\frac{1}{2}, \sqrt{3}\right),$$

entering into our formula,

$$V_{\text{sep/real}}^{\text{HS}} = 2 \int_1^\nu \mathcal{J}_{\text{real}}(\nu)S_{\text{real}}(\nu)d\nu = \int_0^\infty \mathcal{J}_{\text{real}}(\nu)S_{\text{real}}(\nu)d\nu,$$

for the 9-dimensional Hilbert-Schmidt separable volume of the real $4 \times 4$ density matrices [15, eq. (9)]. Here, $B$ denotes the (complete) beta function, and $B_\nu$ the incomplete beta function [29],

$$B_\nu(a, b) = \int_0^\nu w^{a-1}(1 - w)^{b-1}dw.$$

Additionally [15, eq. (10)],

$$\mathcal{J}_{\text{real}}(\nu) = \frac{\nu^{3/2} (12 (\nu (\nu + 2) (\nu^2 + 14\nu + 8) + 1) \log (\sqrt{\nu}) - 5 (5\nu^4 + 32\nu^3 - 32\nu - 5))}{3780(\nu - 1)^9}$$

is the (highly oscillatory near $\nu = 1$ [15, Fig. 1]) jacobian function resulting from the transformation to the $\nu$ variable of the Bloore jacobian $(\Pi_{i=1}^4 \rho_{ii})^{\frac{3}{2}}$. (Perhaps we should refer to $\mathcal{J}_{\text{real}}(\nu)$ as a marginal jacobian, since it is the result of the integration of a three-dimensional jacobian function over two, say $\rho_{11}$ and $\rho_{22}$, variables.)

C. Computational limitations

Although we were able to implement the three (six-variable) nonnegativity conditions ((2), (3) and (4)) exactly in Mathematica in [15], for density matrices of the form $(\Pi)$, we found that additionally incorporating the fourth Peres-Horodecki (separability) one (5) — even holding $\nu$ fixed at specific values — seemed to yield a computationally intractable problem. In fact, after the completion of [15], we consulted with A. Strzebonski (the resident expert on these matters at Wolfram Inc.), and he wrote in regard to our problem that “It
looks like the [nine-dimensional four-condition separable real density matrix] problem is well out of range for CAD [the cylindrical algorithmic decomposition \([30]\)]. The algorithm is doubly exponential in the number of variables. Six variables is a lot for CAD, so only very, very simple systems with six variables can be solved. Adding one more inequality of total degree 4 makes a huge difference. After an hour the algorithm is still in the projection phase at 4 variables (it needs to go down to univariate polynomials) and the projection polynomials already are huge: the last resultant computed has degree 60 and 9520 terms, and the 3-variable projection set already has 890 such polynomials..."

D. Research design and objectives

In light of the apparent present computational intractability in obtaining exact results in the 9-dimensional real (and \(a fortiori\) 15-dimensional complex) two-qubit cases, we adjusted the research program pursued in \([15]\). We now sought to determine how far we would have to curtail the dimension (the number of free parameters) of the two-qubit systems in order to be able to obtain exact results using the same basic investigative framework. Such results — in addition to their own intrinsic interest — might help us understand those previously obtained (basically numerically) in the full 9-dimensional real and 15-dimensional complex cases \([15]\).

To pursue such a strategem, we chose to nullify various \(m\)-subsets of the six symmetrically-located off-diagonal pairs in the 9-parameter real density matrix \((1)\), and tried to exactly implement the so-reduced non-negativity conditions \((2), (3), (4)\) and \((5)\) — both the first three (to obtain HS total volumes) and then all four jointly (to obtain HS separable volumes). We leave the four diagonal entries themselves alone in all our analyses, so if we nullify \(m\) pairs of symmetrically-located off-diagonal entries, we are left in a \((9-m)\)-dimensional setting. We consider the various combinatorially distinct scenarios individually, though it would appear that we also could have grouped them into classes of scenarios equivalent under local operations, and simply analyzed a single representative member of each equivalence class.

We will be examining a number of scenarios of various dimensionalities (that is, differing numbers of variables parameterizing \(\rho\)). In all of them, we will seek to find the univariate function \(S_{scenario}(\nu)\) (our primary computational and theoretical challenge) and the constant
\(c_{\text{scenario}}\), such that
\[
V_{\text{sep/scenario}}^{\text{HS}} = \int_0^\infty S_{\text{scenario}}(\nu) J_{\text{scenario}}(\nu) d\nu, \tag{16}
\]
and
\[
V_{\text{tot/scenario}}^{\text{HS}} = c_{\text{scenario}} \int_0^\infty J_{\text{scenario}}(\nu) d\nu. \tag{17}
\]
Given such a pair of volumes, one can immediately calculate the corresponding HS separability probability,
\[
P_{\text{sep/scenario}}^{\text{HS}} = \frac{V_{\text{sep/scenario}}^{\text{HS}}}{V_{\text{tot/scenario}}^{\text{HS}}}. \tag{18}
\]
Let us note that in the full 9-dimensional real and 15-dimensional complex two-qubit cases recently studied in [15], it was quite natural to expect that \(S_{\text{real}}(\nu) = S_{\text{real}}(\frac{1}{\nu})\) (and \(S_{\text{complex}}(\nu) = S_{\text{complex}}(\frac{1}{\nu})\)). But, here, in our lower-dimensional scenarios, the nullification of entries that we employ, breaks symmetry (duality), so we can not realistically expect such a reciprocity property to hold, in general. Consequently, we adopt the more general, broader formula in (13) as our working formula (16).

II. QUBIT-QUBIT ANALYSES

To begin, let us make the simple observation that since the partial transposition operation on a \(4 \times 4\) density matrix interchanges only the (1,4) and (2,3) entries (and the (4,1) and (3,2) entries), any scenario which does not involve at least one of these entries must only yield separable states.

A. Five nullified pairs of off-diagonal entries — 6 scenarios

1. 4-dimensional real case — \(P_{\text{sep}}^{\text{HS}} = \frac{3\pi}{16}\)

There are, of course, six ways of nullifying five of the six off-diagonal pairs of entries of \(\rho\). Of these, only two of the six yield any non-separable (entangled) states. In the four trivial (fully separable) scenarios, the lower-dimensional counterpart to \(S_{\text{real}}(\nu)\) was of the form \(S_{\text{scenario}}(\nu) = c_{\text{scenario}} = 2\).

In one of the two non-trivial scenarios, having the (2,3) and (3,2) pair of entries of \(\rho\) left
intact (not nullified), the separability function was

\[
S_{[2,3]}(\nu) = \begin{cases} 
2\sqrt{\nu} & 0 \leq \nu \leq 1 \\
2 & \nu > 1
\end{cases}
\] (19)

(It is of interest to note that \(B_\nu(\frac{1}{2}, 1) = 2\sqrt{\nu}\), while in [15], we had conjectured that \(S_{\text{real}}(\nu) \propto B_\nu(\frac{1}{2}, \sqrt{3})\) and \(S_{\text{complex}}(\nu) \propto B_\nu(\frac{2\sqrt{6}}{5}, \frac{\sqrt{2}}{5})\).)

In the other non-trivial scenario, with the (1,4) and (4,1) pair being the one not nullified, the separability function was — in a dual manner (mapping \(f(\nu)\) for \(\nu \in [0, 1]\) into \(f(\frac{1}{\nu})\) for \(\nu \in [1, \infty]\)) — equal to

\[
S_{[1,4]}(\nu) = \begin{cases} 
2 & 0 \leq \nu \leq 1 \\
\frac{2}{\sqrt{\nu}} & \nu > 1
\end{cases}
\] (20)

In both of these scenarios (having \(c_{\text{scenario}} = 2\)) for the total (separable and non-separable) HS volume, we obtained \(V_{\text{HS}}^{\text{tot}} = \frac{\pi}{48} \approx 0.0654498\) and \(V_{\text{sep}}^{\text{HS}} = \frac{\pi^2}{256} \approx 0.0385531\). The corresponding HS separability probability for the two non-trivial (dual) scenarios is, then, \(\frac{3\pi}{16} \approx 0.589049\).

2. 5-dimensional complex case — \(P_{\text{sep}}^{\text{HS}} = \frac{1}{3}\)

Although our study here was initially intended to concentrate only on \(4 \times 4\) density matrices with solely real entries, at a later point in our analyses, we returned to (first) the \(m = 5\) case, but now with the single non-nullified pair of symmetrically-located entries being complex in nature (so, obviously we have five variables/parameters in toto to consider, rather than four).

Again, we have only the same two scenarios (of the six combinatorially possible) being separably non-trivial. Based on the (2,3) and (3,2) pair of entries, the relevant function (with the slight change of notation to indicate complex entries) was

\[
S_{[\tilde{2},3]}(\nu) = \begin{cases} 
\pi \nu & 0 \leq \nu \leq 1 \\
\pi & \nu > 1
\end{cases}
\] (21)

and, dually,

\[
S_{[\tilde{1},4]}(\nu) = \begin{cases} 
\frac{\pi}{\nu} & 0 \leq \nu \leq 1 \\
\pi & \nu > 1
\end{cases}
\] (22)
So, the function $\sqrt{\nu}$, which appeared ((19), (20)) in the corresponding scenarios restricted to real entries, is replaced by $\nu$ itself in the complex counterpart. (We note that $B_{\nu}(1, 1) = \nu$.)

For both of these complex scenarios, we had $V_{\text{tot}}^{HS} = \frac{\pi}{120}$ and $V_{\text{sep}}^{HS} = \frac{\pi}{360}$, for a particularly simple HS separability probability of $\frac{1}{3}$.

3. 7-dimensional quaternionic case — $P_{\text{sep}}^{HS} = \frac{1}{10}$

Here we allow the single pair of non-null off-diagonal entries to be quaternionic in nature [31, 32, 33, sec. IV]. We found

$$S_{[\widetilde{(2,3)}]}(\nu) = \begin{cases} \frac{\pi^2 \nu^2}{2} & 0 \leq \nu \leq 1 \\ \frac{\pi^2}{2} & \nu > 1 \end{cases} \tag{23}$$

and, dually,

$$S_{[\widetilde{(1,4)}]}(\nu) = \begin{cases} \frac{\nu^2}{2} & 0 \leq \nu \leq 1 \\ \frac{\pi^2 \nu^2}{2} & \nu > 1 \end{cases} \tag{24}$$

(We note that $B_{\nu}(2, 1) = \frac{\nu^2}{2}$.) For both scenarios, we had $V_{\text{tot}}^{HS} = \frac{\pi^2}{360}$, $V_{\text{sep}}^{HS} = \frac{\pi^2}{3600}$, giving us $P_{\text{sep}}^{HS} = \frac{1}{10}$ — which is the smallest probability we will report in this entire paper.

So, in our first set of simple ($m = 5$) scenarios, we observe a decrease in the probabilities of separability from the real to the complex to the quaternionic case, as well as a progression from $\sqrt{\nu}$ to $\nu$ to $\nu^2$ in the functional forms occurring in the corresponding HS separability probability functions.

The exponents of $\nu$ in this progression, that is $1/2, 1, 2$ bear an evident relation to the Dyson indices [34], 1, 2, 4, corresponding to the Gaussian orthogonal, unitary and symplectic ensembles [35]. Certainly, this observation bears further investigation, in particular since the foundational work of Życzkowski and Sommers [17]) in computing the HS (separable plus nonseparable) volumes itself relies strongly on random matrix theory. (“[T]hese explicit results may be applied for estimation of the volume of the set of entangled [emphasis added] states” [17, p. 10125].) However, this theory is framed in terms of the eigenvalues and eigenvectors of random matrices — which do not appear explicitly in the Bloore parameterization — so, it is not altogether transparent in what manner one might proceed. (But for the $m = 5$ highly sparse density matrices for this set of scenarios, one can explicitly transform between the eigenvalues and the Bloore parameters.)
B. Four nullified pairs of off-diagonal entries — 15 scenarios

1. 5-dimensional real case — $P_{sep}^{HS} = 5 \cdot \frac{16}{3\pi^2}$

Here, there are fifteen possible scenarios, all with $V_{tot}^{HS} = \frac{\pi^2}{480}$. Six of them are trivial (separability probabilities of 1), in which $c_{\text{scenario}}$ is either $\pi$ (scenarios [(1,2), (1,3)], [(1,2), (2,4)], [(1,3), (3,4)] and [(2,4), (3,4)]) or 4 (scenarios [(1,2), (3,4)] and [(1,3), (2,4)]). Eight of the nine non-trivial scenarios all have — similarly to the 4-dimensional analyses (sec. II A 1) — separability functions $S(\nu)$ either of the form,

$$S_{\text{scenario}}(\nu) = \begin{cases} \pi \sqrt{\nu} & 0 \leq \nu \leq 1 \\ \pi & \nu > 1 \end{cases}, \quad (25)$$

(for scenarios [(1,2), (2,3)], [(1,3), (2,3)], [(2,3), (2,4)] and [(2,3), (3,4)]) or, dually,

$$S_{\text{scenario}}(\nu) = \begin{cases} \pi & 0 \leq \nu \leq 1 \\ \frac{\pi}{\sqrt{\nu}} & \nu > 1 \end{cases} \quad (26)$$

(for scenarios [(1,2), (1,4)], [(1,3), (1,4)], [(1,4), (2,4)] and [(1,4), (3,4)]). The corresponding HS separability probabilities, for all eight of these non-trivial scenarios, are equal to $\frac{5}{8} = 0.625$. This result was, in all the eight cases, computed by taking the the ratio of $V_{sep}^{HS} = \frac{\pi^2}{768}$ to $V_{tot}^{HS} = \frac{\pi^2}{480}$.

In the remaining (ninth) non-trivially entangled case — based on the non-nullified dyad [(1,4),(2,3)] — we have, taking the ratio of $V_{sep}^{HS} = \frac{1}{90}$ to $V_{tot}^{HS} = \frac{\pi^2}{480}$, a quite different Hilbert–Schmidt separability probability of $\frac{16}{3\pi^2} \approx 0.54038$. This isolated scenario (with $c_{\text{scenario}} = 4$) can also be distinguished from the other eight partially entangled scenarios, in that it is the only one for which entanglement occurs for both $\nu < 1$ and $\nu > 1$. We have

$$S_{[(1,4),(2,3)]}(\nu) = \begin{cases} 4\sqrt{\nu} & 0 \leq \nu \leq 1 \\ \frac{4}{\sqrt{\nu}} & \nu > 1 \end{cases} \quad (27)$$

By way of illustration, in this specific case, we have the scenario-specific marginal jacobian function,

$$J_{[(1,4),(2,3)]}(\nu) = -\frac{\sqrt{\nu}(-3\nu^2 + (\nu(\nu + 4) + 1)\log(\nu) + 3)}{30(\nu - 1)^5}. \quad (28)$$
2. 6-dimensional mixed (real and complex) case — $P_{sep}^{HS} = \frac{105\pi}{512} \cdot \frac{135\pi}{1024} \cdot \frac{3}{8}$

Here, we again nullify all but two of the off-diagonal entries ($m = 4$) of $\rho$, but allow the first of the two non-nullified entries to be complex in nature. Making (apparently necessary) use of the circular/trigonometric transformation $\rho_{11} = r^2 \sin^2 \theta$, $\rho_{22} = r^2 \cos^2 \theta$, we were able to obtain an interesting variety of exact results. One of these takes the form,

$$S_{[(1,2),(1,4)]}^{\tilde{1}}(\nu) = S_{[(1,3),(1,4)]}^{\tilde{1}}(\nu) = \begin{cases} \left\{ \frac{4\pi}{3}, 0 \leq \nu \leq 1 \right\} \\ \left\{ \frac{4\pi}{3\sqrt{\nu}}, \nu > 1 \right\} \end{cases}. \quad (29)$$

Now, we have $V_{tot}^{HS} = \frac{\pi^2}{1440}$ and $V_{sep}^{HS} = \frac{7\pi^3}{49152}$, so $P_{sep}^{HS} = \frac{105\pi}{512} \approx 0.644272$. The two dual scenarios — having the same three results — are $[(1,2), (2,3)]$ and $[(1,3), (2,3)]$.

Additionally, we have an isolated scenario,

$$S_{[(1,4),(2,3)]}^{\tilde{1}}(\nu) = \begin{cases} \left\{ 2\pi \sqrt{\nu}, 0 \leq \nu \leq 1 \right\} \\ \left\{ \frac{2\pi}{\nu}, \nu > 1 \right\} \end{cases}, \quad (30)$$

for which, $V_{tot}^{HS} = \frac{\pi^2}{1440}$ and $V_{sep}^{HS} = \frac{3\pi^3}{3840}$, so $P_{sep}^{HS} = \frac{135\pi}{1024} \approx 0.414175$. (Note the presence of both $\sqrt{\nu}$ and $\nu$ in (30) — apparently related to the mixed [real and complex] nature of this scenario (cf. (33)).)

Further,

$$S_{[(1,4),(2,4)]}^{\tilde{1}}(\nu) = \begin{cases} \left\{ \frac{4\pi}{3}, 0 \leq \nu \leq 1 \right\} \\ \left\{ \frac{4\pi}{3\sqrt{\nu}}, \nu > 1 \right\} \end{cases}, \quad (31)$$

the dual scenarios being $[(2,3), (2,4)]$ and $[(2,3), (3,4)]$. For all four of these scenarios, $V_{tot}^{HS} = \frac{\pi^2}{1440}$ and $V_{sep}^{HS} = \frac{\pi^2}{3840}$, so $P_{sep}^{HS} = \frac{3}{8} = 0.375$.

3. 7-dimensional complex case — $P_{sep}^{HS} = \frac{2}{9}$

Here, in an $m = 4$ setting, we nullify four of the six off-diagonal pairs of the $4 \times 4$ density matrix, allowing the remaining two pairs both to be complex. We have (again observing a shift from $\sqrt{\nu}$ in the real case to $\nu$ in the complex case)

$$S_{[(1,2),(1,4)]}^{\tilde{1}}(\nu) = S_{[(1,3),(1,4)]}^{\tilde{1}}(\nu) = S_{[(1,4),(2,4)]}^{\tilde{1}}(\nu) = S_{[(1,4),(3,4)]}^{\tilde{1}}(\nu) = \begin{cases} \frac{\pi^2}{2}, 0 \leq \nu \leq 1 \\ \frac{\pi^2}{2\nu}, \nu > 1 \end{cases}. \quad (32)$$

Since $V_{tot}^{HS} = \frac{\pi^2}{5040}$ and $V_{sep}^{HS} = \frac{\pi^2}{12000}$, we have $P_{sep}^{HS} = \frac{2}{9} = 0.4$. We have the same three outcomes for the four dual scenarios $[(1,2), (2,3)], [(1,3), (2,3)], [(2,3), (2,4)]$ and $[(2,3), (3,4)]$.\n
as well as — rather remarkably — for the (again isolated [cf. (30)]) scenario [(1, 4), (2, 3)], having the (somewhat different) separability function (manifesting entanglement for both \( \nu < 1 \) and \( \nu > 1 \)),

\[
S_{[(1,4),(2,3)]}(\nu) = \begin{cases} 
\frac{\pi^2 \nu}{2} & 0 \leq \nu \leq 1 \\
\frac{\pi^2}{\nu} & \nu > 1
\end{cases}.
\]  

(33)

(However, \( c_{\text{scenario}} = \pi^2 \) for this isolated scenario, while it equals \( \frac{\pi^2}{2} \) for the other eight.) The remaining six (fully separable) scenarios (of the fifteen possible) simply have \( P_{sep}^{HS} = 1 \).

4. 8-dimensional mixed (real and quaternionic) case

We report here that

\[
c_{[(\tilde{1}, 2), (1, 4)]} = \frac{8\pi^2}{15}, \quad c_{[(1,2), (\tilde{1}, 4)]} = 32, \tag{34}
\]

where as before the wide tilde notation denote the quaternionic off-diagonal entry.

C. Three nullified pairs of off-diagonal entries — 20 scenarios

1. 6-dimensional real case — \( P_{sep}^{HS} = 2 - \frac{435\pi^4}{1024\pi^4} \approx \frac{9}{16} \)

Here \( (m = 3) \), there are twenty possible scenarios — nullifying triads of off-diagonal pairs in \( \rho \). Of these twenty, there are four totally separable scenarios — corresponding to the non-nullified triads [[1,2], (1,3), (2,4)], [[1,2], (1,3), (3,4)], [(1,2), (2,4), (3,4)] and [[1,3], (2,4), (3,4)] — with \( c_{\text{scenario}} = \frac{\pi^2}{2} \) and \( V_{tot}^{HS} = V_{sep}^{HS} = \frac{\pi^3}{5760} \). To proceed further in this 6-dimensional case — in which we began to encounter some computational difficulties — we sought, again, to enforce the four nonnegativity conditions (2, 3, 1, 5), but only after setting \( \nu \) to specific values, rather than allowing \( \nu \) to vary. We chose the nine values \( \nu = \frac{1}{5}, \frac{2}{5}, \frac{3}{5}, \frac{4}{5}, 1, 2, 3, 4 \) and 5. Two of the scenarios (with the triads [[1,2], (2,3), (3,4)] and [[1,3],(2,3), (2,4)] could, then, be seen to fit unequivocally into our earlier observed predominant pattern, having the piecewise separability function,

\[
S_{[(1,2), (2,3), (3,4)]}(\nu) = S_{[(1,3), (2,3), (2,4)]}(\nu) = \begin{cases} 
\frac{\pi^2 \nu}{2} & 0 \leq \nu \leq 1 \\
\frac{\pi^2}{\nu} & \nu > 1
\end{cases}.
\]  

(35)
FIG. 1: Plot of $S_{[(1,2),(1,4),(2,3)]}(\nu)$ and the close fitting function (37). The former function slightly
dominates the latter except at $\nu = 1$, where they both equal $\frac{\pi^2}{2} \approx 4.9348$.

We, then, computed for these two scenarios that $V_{HS}^{tot} = \frac{\pi^3}{5760} \approx 0.00538303$ and (again making use of the transformation $\rho_{11} = r^2 \sin \theta^2$, $\rho_{22} = r^2 \cos \theta^2$) that $V_{sep}^{HS} = 2 \left( \frac{\pi^3}{5760} - \frac{29\pi^4}{786432} \right) \approx 0.00358207$. This gives us $P_{sep}^{HS} = 2 - \frac{435\pi}{1024} \approx 0.665437$. For two dual dyads, we have the same volumes and separability probability and, now, the piecewise separability function,

$$S_{[(1,2),(1,4),(2,3)]}(\nu) = S_{[(1,3),(1,4),(2,3)]}(\nu) = \begin{cases} \frac{\pi^2}{2} & 0 \leq \nu \leq 1 \\ \frac{\pi^2}{2\sqrt{\nu}} & \nu > 1 \end{cases} \quad (36)$$

Additionally, in Fig. II we are able to plot $S_{[(1,2),(1,4),(2,3)]}(\nu)$ along with its close fit to

$$S_{fit}(\nu) = \begin{cases} \frac{\pi^2 \sqrt{\nu}}{2} & 0 \leq \nu \leq 1 \\ \frac{\pi^2}{2\sqrt{\nu}} & \nu > 1 \end{cases} \quad (37)$$

(The analogous plots for the scenarios $[(1,3), (1,4), (2,3)]$ and $[(1,2), (1,3), (2,3)]$ appear to be precisely the same in character as Fig. II.) If we use the close fit (37) as a proxy for $S_{[(1,2),(1,4),(2,3)]}(\nu)$, we obtain an approximate HS separability probability of $\frac{9}{16} = \frac{\pi^3}{720} = 0.6625$.

We have not, to this point, been able to explicitly and succinctly characterize the functions $S_{scenario}(\nu)$ for non-trivial fully real $m = 3$ scenarios other than the dual pair (35), (36).

In all the separably non-trivial scenarios so far presented and discussed, we have had the relationship $S_{scenario}(1) = c_{scenario}$. However, in our present $m = 3$ setting (three pairs of nullified off-diagonal entries), we have situations in which $S_{scenario}(1) < c_{scenario}$. The values of $c_{scenario}$ in the sixteen non-trivial fully real $m = 3$ scenarios are either $\frac{\pi^2}{2} \approx 4.9348$ (twelve
occurrences) or \( \frac{4\pi}{3} \approx 4.18879 \) (four occurrences — \([1,2), (1,3), (1,4)\], \([1,2), (2,3), (2,4)\], \([1,3), (2,3), (3,4)\] and \([1,4), (2,4), (3,4)\]). In all four of the latter \( \left( \frac{4\pi}{3} \right) \) occurrences, though, we have the inequality,

\[
S_{\text{scenario}}(1) = \frac{1}{24} (12 + 16\pi + 3\pi^2) \approx 3.8281 < \frac{4\pi}{3} \approx 4.18879,
\]

as well as a parallel inequality for four of the twelve former \( \left( \frac{\pi^2}{2} \right) \) cases. The implication of these inequalities for those eight scenarios is that at \( \nu = 1 \) (the value associated with the fully mixed [separable] classical state), that is, when \( \rho_{11}\rho_{44} = \rho_{22}\rho_{33} \), there do exist non-separable states.

2. 7-dimensional mixed (one complex and two real) case — \( P^{HS}_{sep} = \frac{11}{16} \)

Here, in an \( m = 3 \) setting, we take the first entry of the non-nullified triad to be complex and the other two real. Of the twenty possible scenarios, four —\( [(1\tilde{2}), (1,3), (1,4)], [(1\tilde{2}), (2,3), (2,4)], [(1\tilde{3}), (2,3), (3,4)] \) and \([ (1\tilde{4}), (2,4), (3,4)] \) — had \( c_{\text{scenario}} = \frac{\pi^2}{2} \approx 4.9348 \) and these four all had the same (lesser) value of

\[
S_{\text{scenario}}(1) = \frac{56}{27} + \frac{\pi^2}{4} \approx 4.54148.
\]

There were seven scenarios with \( c_{\text{scenario}} = \frac{16\pi}{9} \approx 5.58505 \). Three of them — \([ (1\tilde{2}), (1,3), (2,4)], [(1\tilde{1}), (1,4), (2,3)] \) and \([ (1\tilde{3}), (1,4), (2,3)] \) — had \( S_{\text{scenario}}(1) = \frac{16\pi}{9} \) (manifesting equality), while four — \([ (1\tilde{2}), (1,3), (2,3)], [(1\tilde{2}), (1,4), (2,4)], [(1\tilde{3}), (1,4), (3,4)] \) and \([ (2\tilde{3}), (2,4), (3,4)] \) — had the result (39) (manifesting inequality).

The remaining nine of the twenty scenarios all had \( c_{\text{scenario}} = S_{\text{scenario}}(1) = \frac{2\pi^2}{3} \approx 6.57974 \). For one of them, we obtained

\[
S_{[(1\tilde{2}), (2,3), (3,4)]}(\nu) = \begin{cases} 
\frac{2\pi^2}{3} & \nu \geq 1 \\
\frac{2\pi^2\sqrt{\nu}}{3} & 0 < \nu < 1
\end{cases}
\]

with associated values of \( V^{HS}_{tot} = \frac{\pi^3}{20160} \), \( V^{HS}_{sep} = \frac{11\pi^3}{322560} \) and \( P^{HS}_{sep} = \frac{11}{16} \approx 0.6875 \). A dual scenario to this one that we were able to find was \([ (1,2), (1,4), (3,4)] \). The separability functions — and, hence, separability probabilities — for the other eighteen scenarios, however, are unknown to us at present.
3. 8-dimensional mixed (two complex and one real) case

Our sole result in this category is

\[ c_{[(\tilde{1},2), (\tilde{1},3), (1,4)]} = \frac{8\pi^2}{15}. \] (41)

4. 9-dimensional complex case

Now, we have three off-diagonal complex entries, requiring six parameters for their specification. According to the remarks of Strzebonski (sec. [C]), this is about the limit in the number of free off-diagonal parameters for which we might hopefully be able to determine associated separability functions.

As initial findings, we obtained

\[ S_{[(\tilde{1},4), (2,\tilde{3}), (2,\tilde{4})]}(1) = c_{[(\tilde{1},4), (2,\tilde{3}), (2,\tilde{4})]} = \frac{\pi^3}{4}, \] (42)

and also for scenarios \([(\tilde{1},2), (1,\tilde{4}), (3,\tilde{4})], [(\tilde{1},3), (1,\tilde{4}), (2,\tilde{4})], [(1,\tilde{4}), (2,\tilde{3}), (3,\tilde{4})]\), while

\[ c_{[(\tilde{1},2), (\tilde{1},3), (1,4)]} = c_{[(1,3), (2,\tilde{3}), (\tilde{3},4)]} = c_{[(1,4), (\tilde{2},\tilde{3}), (\tilde{2},\tilde{4})]} = \frac{\pi^3}{6}. \] (43)

D. Two or fewer nullified pairs of off-diagonal entries

1. 7-dimensional real case

The \([(1,2), (1,3), (2,4), (3,4)]\) scenario is the only fully separable one of the fifteen possible \((m = 2)\). For all the other fourteen non-trivial scenarios, there are non-separable states both for \(\nu < 1\) and \(\nu > 1\). For all fifteen scenarios, we have \(c_{\text{scenario}} = \frac{2\pi^2}{3} \approx 6.57974\). Otherwise, we have not so far been able to extend the analyses above to this \(m = 2\) fully real case (and \textit{a fortiori} the \(m = 1\) fully real case), even to determine specific values of \(S_{\text{scenario}}(1)\).

2. 8-dimensional real case

Here we have \(c_{\text{scenario}} = \frac{8\pi^2}{9} \approx 8.77298\) for all the six possible (separably non-trivial) scenarios \((m = 1)\). Let us note that this is, in terms of preceding values of these constants (for the successively lower-dimensional fully real scenarios), \(\frac{8\pi^2}{9} = \frac{4}{3}(\frac{2\pi^2}{3})\), while \(\frac{2\pi^2}{3} = \frac{4}{3}(\frac{\pi^2}{2})\).
Also, \( \frac{32\pi^2}{27} = \frac{4}{3}(\frac{8\pi^2}{9}) \), the further relevance of which will be apparent in relation to our discussion of the full 9-dimensional real scenario (sec. VIII).

III. QUBIT-QUTRIT ANALYSES

The cancellation property, we exploited above, of the Bloore parameterization — by which the determinant and principal minors of density matrices can be factored into products of (nonnegative) diagonal entries and terms just involving off-diagonal parameters \( (z_{ij}) \) — clearly extends to \( n \times n \) density matrices. It initially appeared to us that the advantage of the parameterization in studying the two-qubit HS separability probability question would diminish if one were to examine the two-qubit separability problem for other (possibly monotone) metrics than the HS one, or even the qubit-qutrit HS separability probability question. But upon some further analysis, we have found that the nonnegativity condition for the determinant of the partial transpose of a real \( 6 \times 6 \) (qubit-qutrit) density matrix (cf. (2)) can be expressed in terms of the corresponding \( z_{ij} \)'s and two ratio variables (thus, not requiring the five independent diagonal variables individually),

\[
\nu_1 = \frac{\rho_{11}\rho_{55}}{\rho_{22}\rho_{44}}, \quad \nu_2 = \frac{\rho_{22}\rho_{66}}{\rho_{33}\rho_{55}},
\]

rather than simply one (\( \nu \)) as in the \( 4 \times 4 \) case. (We compute the qubit-qutrit partial transpose by transposing in place the four \( 3 \times 3 \) blocks of \( \rho \), rather than — as we might alternatively have done — the nine \( 2 \times 2 \) blocks.)

A. Fourteen nullified pairs of off-diagonal entries — 15 scenarios

1. 6-dimensional real case — \( P_{sep}^{HS} = \frac{3\pi}{16} \)

To begin our examination of the qubit-qutrit case, we study the \( (m = 14) \) scenarios, in which only a single pair of real entries is left intact and all other off-diagonal pairs of the \( 6 \times 6 \) density matrix are nullified. (We not only require that the determinant of the partial transpose of \( \rho \) be nonnegative for separability to hold — as suffices in the qubit-qubit case, given that \( \rho \) itself is a density matrix [36, 37] — but also, per the Sylvester criterion, a nested series of principal leading minors of \( \rho \).) We have six separably non-trivial scenarios. (For all of them, \( V_{tot}^{HS} = \frac{\pi}{1440} \).)
Firstly, we have the separability function,

\[
S_{([1,5])}^{6 \times 6}(\nu_1) = \begin{cases} 
2 & \nu_1 \leq 1 \\
\frac{2}{\sqrt{\nu_1}} & \nu_1 > 1
\end{cases}
\] (45)

The dual scenario to this is \([2,4]\)]. Further,

\[
S_{([1,6])}^{6 \times 6}(\nu_1, \nu_2) = \begin{cases} 
2 & \nu_1 \nu_2 \leq 1 \\
\frac{2}{\sqrt{\nu_1 \nu_2}} & \nu_1 \nu_2 > 1
\end{cases}
\] (46)

with the dual scenario here being \([3,4]\)]. Finally,

\[
S_{([2,6])}^{6 \times 6}(\nu_2) = \begin{cases} 
2 & \nu_2 \leq 1 \\
\frac{2}{\sqrt{\nu_2}} & \nu_2 > 1
\end{cases}
\] (47)

having the dual \([3,5]\)].

The remaining nine possible scenarios — the same as their complex counterparts in the immediate next analysis — are all fully separable in character.

We have found that \(V_{HS}^{sep} = \frac{\pi^2}{7680}\) for the six non-trivially separable scenarios here, so \(P_{sep}^{HS} = \frac{3s}{16} \approx 0.589049\), as in the qubit-qubit analogous case (sec. II A 1).

2. 7-dimensional complex case — \(P_{sep}^{HS} = \frac{1}{3}\)

Now, we allow the single non-nullified pair of off-diagonal entries to be complex in nature (the two paired entries, of course, being complex conjugates of one another). \(V_{tot}^{HS} = \frac{\pi}{5040}\) for this series of fifteenb scenarios.) Then, we have (its dual being \([2,4]\])

\[
S_{([1,5])}^{6 \times 6}(\nu_1) = \begin{cases} 
\pi & \nu_1 \leq 1 \\
\frac{\pi}{\nu_1} & \nu_1 > 1
\end{cases}
\] (48)

Further, we have (with the dual \([3,4]\])

\[
S_{([1,6])}^{6 \times 6}(\nu_1, \nu_2) = \begin{cases} 
\pi & \nu_1 \nu_2 \leq 1 \\
\frac{\pi}{\nu_1 \nu_2} & \nu_1 \nu_2 > 1
\end{cases}
\] (49)

and (its dual being \([3,5]\])

\[
S_{([2,6])}^{6 \times 6}(\nu_2) = \begin{cases} 
\pi & \nu_2 \leq 1 \\
\frac{\pi}{\nu_2} & \nu_2 > 1
\end{cases}
\] (50)
For all six of these scenarios, $V_{sep} = \frac{\pi}{15120}$, so $P_{sep}^{HS} = \frac{1}{3}$.

B. Thirteen nullified pairs of off-diagonal entries — 105 scenarios

1. 7-dimensional real case — $P_{sep}^{HS} = \frac{5}{8} \cdot \frac{5}{16} \cdot \frac{3\pi}{32} \cdot \frac{16}{3\pi^2}$

Continuing along similar lines ($m = 13$), we have 105 combinatorially distinct possible scenarios. Among the separably non-trivial scenarios, we have

\[
S_{[(1,2),(1,5)]}^{6\times6}(\nu_1) = S_{[(1,4),(1,5)]}^{6\times6}(\nu_1) = \begin{cases} 
\pi & \nu_1 \leq 1 \\
\frac{\pi}{\sqrt{\nu_1}} & \nu_1 > 1
\end{cases}
\]

(duals being $[(1,2),(2,4)]$ and $[(1,4),(2,4)]$). We computed $V_{tot}^{HS} = \frac{\pi^2}{20610}$, $V_{sep}^{HS} = \frac{\pi^2}{32256}$, so $P_{sep}^{HS} = \frac{5}{8} = 0.625$ for these scenarios.

Also,

\[
S_{[(1,3),(1,6)]}^{6\times6}(\nu_1, \nu_2) = S_{[(1,4),(1,6)]}^{6\times6}(\nu_1, \nu_2) = \begin{cases} 
\pi & \nu_1 \nu_2 < 1 \\
\frac{\pi}{\sqrt{\nu_1 \nu_2}} & \nu_1 \nu_2 \geq 1
\end{cases}
\]

We, then, have $V_{tot}^{HS} = \frac{\pi^2}{20610}$, $V_{sep}^{HS} = \frac{\pi^2}{64512}$, so $P_{sep}^{HS} = \frac{5}{16} = 0.3125$.

Additionally,

\[
S_{[(1,4),(2,6)]}^{6\times6}(\nu_2) = \begin{cases} 
4 & \nu_2 \leq 1 \\
\frac{4}{\sqrt{\nu_2}} & \nu_2 > 1
\end{cases}
\]

For this scenario, we have $V_{tot}^{HS} = \frac{\pi^2}{20610}$, $V_{sep}^{HS} = \frac{\pi^2}{215040}$, so $P_{sep}^{HS} = \frac{3\pi}{32} \approx 0.294524$.

Further still,

\[
S_{[(1,5),(2,4)]}^{6\times6}(\nu_1) = \begin{cases} 
4 & \nu_1 \nu_2 < 1 \\
\frac{4}{\sqrt{\nu_1 \nu_2}} & \nu_1 \nu_2 \geq 1
\end{cases}
\]

For this scenario, we have $V_{tot}^{HS} = \frac{\pi^2}{20610}$, $V_{sep}^{HS} = \frac{1}{3780}$, so $P_{sep}^{HS} = \frac{16}{3\pi^2} \approx 0.54038$.

Further,

\[
S_{[(1,2),(2,6)]}^{6\times6}(\nu_2) = \begin{cases} 
\pi & \nu_2 \leq 1 \\
2 \left( \cos^{-1} \left( \sqrt{1 - \frac{1}{\nu_2}} \right) + \frac{\nu_2^{-1}}{\nu_2} \right) & \nu_2 > 1
\end{cases}
\]

The separability function for $[(1,3),(1,5)]$ is obtained from this one by replacing $\nu_2$ by $\nu_1$.

Also,

\[
S_{[(1,2),(3,4)]}^{6\times6}(\nu_1, \nu_2) = \begin{cases} 
\pi & \nu_1 \nu_2 \leq 1 \\
\frac{\pi}{\sqrt{\nu_1 \nu_2}} & \nu_1 \nu_2 > 1
\end{cases}
\]
The separability function for $[(1,2),(3,5)]$ can be obtained from this one by setting $\nu_1 = 1$.

2. 8-dimensional mixed (real and complex) case — $P_{sep}^{HS} = \frac{105\pi}{512}$

Further, we have (with $V_{tot}^{HS} = \frac{\pi^3}{38880}$ for all scenarios),

$$S^{6 \times 6}_{[(1,2),(2,4)]}(\nu_1) = S^{6 \times 6}_{[(1,4),(2,4)]}(\nu_1) = \begin{cases} \frac{4\pi \sqrt{\nu_1}}{3} & 0 < \nu_1 < 1 \\ 2\pi - \frac{2\pi}{3\nu_1} & \nu_1 > 1 \end{cases}$$

(57)

Since $V_{sep}^{HS} = \frac{\pi^3}{393216}$, we have $P_{sep}^{HS} = \frac{105\pi}{512} \approx 0.644272$ for both these scenarios.

Further,

$$S^{6 \times 6}_{[(1,3),(2,4)]}(\nu_1) = \begin{cases} \frac{4\pi \sqrt{\nu_1}}{3} & 0 < \nu_1 < 1 \\ 2\pi - \frac{2\pi}{3\nu_1} & \nu_1 > 1 \end{cases}$$

(58)

and

$$S^{6 \times 6}_{[(1,3),(3,4)]}(\nu_1, \nu_2) = S^{6 \times 6}_{[(1,4),(3,4)]}(\nu_1, \nu_2) = \begin{cases} \frac{4\pi \sqrt{\nu_1 \nu_2}}{3} & \nu_1 \nu_2 \geq 1 \\ \frac{1}{3} \pi \sqrt{\nu_1 \nu_2} & 0 < \nu_1 \nu_2 < 1 \end{cases}$$

(59)

Additionally,

$$S^{6 \times 6}_{[(2,3),(3,4)]}(\nu_1, \nu_2) = \begin{cases} \frac{4\pi}{3} & \nu_1 \nu_2 \geq 1 \\ \frac{2\pi}{3} \sqrt{\nu_1 \nu_2} (3 - \nu_1 \nu_2) & 0 < \nu_1 \nu_2 < 1 \end{cases}$$

(60)

and

$$S^{6 \times 6}_{[(1,2),(3,4)]}(\nu_1, \nu_2) = \begin{cases} \frac{4\pi}{3} & \nu_1 \nu_2 = 1 \\ \frac{4}{3} \pi \sqrt{\nu_1 \nu_2} & 0 < \nu_1 \nu_2 < 1 \end{cases}$$

(61)

We have also obtained the separability function (Fig. 2)

$$S^{6 \times 6}_{[(2,3),(2,4)]}(\nu_1) = \begin{cases} \frac{4\pi}{3} & \nu_1 \geq 1 \\ \frac{2\pi}{3} (3 - \nu_1) \sqrt{\nu_1} & 0 < \nu_1 < 1 \end{cases}$$

(62)

Of the 105 possible scenarios, sixty had $S^{6 \times 6}_{scenario}(1,1) = c_{scenario} = \frac{4\pi}{3}$, thirty-three had $S^{6 \times 6}_{scenario}(1,1) = c_{scenario} = 2\pi$, and twelve (for example, $[(3,4),(5,6)]$) had $S^{6 \times 6}_{scenario}(1,1) = \frac{4\pi}{3} < c_{scenario} = 2\pi$. 

23
3. 9-dimensional complex case — \( P_{sep}^{HS} = \frac{1}{3}; \frac{2}{5} \)

We have obtained the results

\[
S_{[1,2),(2,4)]}^{6 \times 6}(\nu_1) = S_{[1,4),(2,4)]}^{6 \times 6}(\nu_1) = \begin{cases} \frac{\pi^2 \nu_1}{2} & 0 \leq \nu_1 \leq 1 \\ \frac{\pi^2}{2} \nu_1 & \nu_1 > 1 \end{cases}, \quad (63)
\]

Since \( V_{tot}^{HS} = \frac{\pi^2}{362880} \) and \( V_{sep}^{HS} = \frac{\pi^2}{907200} \), we have here \( P_{sep}^{HS} = \frac{2}{5} = 0.4 \). We have the same three outcomes also based on the separability function,

\[
S_{[1,4),(3,4)]}^{6 \times 6}(\nu_1, \nu_2) = \begin{cases} \frac{\pi^2}{2} \nu_1 \nu_2 & \nu_1 \nu_2 \geq 1 \\ \frac{1}{2} \pi^2 \nu_1 \nu_2 & \nu_1 \nu_2 < 1 \end{cases}, \quad (64)
\]

Further,

\[
S_{[(1,2),(3,4)]}^{6 \times 6}(\nu_1, \nu_2) = \begin{cases} \frac{2 \pi^2 \nu_1 \nu_2 - \pi^2}{2 \nu_1 \nu_2} & \nu_1 \nu_2 > 1 \\ \frac{1}{2} \pi^2 \nu_1 \nu_2 & 0 < \nu_1 \nu_2 \leq 1 \end{cases}, \quad (65)
\]

and

\[
S_{[(1,3),(2,4)]}^{6 \times 6}(\nu_1) = \begin{cases} \frac{\pi^2 \nu_1}{2} & 0 < \nu_1 \leq 1 \\ \pi^2 - \frac{\pi^2}{2 \nu_1} & \nu_1 > 1 \end{cases}. \quad (66)
\]

For both of these last two scenarios, we have \( V_{tot}^{HS} = \frac{\pi^2}{362880} \) and \( V_{sep}^{HS} = \frac{\pi^2}{362880} \), leading to \( P_{sep}^{HS} = \frac{1}{3} \approx 0.33333 \). Also, we have these same three outcomes based on the separability function,

\[
S_{[(2,3),(3,4)]}^{6 \times 6}(\nu_1, \nu_2) = \begin{cases} \frac{\pi^2}{2} \nu_1 \nu_2 & \nu_1 \nu_2 \geq 1 \\ \frac{1}{2} \pi^2 \nu_1 \nu_2 (2 - \nu_1 \nu_2) & 0 < \nu_1 \nu_2 < 1 \end{cases}. \quad (67)
\]
Of the 105 possible scenarios — in complete parallel to those in the immediately pre-
ceeding section — sixty had $S_{\text{scenario}}^{6 \times 6}(1, 1) = c_{\text{scenario}} = \frac{\pi^2}{2}$, thirty-three had $S_{\text{scenario}}^{6 \times 6}(1, 1) = c_{\text{scenario}} = \pi^2$, and twelve (for example, $[(3, 4), (5, 6)]$) had $S_{\text{scenario}}^{6 \times 6}(1, 1) = \frac{\pi^2}{2} < c_{\text{scenario}} = \pi^2$.

Our results in this (9-dimensional) section and the (8-dimensional) one immediately pre-
ceeding it are still incomplete with respect to various scenario-specific separability functions
and, thus, the associated HS separability properties.

C. Twelve nullified pairs of off-diagonal entries — 455 scenarios

1. 8-dimensional real case

Now, we allow three of the off-diagonal pairs of entries to be non-zero, but also require
them to be simply real. We found the separability function

$$S_{[(1,2),(1,3),(3,4)]}(\nu_1, \nu_2) = S_{[(1,2),(1,4),(3,4)]}(\nu_1, \nu_2) =$$

$$\begin{cases}
\frac{4\pi}{3} \\ \frac{4\pi}{3} \sqrt{\nu_1\nu_2} \\ \frac{4\pi}{3} \left(3 \sec^{-1} \left(\sqrt{\frac{\nu_1}{\nu_2}}\right) + 4\sqrt{\nu_1\nu_2} + \frac{\sqrt{\nu_1\nu_2-1}}{\nu_1\nu_2} - 4\sqrt{\nu_1\nu_2 - 1}\right)
\end{cases}
\begin{array}{l}
\frac{1}{\nu_1} = \nu_2 \wedge \nu_1 > 0 \\
\nu_1 > 0 \wedge \frac{1}{\nu_1} > \nu_2 \wedge \nu_2 > 0 . \\
\nu_1 > 0 \wedge \frac{1}{\nu_1} < \nu_2 .
\end{array}
$$

Also, we have

$$S_{[(1,3),(1,4),(2,4)]}(\nu_1) =$$

$$\begin{cases}
\frac{4\pi}{3} \\ \frac{4\pi}{3} \left(3 \sin^{-1} \left(\sqrt{\frac{1 - \frac{1}{\nu_1}}{3\nu_1}}\right) - 4\sqrt{\nu_1 - 1}\right) + \sqrt{\nu_1}\nu_1 + \sqrt{\nu_1 - 1}\nu_1 - 1)
\end{cases}
\begin{array}{l}
\nu_1 = 1 \\
0 < \nu_1 < 1 .
\end{array}
$$

IV. QUTRIT-QUTRIT ANALYSES

In the qubit-qubit ($4 \times 4$ density matrix) case, we were able to express the condition (5) that the determinant of the partial transpose of $\rho$ be nonnegative in terms of one supplementary variable ($\nu$), given by (6), rather than three independent diagonal entries. Similarly, in the qubit-qutrit ($6 \times 6$ density matrix) case, we could employ two supplementary variables ($\nu_1, \nu_2$), given by (44), rather than five independent diagonal entries.
For the qutrit-qutrit (9 × 9 density matrix) case, rather than eight independent diagonal entries, we found that one can employ the four supplementary variables,

\[ \begin{align*}
\nu_1 &= \frac{\rho_{11}\rho_{55}}{\rho_{22}\rho_{44}}, \\
\nu_2 &= \frac{\rho_{22}\rho_{66}}{\rho_{33}\rho_{55}}, \\
\nu_3 &= \frac{\rho_{33}\rho_{88}}{\rho_{55}\rho_{77}}, \\
\nu_4 &= \frac{\rho_{55}\rho_{99}}{\rho_{66}\rho_{88}}.
\end{align*} \] (70)

A. Thirty-five nullified pairs of off-diagonal entries — 36 scenarios

1. 10-dimensional complex case — \( P_{PPT}^{HS} = \frac{1}{3}; \frac{1}{9} \)

Here, we nullify all but one of the thirty-six pairs of off-diagonal entries of the 9 × 9 density matrix \( \rho \). We allow this solitary pair to be composed of complex conjugates. Since the Peres-Horodecki positive partial transposition (PPT) criterion is not sufficient to ensure separability, we accordingly modify our notation.

Our first result is

\[ S_{9 \times 9}^{[(1,5)]}(\nu_1) = \begin{cases} 
\pi & \nu_1 \leq 1 \\
\frac{\pi}{\nu_1} & \nu_1 > 1
\end{cases} \] (71)

(a dual scenario being \([ (2,4) ] \)). We have \( V_{tot}^{HS} = \frac{\pi}{3628800}, V_{PPT}^{HS} = \frac{\pi}{10886400} \), so \( P_{PPT}^{HS} = \frac{1}{3} \).

The same three outcomes are obtained based on the PPT function

\[ S_{9 \times 9}^{[(1,6)]}(\nu_1, \nu_2) = \begin{cases} 
\pi & \nu_1\nu_2 \leq 1 \\
\frac{\pi}{\nu_1\nu_2} & \nu_1\nu_2 > 1
\end{cases} \] (72)

On the other hand, we have \( V_{tot}^{HS} = \frac{\pi}{3628800}, V_{PPT}^{HS} = \frac{\pi}{21772800} \), and \( P_{PPT}^{HS} = \frac{1}{6} \) based on the PPT function

\[ S_{9 \times 9}^{[(6,8)]} (\nu_4) = \begin{cases} 
\pi & \nu_4 \geq 1 \\
\pi\nu_4 & 0 < \nu_4 < 1
\end{cases} \] (73)

Of the thirty-six combinatorially possible scenarios, thirteen had \( P_{PPT}^{HS} = \frac{1}{3} \), while four had \( P_{PPT}^{HS} = \frac{1}{3} \), and the remaining nineteen were fully separable in nature.

B. Thirty-four nullified pairs of off-diagonal entries — 630 scenarios

1. 12-dimensional complex case — \( P_{PPT}^{HS} = \frac{1}{3}; \frac{7}{36} \)

Since the number of combinatorially possible scenarios was so large, we randomly generated scenarios to examine.
Firstly, we found

\[ S_{9 \times 9}^{(1,4),(3,5)}(\nu_2) = \begin{cases} \pi^2 & \nu_2 \geq 1 \\ \pi^2 \nu_2 & 0 < \nu_2 < 1 \end{cases} \]  \hspace{1cm} (74) \]

For this scenario, we had \( V_{tot}^{HS} = \frac{\pi^2}{479001600}, V_{PPT}^{HS} = \frac{\pi^2}{1437004800} \), giving us \( P_{PPT}^{HS} = \frac{1}{3} \).

Also, we found

\[ S_{9 \times 9}^{(2,9),(6,9)}(\nu_2, \nu_4) = \begin{cases} \frac{\pi^2}{2} & \nu_2 \nu_4 \leq 1 \\ \frac{\pi^2(2\nu_2\nu_4-1)}{2\nu_2^2\nu_4^2} & \nu_2 \nu_4 > 1 \end{cases} \]  \hspace{1cm} (75) \]

For this scenario, we had \( V_{tot}^{HS} = \frac{\pi^2}{479001600}, V_{PPT}^{HS} = \frac{\pi^2}{2052864000} \), giving us \( P_{PPT}^{HS} = \frac{7}{30} \approx 0.23333 \).

V. QUBIT-QUBIT-QUBIT ANALYSES, I

For initial relative simplicity, let us regard an \( 8 \times 8 \) density matrix \( \rho \) as a bipartite system, a composite of a four-level system and a two-level system. Then, we can compute the partial transposition of \( \rho \), transposing in place its four \( 4 \times 4 \) blocks. The nonnegativity of this partial transpose can be expressed using just three ratio variables,

\[ \nu_1 = \frac{\rho_{11}\rho_{66}}{\rho_{22}\rho_{55}} \quad \nu_2 = \frac{\rho_{22}\rho_{77}}{\rho_{33}\rho_{66}} \quad \nu_3 = \frac{\rho_{33}\rho_{88}}{\rho_{44}\rho_{77}} \]  \hspace{1cm} (76) \]

rather than seven independent diagonal entries.

A. Twenty-seven nullified pairs of off-diagonal entries — 28 scenarios

1. 9-dimensional complex case — \( P_{PPT}^{HS} = \frac{1}{3} \)

We have the PPT function

\[ S_{8 \times 8}^{\{1,6\}}(\nu_1) = \begin{cases} \pi & \nu_1 \leq 1 \\ \pi \nu_1 & \nu_1 > 1 \end{cases} \]  \hspace{1cm} (77) \]

(Scenario \( [(2,5)] \) was dual to this one.) For this scenario, \( V_{tot}^{HS} = \frac{\pi}{362880}, V_{PPT}^{HS} = \frac{\pi}{1088640} \), yielding \( P_{PPT}^{HS} = \frac{1}{3} \). There were twelve scenarios, in toto, with precisely these three outcomes. The other sixteen were all fully separable in nature.
B. Twenty-six nullified pairs of off-diagonal entries — 378 scenarios

1. 11-dimensional complex case — \( P_{PPT}^{HS} = \frac{1}{3}; \frac{1}{9} \)

Again, because of the large number of possible scenarios, we chose them randomly for inspection.

Firstly, we obtained

\[
\mathcal{S}^{8\times8}_{[(3,5),(6,8)]}(\nu_1, \nu_2) = \begin{cases} 
\pi^2 & \nu_1 > 0 \land \frac{1}{\nu_1} \leq \nu_2 \\
\pi^2 \nu_1 \nu_2 & \nu_1 > 0 \land \frac{1}{\nu_1} > \nu_2 \lor \nu_2 > 0 
\end{cases}.
\]

(Of course, the symbols “\( \land \)” and “\( \lor \)” used by Mathematica in its output, denote the logical connectives “and” (conjunction) and “or” (intersection) of propositions.) For this scenario, we had \( V^{HS}_{tot} = \frac{\pi^2}{39916800}, V^{HS}_{PPT} = \frac{\pi^2}{119750400} \), giving us \( P_{PPT}^{HS} = \frac{1}{3} \).

Also,

\[
\mathcal{S}^{8\times8}_{[(2,5),(4,7)]}(\nu_1, \nu_2) = \begin{cases} 
\pi^2 & \nu_1 \geq 1 \land \nu_3 \geq 1 \\
\pi^2 \nu_1 & 0 < \nu_1 < 1 \land \nu_3 \geq 1 \\
\pi^2 \nu_3 & \nu_1 \geq 1 \land 0 < \nu_3 < 1 \\
\pi^2 \nu_1 \nu_3 & 0 < \nu_1 < 1 \land 0 < \nu_3 < 1 
\end{cases}.
\]

For this scenario, we had \( V^{HS}_{tot} = \frac{\pi^2}{39916800}, V^{HS}_{PPT} = \frac{\pi^2}{359251200} \), giving us \( P_{PPT}^{HS} = \frac{1}{9} \).

We also found the PPT function

\[
\mathcal{S}^{8\times8}_{[(1,3),(4,7)]}(\nu_1) = \begin{cases} 
\frac{\pi^2}{2} & \nu_3 = 1 \\
\frac{\pi^2 \nu_3}{2} & 0 < \nu_3 < 1 \\
\pi \left( \cos^{-1} \left( \sqrt{1 - \frac{1}{\nu_3}} \right) - \csc^{-1} \left( \sqrt{\nu_3} \right) \right) \nu_3 + \pi^2 - \frac{\pi^2}{2\nu_3} & \nu_3 > 1 
\end{cases}.
\]

VI. QUBIT-QUBIT-QUBIT ANALYSES. II

Here we regard the \( 8 \times 8 \) density matrix as a tripartite composite of three two-level systems, and compute the partial transpose by transposing in place the eight \( 2 \times 2 \) blocks of \( \rho \). (For symmetric states of three qubits, positivity of the partial transpose is sufficient to ensure separability \[38\].) Again the nonnegativity of the determinant could be expressed using three (different) ratio variables,

\[
\nu_1 = \frac{\rho_{11}\rho_{44}}{\rho_{22}\rho_{33}}; \quad \nu_2 = \frac{\rho_{44}\rho_{55}}{\rho_{33}\rho_{66}}; \quad \nu_3 = \frac{\rho_{55}\rho_{88}}{\rho_{66}\rho_{77}}.
\]

28
A. Twenty-seven nullified pairs of off-diagonal entries — 28 scenarios

1. 9-dimensional complex case — \( P_{PPT}^{HS} = \frac{1}{3} \)

There were, again, twelve of twenty-eight scenarios with non-trivial separability properties, all with \( V_{tot}^{HS} = \frac{\pi}{362880}, V_{PPT}^{HS} = \frac{\pi}{1088640} \), yielding \( P_{PPT}^{HS} = \frac{1}{3} \). One of these was

\[
S_{8 \times 8}^{(1,4)}(\nu_1) = \begin{cases} 
\pi \nu_1 \leq 1 \\
\frac{\pi}{\nu_1} \nu_1 > 1 
\end{cases}.
\]  

(82)

2. 11-dimensional complex case — \( P_{PPT}^{HS} = \frac{17}{60}, \frac{1}{3} \)

We obtained the PPT function

\[
S_{8 \times 8}^{(1,8),(5,7)}(\nu_1, \nu_2, \nu_3) = \begin{cases} 
\frac{\pi^2}{2} \nu_2 \nu_1 = \nu_3 \wedge \nu_1 > 0 \wedge \nu_2 > 0 \\
\pi^2 \nu_2 > 0 \wedge (\nu_1 = 0 \wedge \nu_3 \geq 0) \vee (\nu_3 = 0 \wedge \nu_1 > 0) \\
\frac{\pi^2 \nu_2}{4 \nu_1 \nu_3} \nu_1 < 0 \wedge \nu_2 > 0 \wedge \frac{\nu_2}{\nu_1} < \nu_3 \\
\pi^2 - \frac{\pi^2 \nu_2 \nu_3}{2 \nu_2} \nu_1 > 0 \wedge \nu_2 > 0 \wedge \frac{\nu_2}{\nu_1} > \nu_3 \wedge \nu_3 > 0 
\end{cases}.
\]  

(83)

For this we had \( V_{tot}^{HS} = \frac{\pi^2}{39916800}, V_{PPT}^{HS} = \frac{17\pi^2}{239500800} \), giving us \( P_{PPT}^{HS} = \frac{17}{60} \approx 0.283333 \).

Additionally,

\[
S_{8 \times 8}^{(1,4),(7,8)}(\nu_1) = \begin{cases} 
\pi^2 \nu_1 \leq 1 \\
\frac{\pi^2}{\nu_1} \nu_1 > 1 
\end{cases}.
\]  

(84)

Here, we had \( V_{tot}^{HS} = \frac{\pi^2}{39916800}, V_{PPT}^{HS} = \frac{17\pi^2}{119750400} \), giving us \( P_{PPT}^{HS} = \frac{1}{3} \).

Another PPT function we were able to find was

\[
S_{8 \times 8}^{(3,4),(3,8)}(\nu_2, \nu_3) = \begin{cases} 
\frac{\pi^2}{2} \nu_2 > 0 \wedge (\nu_3 = \nu_2 \lor (\nu_2 > \nu_3 \wedge \nu_2 < 2\nu_3) \lor (\nu_2 > 2\nu_3 \wedge \nu_3 \geq 0)) \\
\frac{\pi^2 \nu_3 (2\nu_3 - \nu_2)}{2\nu_3} \nu_2 > 0 \wedge \nu_2 < \nu_3 
\end{cases}.
\]  

(85)
VII. APPROXIMATE APPROACHES TO 9-DIMENSIONAL REAL QUBIT-QUBIT SCENARIO

As we have earlier emphasized (sec. I C), it appears that the simultaneous computational enforcement of the four conditions ((2), (3), (4), (5)) that would yield us the 9-dimensional volume of the separable real two-qubit states appears presently highly intractable. But if we replace (5) by less strong conditions on the nonnegativity of the partial transpose ($\rho^T$), we can achieve some form of approximation to the desired results. So, replacing (5) by the requirement (derived from a $2 \times 2$ principal minor of $\rho^T$) that

$$1 - \nu^2 z_{14}^2 \geq 0,$$

we obtain the approximate separability function (Fig. 3)

$$S_{\text{real}}(\nu) = \begin{cases} \frac{512 \pi^2}{27} & 0 < \nu \leq 1, \\ \frac{256 (3 \pi^2 \nu - \pi^2)}{27 \nu^{3/2}} & \nu > 1. \end{cases}$$

(87)

(In the analyses in this section, we utilize the integration limits on the $z_{ij}$’s [15, eqs. (3)-(5)] yielded by the cylindrical decomposition algorithm [CAD], to reduce the dimensionalities of our constrained integrations.) This yields an upper bound on the separability probability of the real 9-dimensional qubit-qubit states of

$$\frac{1}{2} + \frac{512}{135 \pi^2} \approx 0.88427.$$  

We obtain the same probability if we employ instead of (86) the requirement

$$\nu - \nu^2 z_{23}^2 \geq 0,$$

which yields the dual function to (87), namely,

$$S_{\text{real}}(\nu) = \begin{cases} \frac{512 \pi^2}{27} & \nu \geq 1, \\ \frac{256 \pi^2 (\nu - 3) \sqrt{\nu}}{27 \nu} & 0 < \nu < 1. \end{cases}$$

(89)

(The left-hand sides of (86) and (88) are the only two of the six $2 \times 2$ principal minors of $\rho^T$ that are non-trivially distinct — apart from cancellable nonnegative factors — from the corresponding minors of $\rho$ itself.) If we form a “quasi-separability” function by piecing together the non-constant segments of (86) and (88), we can infer — using a simple symmetry, duality argument — an improved lower bound on the HS separability probability of

$$\frac{1024}{135 \pi^2} \approx 0.76854.$$
A. Analytically-derived beta functions

We have not, to this point of time, been able to jointly enforce the constraints (86) and (88). (Doing so, would amount to solving a constrained four-dimensional integration problem.) However, we had some interesting success in jointly enforcing (86) along with the constraint

$$- z_{12}^2 + 2\sqrt{\nu}z_{13}z_{14}z_{12} - z_{13}^2 - \nu z_{14}^2 + 1 \geq 0,$$

(90)

corresponding to the first of the four principal $3 \times 3$ minors of $\rho^T$. (This amounts to solving a constrained three-dimensional integration problem.) In attempting to jointly enforce these two constraints, we obtained (without, however, being directly able to explicitly derive the separability function over $\mu \in [0, \infty]$) an upper bound on $V_{sep}^{HS}$ (and a consequent upper bound on $P_{sep}^{HS}$ of 0.77213) of

$$\frac{11\pi^4}{2116800} + \int_0^1 \check{J}_{\text{real}}(\mu)s_{\text{real}}(\mu)d\mu \approx 0.00124359.$$  

(91)

Here we have the approximate separability function (monotonically-decreasing for $\mu \in [0, 1]$),

$$s_{\text{real}}(\mu) = \frac{\pi^3 (13B\mu^2 \left(\frac{1}{2}, \frac{3}{2}\right) \mu^2 + (2\mu^2 - 13) B\mu^2 \left(\frac{3}{2}, \frac{1}{2}\right) - 2B\mu^2 \left(\frac{3}{2}, \frac{3}{2}\right))}{3\mu^3}.$$  

(92)

For (apparently necessary) convenience in computation, so that Mathematica only has to deal with integral powers rather than half-integer ones, we use $\mu = \sqrt{\nu}$ (as we did in our original study [27]) and the corresponding jacobian function [27, eq. (10)] (cf. (15)) is

$$\check{J}_{\text{real}}(\mu) = \frac{\mu^4 (12 ((\mu^2 + 2) (\mu^4 + 14\mu^2 + 8) \mu^2 + 1) \log(\mu) - 5 (5\mu^8 + 32\mu^6 - 32\mu^2 - 5))}{1890 (\mu^2 - 1)^9}.$$  

(93)
What is most interesting here, of course, is that we have beta functions (now derived analytically) explicitly appearing in the (approximate) separability function formula (92), while we only previously had numerical evidence for their relevance [15].

Though we sought to enforce additional constraints based on the principal minors of $\rho^T$, in order to obtain tighter upper bounds on $V_{sep}^{HS}$ and $P_{sep}^{HS}$, this did not seem to be computationally possible. (One might also pursue similar “approximate” strategies in the lower-dimensional instances, studied earlier in this paper, still not apparently amenable to exact solutions.)

Also, as was mentioned in the Introduction, we have not yet been able to exploit to derive HS separability functions and probabilities, the simplified integration limits (11) based on the spheroidal parameterization (10) suggested by the geometric discussion of Bloore [18, secs. 6, 7].

VIII. CONCLUDING REMARKS

Though we have regarded the derivation of the scenario-specific separability (and PPT) functions as our primary theoretical and computational challenge, the derivation of the HS separability (and PPT) probabilities from such functions — that is, the performance of an integration over the (n-1)-dimensional simplex spanned by the diagonal entries of the $n \times n$ density matrix $\rho$ — can also be quite difficult. (As a general, somewhat informal observation, real off-diagonal entries in our scenarios tend to yield square roots of the diagonal entries in the integrands, which prove more challenging to integrate than complex off-diagonal entries.)

The qubit-qubit results above motivated us to reexamine previously obtained results (cf. [27, eqs. (12), (13)]) and we would like to make the following observations pertaining to the full 9-dimensional real and 15-dimensional HS separability probability issue. We have the exact results in these two cases that

$$\int_0^\infty J_{\text{real}}(\nu) = 2\int_0^1 J_{\text{real}}(\nu) = \frac{\pi^2}{1146880} \approx 8.60561 \cdot 10^{-6}$$  (94)

and

$$\int_0^\infty J_{\text{complex}}(\nu) = 2\int_0^1 J_{\text{complex}}(\nu) = \frac{1}{1009008000} \approx 9.91072 \cdot 10^{-10}. \ (95)$$

Now, to obtain the corresponding total (separable plus nonseparable) HS volumes [17], that is, $\frac{\pi^4}{60480} \approx 0.0016106$ and $\frac{e^6}{85135000} \approx 1.12925 \cdot 10^{-6}$, one must multiply (94) and (95) by the
factors of $C_{\text{real}} = \frac{512\pi^2}{27} = \frac{2^8\pi^2}{3^3} \approx 187.157$ and $C_{\text{complex}} = \frac{32\pi^6}{27} = \frac{2^5\pi^6}{3^3} \approx 1139.42$, respectively.

To most effectively compare these previously-reported results with those derived above in this paper, one needs to multiply $C_{\text{real}}$ and $S_{\text{real}}(\nu)$, by $2^{-4} = \frac{1}{16}$ and in the complex case by $2^{-7} = \frac{1}{128}$. Doing so, for example, would adjust $C_{\text{real}}$ to equal $c_{\text{real}} = \frac{32\pi^2}{27} \approx 11.6973$, which we note, in line with our previous series of calculations [sec. II D 2] is equal to $\frac{4}{3}(\frac{8\pi^2}{9})$.

(Andai [39] also computed the same volumes — up to a normalization factor — as Sommers and Życzkowski [17].) Now, our estimates from [15] are that $S_{\text{real}}(1) = 114.62351 < C_{\text{real}}$ and $S_{\text{complex}}(1) = 387.50809 < C_{\text{complex}}$. These results would appear — as remarked above — to be a reflection of the phenomena that there are non-separable states for both the 9- and 15-dimensional scenarios at $\nu = 1$ (the locus of the fully mixed, classical state).

If we take as a trial function,

$$S_{\text{real}}(\nu) = 114.62351 \left( \begin{cases} \sqrt{\nu} & 0 \leq \nu \leq 1 \\ \frac{1}{\sqrt{\nu}} & \nu > 1 \end{cases} \right) \tag{96}$$

and insert it into our formula (13), as at least the lower-dimensional real results in Fig. II and (27) might suggest trying, we obtain the outcome, $V_{\text{sep/real}}^{\text{HS}} = 0.000613694$ and (using the known $V_{\text{tot/real}}^{\text{HS}}$) an associated HS separability probability of 0.381034. This — as we expected — is certainly not in accord with the numerical results of [15, sec. V.A.2]. The HS real separability probability was estimated there to be $P_{\text{sep/real}}^{\text{HS}} = 0.4538838$ and $S_{\text{real}}(\nu)$ (cf. (12)) was estimated to be closely proportional to the incomplete beta function $B_{\nu}(\frac{1}{2}, \sqrt{3})$ and not the quite different function $\sqrt{\nu} \propto B_{\nu}(\frac{1}{2}, 1)$, as our small exercise here assumes.

So, we may say, in partial summary that we have been able to obtain certain exact two-qubit HS separability probabilities in dimensions seven or less, making use of the advantageous Bloore parameterization [18], but not yet in dimensions greater than seven. This, however, is considerably greater than simply the three dimensions (parameters) we were able to achieve [7] in a somewhat comparable study based on the generalized Bloch representation parameterization [40, 41]. In [7] — extending an approach of Jakóbczyk and Siennicki [41] — we primarily studied two-dimensional sections of a set of generalized Bloch vectors corresponding to $n \times n$ density matrices, for $n = 4, 6, 8, 9$ and 10. For $n > 4$, by far the most frequently recorded HS separability [or positive partial transpose (PPT) for $n > 6$] probability was $\frac{3}{4} \approx 0.785398$. A very wide range of exact HS separability and PPT probabilities were tabulated.
Immediately below is just one of many matrix tables (this one being numbered (5) in [3]) presented in [7] (which due to its large size has been left simply as a preprint, rather than submitted directly to a journal). This table gives the HS separability probabilities for the qubit-qutrit case. In the first column are given the identifying numbers of a pair of generalized Gell-mann matrices (generators of \( SU(6) \)). In the second column of (97) are shown the number of distinct unordered pairs of \( SU(6) \) generators which share the same total (separable and nonseparable) HS volume, as well as the same separable HS volume, and consequently, identical HS separability probabilities. The third column gives us these HS total volumes, the fourth column, the HS separability probabilities and the last (fifth) column, numerical approximations to the exact probabilities (which, of course, we see — being probabilities — do not exceed the value 1). (Due to space/page width constraints, we were unable to generally present in these data arrays the HS separable volumes too, though they can, of course, be deduced from the total volume and the separability probability.)

\[
\begin{pmatrix}
\{1,13\} & 48 & \frac{4}{9} & \frac{\pi}{4} & 0.785398 \\
\{3,11\} & 4 & \frac{8\sqrt{2}}{27} & \frac{1}{\sqrt{2}} & 0.707107 \\
\{3,13\} & 4 & \frac{4}{9} & \frac{5}{\sqrt{6}} & 0.833333 \\
\{3,25\} & 4 & \frac{8\sqrt{2}}{27} & \frac{5}{4\sqrt{2}} & 0.883883 \\
\{8,13\} & 4 & \frac{2}{3} & \frac{1}{\sqrt{3}} & \sqrt{\frac{2}{3}} & 0.577350 \\
\{8,25\} & 4 & \frac{\sqrt{7}}{3} & \sqrt{\frac{2}{3}} & 0.816497 \\
\{11,15\} & 4 & \frac{4\sqrt{2\pi}}{27} & \frac{1}{3} + \frac{3\sqrt{2}}{4\pi} & 0.746830 \\
\{11,24\} & 2 & \frac{25\sqrt{2}}{72} & \frac{2}{3} + \frac{1}{2}\sin^{-1}\left(\frac{\sqrt{2}}{3}\right) & 0.863648 \\
\{13,24\} & 2 & \frac{25\sqrt{2}}{72} & \frac{8}{75} \left(-2 + 5\sqrt{5}\right) & 0.979236 \\
\{13,35\} & 4 & \frac{4\sqrt{7}}{5} & \frac{1}{12} \left(5 + 3\sqrt{5} \csc^{-1}\left(\frac{3}{\sqrt{5}}\right)\right) & 0.886838 \\
\{15,16\} & 4 & \frac{32\sqrt{3}}{81} & \frac{1}{12} \left(9\sqrt{3} + 4\pi\right) & 0.879838 \\
\{16,24\} & 2 & \frac{25}{144} \sqrt{\frac{2\pi}{3}} & \frac{4+5\sin^{-1}\left(\frac{\sqrt{2}}{3}\right)}{8\pi} & 0.549815 \\
\{20,24\} & 2 & \frac{25}{144} \sqrt{\frac{2\pi}{3}} & \frac{92+75\sin^{-1}\left(\frac{\sqrt{2}}{3}\right)}{75\pi} & 0.685627 \\
\{24,25\} & 2 & \frac{25}{27\sqrt{2}} & 1 - \frac{2}{5\sqrt{5}} & 0.821115 \\
\{24,27\} & 2 & \frac{25}{27\sqrt{2}} & \frac{92+75\cos^{-1}\left(\frac{3}{5}\right)}{80\sqrt{5}} & 0.903076 \\
\{25,35\} & 4 & \frac{\sqrt{7}}{5} & \sqrt{\frac{5+3\csc^{-1}\left(\frac{3}{\sqrt{5}}\right)}{3\pi}} & 0.504975 \\
\end{pmatrix}
\]

It might be of interest to address separability problems that appear to be computationally
intractable in the generalized Bloch representation by transforming them into the Bloore parameterization.

We leave the reader with the intriguing questions, still left unanswered: do simple, exact formulas exist for the Hilbert-Schmidt — and/or Bures, Kubo-Mori, Wigner-Yanase, . . . (cf. [9]) — separability probabilities for the full 9-dimensional and 15-dimensional convex sets of real and complex $4 \times 4$ density matrices (and the 20-dimensional and 35-dimensional convex sets of real and complex $6 \times 6$ density matrices)? Further, are there helpful intuitions — above and beyond the direct implementation of our formulas (16) and (17) — that can aid in understanding the abundance of elegant, simple results occurring in this general research area?

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