Moment-based evidence for simple rational-valued Hilbert–Schmidt generic $2 \times 2$ separability probabilities

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Abstract

Employing the Hilbert–Schmidt measure, we explicitly compute and analyze a number of determinantal product (bivariate) moments $|\rho|^k|\rho^{PT}|^n$, $k, n = 0, 1, 2, 3, \ldots$, with $PT$ denoting the partial transpose, for both generic (9-dimensional) two-rebit ($\alpha = 1$) and generic (15-dimensional) two-qubit ($\alpha = 1$) density matrices $\rho$. The results are, then, incorporated into a general formula, parameterized by $k, n$ and $\alpha$, with the case $\alpha = 2$, presumptively corresponding to generic (27-dimensional) quaternionic systems. Holding the Dyson-index-like parameter $\alpha$ fixed, the induced univariate moments $(|\rho||\rho^{PT}|)^n$ and $|\rho^{PT}|^n$ are inputted into a Legendre-polynomial-based (least-squares) probability-distribution reconstruction algorithm of Provost (2005 Mathematica J. 9 727), yielding $\alpha$-specific separability-probability estimates.

Since, as the number of inputted moments grows, estimates based on the variable $|\rho||\rho^{PT}|$ strongly decrease, while ones employing $|\rho^{PT}|$ strongly increase (and converge faster), the gaps between upper and lower estimates diminish, yielding sharper and sharper bounds. Remarkably, for $\alpha = 2$, with the use of 2325 moments, a separability-probability lower bound 0.999 999 987 as large as $2^{323} \approx 0.080 4954$ is found. For $\alpha = 1$, based on 2415 moments, a lower bound results that is 0.999 997 066 times as large as $8^{147} \approx 0.242 424$, a (simpler still) fractional value that had previously been conjectured (Slater 2007 J. Phys. A: Math. Theor. 40 14279). Furthermore, for $\alpha = \frac{1}{2}$, employing 3310 moments, the lower bound is 0.999 955 times as large as $29^{164} = 0.453 125$, a rational value previously considered (Slater 2010 J. Phys. A: Math. Theor. 43 195302).

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(Some figures may appear in colour only in the online journal)
1. Introduction

In a much cited paper [1], Życzkowski, Horodecki, Sanpera and Lewenstein expanded upon ‘three main reasons’—‘philosophical’, ‘practical’ and ‘physical’—for attempting to evaluate the probability that mixed states of composite quantum systems are separable in nature. Pursuing such a research agenda, it was conjectured [2, section IX]—based on ‘a confluence of numerical and theoretical results’—that the separability probabilities of generic (15-dimensional) two-qubit and (9-dimensional) two-rebit quantum systems, in terms of the Hilbert–Schmidt/Euclidean/flat measures [3, 4], are \( \frac{8}{33} \approx 0.242424 \) and \( \frac{8}{17} \approx 0.470588 \), respectively. In this study, we shall avail ourselves of newly proposed formulas (appendix D) for (bivariate) moments of products of determinants of density matrices (\( \rho \)) and of their partial transposes (\( \rho^{PT} \)) [5, 6] to investigate these hypotheses from a novel perspective, as well as extend our analyses beyond the strictly two-rebit and two-qubit frameworks. (To be fully explicit, we note here that both (symmetric) two-rebit and (Hermitian) two-qubit 4 \( \times \) 4 density matrices \( \rho \) have unit trace and nonnegative eigenvalues, while their partial transposes \( \rho^{PT} \) can be obtained by transposing in place the four 2 \( \times \) 2 blocks of \( \rho \). The Hilbert–Schmidt (HS) metric—from which the corresponding measure can, of course, be derived—is defined by the line element squared, \( \frac{1}{2} Tr((d\rho)^2) \) [4, equation (14.29)].)

Reconstructions of probability distributions based on these product moment formulas do prove to be highly supportive of the specific HS two-qubit conjecture (section 8.2), while definitively ruling out its two-rebit counterpart (section 8.1), but emphatically not a later advanced value of \( \frac{26}{33} \approx 0.787879 \) [7, p 6]. Extending these analyses from the real (\( \alpha = \frac{1}{2} \)) and complex (\( \alpha = 1 \)) cases to the (presumptively, since we lack relevant computer-algebraic determinantal moment calculations) generic (27-dimensional) quaternionic (\( \alpha = 2 \)) instance [8–11], in which the off-diagonal entries of the 4 \( \times \) 4 density matrices can be quaternions, we find that the value \( \frac{26}{33} \approx 0.787879 \) fits our moment-based computations, may we say, amazingly well (section 8.5). Nevertheless, the apparently formidable challenges of rigorously proving the determinantal moment formulas and/or the conjectured simple fractional separability probabilities certainly remain. (To again be explicit, the only rigorously demonstrated results reported in this paper are those we have been able to obtain through computer algebraic (Mathematica) methods—using the Cholesky-decomposition parameterization of \( \rho \)—for the moments of \( |\rho|^4 |\rho^{PT}|^n \) for \( n = 1, 2, \ldots, 13 \) for the two-rebit systems and \( n = 1, 2, 3, 4 \) for the two-qubit systems (section 2), and \( n = 1 \) for their qubit–qutrit [6 \( \times \) 6] counterparts (section 6), as well as \( n = 1, \ldots, 10 \) for minimally degenerate two-rebit systems (section 7). Aside from the presentation and discussion of these results, the paper is concerned with the (unproven) generalization to arbitrary \( n \) of these specific results, and its apparent successful application in probability-distribution reconstruction procedures (section 8). This latter step is taken in order to examine anew and extend certain conjectures as to the specific values of the separability probabilities, the properties of which were first investigated by Życzkowski, Horodecki, Sanpera and Lewenstein [1].)

In marked contrast to the finite-dimensional focus in this study on 2 \( \times \) 2 quantum systems (and, marginally, on 2 \( \times \) 3 systems (section 6)), let us note the (asymptotically based) conclusion of Ye that ‘the probability of finding separable quantum states within quantum states is extremely small and the Peres–Horodecki PPT criterion as tools to detect separability is imprecise for large \( N \), in the sense of both HS and Bures volumes’ [12, p 14]. (The Bures distance measures the length of a curve within the cone of positive operators on the Hilbert space [4, section 9.4], while the Bures volume of the set of mixed states is remarkably equal to the volume of an \((N^2 - 1)\)-dimensional hypersphere of radius \( \frac{1}{2} \) [4, p 351].) Also,
contrastingly, to the predominantly ‘nondegenerate/full-rank’ objectives here (cf section 7), Ruskai and Werner have demonstrated that ‘bipartite states of low rank are almost surely entangled’ [13].

2. Density-matrix determinantal product moments

Let us begin our investigation into the indicated statistical aspects of the ‘geometry of quantum states’ [4, 14] by noting the following two special cases—which will be extended in certain bivariate directions—of the (univariate determinantal moment) formulas [15, equation (3.2)] (cf [16, theorem 4]):

\[
\langle |\rho|^{k}\rangle_{\text{two-rebit}/\text{HS}} = 945 \left(4^{k-2} \frac{\Gamma(2k + 2)\Gamma(2k + 4)}{\Gamma(4k + 10)}\right)
\]

and

\[
\langle |\rho|^{k}\rangle_{\text{two-qubit}/\text{HS}} = 108972 864 000 \frac{\Gamma(k + 1)\Gamma(k + 2)\Gamma(k + 3)\Gamma(k + 4)}{\Gamma(4(k + 4))},
\]

\(k = 0, 1, 2, \ldots\) The bracket notation \(\langle \rangle\) is employed to denote the expected value, while \(\rho\) indicates a generic (symmetric) two-rebit or generic (Hermitian) two-qubit (4 \(\times\) 4) density matrix. The expectation is taken with respect to the probability distribution determined by the HS/Euclidean/flat metric on either the 9-dimensional space of generic two-rebit or the 15-dimensional space of generic two-qubit systems [3, 4].

At the outset of our study, we were able to compute seventeen (thirteen two-rebit and four two-qubit) non-trivial (bivariate) extensions of these two formulas, involving now in addition to \(\rho\) the quantum-theoretically important determinant \(|\rho^{PT}|\). (The nonnegativity of \(|\rho^{PT}|\)—as a corollary of the celebrated Peres–Horodeccy results [5, 6]—constitutes a necessary and sufficient condition for separability/disentanglement, when \(\rho\) is a 4 \(\times\) 4 density matrix [17, 18].) At this point of our presentation, we note that three of these seventeen extensions are expressible—incorporating as the last factors on their right-hand sides the two formulas above ((1) and (2))—as

\[
\langle |\rho|^{k}|\rho^{PT}|\rangle_{\text{two-rebit}/\text{HS}} = \frac{(k-1)(k(2k + 11) + 16)}{32(k + 3)(4k + 11)(4k + 13)} \langle |\rho|^{k}\rangle_{\text{two-rebit}/\text{HS}},
\]

\[
\langle |\rho|^{k}|\rho^{PT}|^{2}\rangle_{\text{two-rebit}/\text{HS}} = \frac{k(k(k(4k(k + 12) + 203) + 368) + 709) + 2940) + 4860}{1024(k + 3)(k + 4)(4k + 11)(4k + 13)(4k + 15)(4k + 17)}
\times \langle |\rho|^{k}\rangle_{\text{two-rebit}/\text{HS}}
\]

and

\[
\langle |\rho|^{k}|\rho^{PT}|\rangle_{\text{two-qubit}/\text{HS}} = \frac{k(k + 6) - 42}{8(2k + 9)(4k + 17)(4k + 19)} \langle |\rho|^{k}\rangle_{\text{two-qubit}/\text{HS}}.
\]

These three new formulas were, initially, established by ‘brute force’ computation—that is calculating the first \((k = 0, 1, 2, \ldots, 15\) or so) instances of them, then employing the Mathematica command FindSequenceFunction and verifying the formulas generated on still higher values of \(k\).

Let us note here the ranges of the two variables of central interest, \(|\rho| \in [0, \frac{1}{256}]\) and \(|\rho^{PT}| \in [-\frac{1}{16}, \frac{1}{16}]\). For various analytical and conventional purposes, it is often convenient to have variables defined over the unit interval \([0,1]\). If we so (linearly) transform the two determinantal variables, then the rational factors on the right-hand sides of (3) and (4) get replaced, respectively, by

\[
\frac{8(k(k(34k + 297) + 867) + 842)}{17(k + 3)(4k + 11)(4k + 13)}
\]
3. The mixed/balanced variable $|\rho||\rho^{PT}| = |\rho^{PT}|$

As a special case ($k = 1$) of formula (3), we obtain the rather remarkable moment result, zero, already reported in [19]. The immediate interpretation of this finding is that for the generic two-rebit systems, the two determinants $|\rho|$ and $|\rho^{PT}|$ comprise a pair of nine-dimensional orthogonal polynomials [20–22] with respect to the HS measure. (Orthogonality here does not imply zero correlation. The analogous quantity for generic two-qubit systems is not zero, however, but $-\frac{1}{576 \times 262}$.) In addition to this first ($k = 1$) HS zero moment of the product variable $|\rho||\rho^{PT}|$ in the two-rebit case, we had been able to compute its higher order moments, $k = 2, \ldots, 6$. (The result for $k = 2$, that is, $\frac{5096.347.144.800}{38576}$, can be obtained by direct application of formula (4).)

3.1. Range of the variable

The feasible range of the (mixed/balanced) variable is $|\rho||\rho^{PT}| \in \left[ -\frac{1}{110592}, \frac{1}{110592} \right]$—the lower bound of which $-\frac{1}{110592} = -2^{-12} 3^{-2}$. This lower bound, determined by analyzing a general convex combination of a Bell state and the fully mixed state, can be achieved with the entangled two-rebit density matrix

$$
\rho = \begin{pmatrix}
\frac{1}{6} & \frac{1}{6 \sqrt{2}} & \frac{1}{12} (-1 - \sqrt{3}) & \frac{1}{12} (-1 + \sqrt{3}) \\
\frac{1}{6 \sqrt{2}} & \frac{1}{6} & \frac{1}{3} & \frac{1}{6 \sqrt{2}} \\
\frac{1}{12} (-1 - \sqrt{3}) & \frac{1}{3} & \frac{1}{6} & \frac{1}{6 \sqrt{2}} \\
\frac{1}{12} (-1 + \sqrt{3}) & \frac{1}{6 \sqrt{2}} & \frac{1}{6 \sqrt{2}} & \frac{1}{6}
\end{pmatrix}.
$$

The determinant of $\rho$ here is $\frac{1}{768} (2 \sqrt{3} - 3) \approx 0.000 805 732$ and that of its partial transpose is $\frac{1}{768} (-3 - 2 \sqrt{3}) \approx -0.011 2224$ (their product being $-\frac{1}{110592} \approx -9.04225 \times 10^{-6}$). Both $\rho$ and $\rho^{PT}$ here have three identical eigenvalues ($\frac{1}{12} (3 - \sqrt{3}) \approx 0.105 662$ for $\rho$ and $\frac{1}{12} (3 + \sqrt{3}) \approx 0.394 338$ for $\rho^{PT}$). The isolated eigenvalues for $\rho$ and $\rho^{PT}$ are $\frac{1}{12} (1 + \sqrt{3}) \approx 0.683 013$ and $\frac{1}{12} (1 - \sqrt{3}) \approx -0.183 013$, respectively. The purity (index of coincidence [4, p 56]) of (8) equals $\frac{1}{2}$, so the participation ratio is 2. Its concurrence is $\frac{1}{2} \left( \sqrt{3} - 1 \right) \approx 0.366 025$, while its entanglement of formation is [4, section 15.7]

$$
E_{\text{complex}}[\rho] = \frac{\log(2) (\log(84 + 48 \sqrt{3}) - \sqrt{3} \log(3))}{4 \log (1 + \frac{1}{\sqrt{3}}) \log (1 + \sqrt{3})} \approx 1.216 65.
$$

(In support, we note the computed zeros in the Gaussian quadrature analyses (appendix D.5) of the two-rebit case fit well into the known ranges of $|\rho|$ and $|\rho^{PT}|$.) Alternatively, taking into account the real nature of the entries of $\rho$, in the sense of the ‘foil’ theory of Caves, Fuchs and Runge [23], one has a concurrence of [24, equation (4)] $-\frac{1}{\sqrt{3}}$, and an entanglement of formation [24, equation (2)] of

$$
E_{\text{real}}[\rho] = \frac{\log(2) (\log(1728) + 2 \sqrt{6} \tanh^{-1} \left( \frac{\sqrt{3}}{2} \right))}{6 \log(6 - 2 \sqrt{6}) \log(2(3 + \sqrt{6}))} \approx 6.568 25.
$$

(7)
4. Contour plots of bivariate probability distributions

For the further edification of the reader, we present in figure 1 a numerically generated contour plot of the joint HS (bivariate) probability distribution of $|\rho|$ and $|\rho^{PT}|$ in the two-rebit case, and in figure 2, its two-qubit analog. (A colorized grayscale output is employed, in which larger values appear lighter.) In figure 3, the difference obtained by subtracting the second (two-qubit) distribution from the first (two-rebit) distribution is displayed.

(The black curves in all three contour plots appear to be attempts by Mathematica to establish the nonzero–zero probability boundaries—which would, of course, be of interest to explicitly determine/parameterize, if possible—of the joint domain of $|\rho|$ and $|\rho^{PT}|$.)

These last three figures are based on Hibert–Schmidt sampling (utilizing Ginibre ensembles [15]) of random density matrices, using $10000 = 100^2$ bins. In regard to the two-qubit plot, Życzkowski informally wrote: ‘A high peak in the upper corner means that (a) a majority of the entangled states are ‘little entangled’ (small det$(\rho^T)$) or rather, they are ‘close’ to the boundary of the set, so one eigenvalue is close to zero and the determinant is small; (b) as det$(\rho)$ is also small, it means that these entangled states live close to the boundary of the set of all states (at least one eigenvalue is very small), but this is very much consistent with the observation that the center of the convex body of the two-qubit states is separable (so entangled states have to live ‘close’ to the boundary). Similar reasoning has to hold in the real case as well’.
Figure 2. Contour plot of the joint HS probability distribution of $|\rho|$ (horizontal axis) and $|\rho^{PT}|$ in the two-qubit case. Six hundred million random density matrices were employed.

5. Determinantal product moment formulas

5.1. Two-rebit case

At a still later point in our investigation, we realized that we might make further progress—despite apparent limitations on the number of determinantal moments we could explicitly compute—by exploiting the evident pattern followed by our newly found formulas (3) and (4)—in particular, the structure in their denominators. This encouragingly proved to be the case, as we were able to additionally establish that

$$\langle|\rho|^k|\rho^{PT}|^3\rangle_{\text{two-rebit/HS}} = \frac{A_3}{B_3} \langle|\rho|^k\rangle_{\text{two-rebit/HS}},$$  \hspace{1cm} (11)

where

$$A_3 = 8k^9 + 180k^8 + 1674k^7 + 8559k^6 + 29493k^5 + 84291k^4 + 136801k^3 - 401334k^2 - 2516616k - 3612816$$  \hspace{1cm} (12)

and

$$B_3 = 32768(k+3)(k+4)(k+5)(4k+11)(4k+13) \times (4k+15)(4k+17)(4k+19)(4k+21).$$  \hspace{1cm} (13)

So it then became rather evident that we can write for general nonnegative integer $n$

$$\langle|\rho|^k|\rho^{PT}|^n\rangle_{\text{two-rebit/HS}} = \frac{A_n}{B_n} \langle|\rho|^k\rangle_{\text{two-rebit/HS}},$$  \hspace{1cm} (14)
where both the numerator $A_n$ and the denominator $B_n$ are 3n-degree polynomials (thus, forming a ‘biproper rational function’ [25]) in $k$ (the leading coefficient of $A_n$ being $2^n$), and

$$B_n = 128^n (k + 3) \frac{(2k + \frac{11}{2})_{2n}}{2^n}, \quad (15)$$

where the Pochhammer symbol $(x)_n \equiv \frac{\Gamma(x+n)}{\Gamma(x)} = x(x+1) \cdots (x+n-1)$ is employed. Further still, moving upward to the next level ($n = 4$), we determined that

$$\langle |\rho|^{k} |\rho_{\text{PT}}|^{4} \rangle_{\text{two-rebit/HS}} = \frac{A_4}{B_4} \langle |\rho|^{k} \rangle_{\text{two-rebit/HS}}, \quad (16)$$

where

$$A_4 = 16k^{12} + 576k^{11} + 9112k^{10} + 84 496k^9 + 52 5681k^8 + 23 89416k^7 + 7805 462k^6$$
$$+ 13 904 508k^5 + 6212 189k^4 + 166 748 972k^3 + 1636 873 812k^2$$
$$+ 5496 485 760k + 6610 161 600, \quad (17)$$

and $B_4$ is given by (15) with $n = 4$. The real part of one of the roots of $A_4$ is 2.999 905, suggesting to us some possible interesting asymptotic behavior of the roots of these numerators, $n \to \infty$. In a related predecessor study [19, section II.B.2], we had been able to discern the general structure that the denominators of certain ‘intermediate (rational) functions’ used in computing the (univariate) moments of $\langle |\rho_{\text{PT}}|^{n} \rangle_{\text{two-rebit/HS}}, n = 1, \ldots, 9$, followed.

From our four new two-rebit determinantal moment results (3), (4), (11) and (16), we see that the constant terms in the 3n-degree numerator $A_n$ are $-164 860$, $-3612 816$ and $6610 161 600$ for $n = 1, 2, 3, 4$. Since we had previously computed [19, equations (33)–(41)] the moments of $\langle |\rho_{\text{PT}}|^{n} \rangle_{\text{two-rebit/HS}}, n = 1, \ldots, 9$, we were also immediately able to determine the next five members of this sequence $\{-16, 4860, -3612 816, 6610 161 600\}$. However, no
general rule for this sequence, which would, interestingly, directly allow us to obtain a formula for \(\langle |\rho PT| \rangle_{\text{two-qubit/HS}}\), had yet emerged for them.

Certainly, it would be of interest to conduct analyses parallel to those reported above for metrics of quantum-information-theoretic interest other than the HS, such as the Bures (minimal monotone) metric [4, 16, 26]. The computational challenges involved, however, might, at least in certain respects, be even more substantial.

5.2. Use of Cholesky decomposition in rigorously finding formulas for general \(k\)

After having posted the results above, along with additional ones, as a preprint [27], One of us (CD) detailed a computational proposal that he had outlined somewhat earlier. The particularly attractive feature of this proposal was that it would—holding the exponent \(n\) of \(|\rho PT|\) fixed—be able to compute the adjustment factors for general \(k\), rather than having to do so for sufficient numbers of individual members of the sequence \(k = 1, \ldots, N\), so that we could successfully apply the Mathematica command FindSequenceFunction, as had been our strategy heretofore.

The proposal (appendix D) involved parameterizing \(4 \times 4\) density matrices in terms of their Cholesky decompositions. The parameters (ten in number for the two-rebit case and sixteen for the two-qubit case) would be viewed as points on the surface of a unit (due to the trace requirement) 10-sphere or 16-sphere. The squares of the points lie in a simplex. One can then employ the corresponding Dirichlet probability distributions over the simplices to determine the associated expected values (joint moments). (A further highly facilitating aspect here is that both \(|\rho|\) and the jacobian for the transformation to Cholesky variables are simply monomials in the variables.) Using this approach, we were able to extend our single \((n = 1, \alpha = 1)\) two-qubit result (5) to the \(n = 2\) case,

\[
\langle |\rho|^{k} |\rho PT|^{2} \rangle_{\text{two-qubit/HS}} = \frac{k(k(k(k(k + 15) + 67) + 45) + 220) + 10944}{64(2k + 9)(2k + 11)(4k + 17)(4k + 19)(4k + 21)(4k + 23)} \langle |\rho|^{k} \rangle_{\text{two-qubit/HS}}.
\]

(18)

Additionally, in the following array,

\[
\begin{pmatrix}
-16 & 4860 & -3612816 & 6610161600 & -23680812672000 & 147885533254368000 \\
5 & 2940 & -2516616 & 5496485760 & -21644930613600 & 144374531813568000 \\
9 & 709 & -401334 & 1636873812 & -7755993054000 & 58524043784903280 \\
2 & 368 & 136801 & 166748972 & -1199508017652 & 11977854861441312 \\
-203 & 84291 & 6212189 & -4378482660 & 1052189083196640 \\
-48 & 29493 & 13904508 & 29246867605 & -30302414250528 \\
-4 & 8559 & 7805462 & 7876634465 & -6899036908859 \\
-1 & 1674 & 2389416 & 2649513956 & 3583820785224 \\
-1 & 180 & 525681 & 883461216 & 1632448582425 \\
-1 & 8 & 84496 & 219916945 & 477741210624 \\
-1 & - & 9112 & 40679505 & 118164517947 \\
-1 & - & 576 & 5660714 & 238170088564 \\
-1 & - & 16 & 575800 & 3786901675 \\
-1 & - & - & 40000 & 469728096 \\
-1 & - & - & 1680 & 44685468 \\
-1 & - & - & 32 & 3143808 \\
-1 & - & - & - & 153360 \\
-1 & - & - & - & 4608 \\
-1 & - & - & - & 64
\end{pmatrix}
\]

(19)
we show \((n = 1, \ldots, 6)\), column by column, the \((3n + 1)\) coefficients of the numerator polynomials in ascending order—the entries in the first row corresponding to the constant terms, \ldots—in the two-rebit case.

Additional results for the cases \(n = 7, \ldots, 13\) were found \([27, \text{equations (17)}–(21)]\). The leading (highest order) coefficients in these 13 sets of two-rebit results were found to be expressible in descending order as

\[
C_{3n+1} = 2^n; \quad C_{3n} = 3 \times 2^{n-1} n(n + 2); \quad C_{3n-1} = 2^{n-3} n(n(9n + 32) + 24) - 45; \quad (20)
\]

\[
C_{3n-2} = 2^{n-4} n(n(n(9n^2 + 42n + 52) - 119) - 52) - 60. \quad (21)
\]

From these four formulas, we are able to reconstruct \((n = 1)\) all four entries in the first column of equation (19). Thus, it appears that, in general, \(C_{3n-i}\) is a polynomial in \(n\) of degree \(2(i + 1)\). (For \(i = 3n-1\), we obtain the constant term, of strong interest. With the full knowledge of all the constant terms, and none of the other coefficients, we could obtain the univariate moments \(\langle |\rho_{PT}|^n \rangle_{\text{two-rebit/HS}}\).) Further, we have found that

\[
C_{3n-3} = \frac{1}{5} 2^{n-7} (n - 1)(135n^7 + 855n^6 + 1895n^5 - 1771n^4 - 3091n^3 - 7731n^2 + 32394n), \quad (22)
\]

and

\[
C_{3n-4} = \frac{1}{5} 2^{n-8} (n - 1)m(n(n(n(3n(9n + 59) + 377) - 2887) - 2295) - 10535) + 112 240) - 181 492) + 436 720. \quad (23)
\]

### 5.3. Two-qubit formulas

The numerators of our four sets \((n = 1, 2, 3, 4)\) of two-qubit results (the first two having been obtained by ‘brute force’ Mathematica computations, and the last two, using the Cholesky-decomposition parameterization) are expressible, in similar fashion, as

\[
\begin{pmatrix}
-42 & 10944 & -6929280 & 9247219200 \\
-1 & 4260 & -3684384 & 6039653760 \\
6 & 220 & -456948 & 1342859616 \\
1 & 45 & 80168 & 64072440 \\
- & 67 & 27783 & -13235252 \\
- & 15 & 5373 & 1080858 \\
- & 1 & 1458 & 1160375 \\
- & - & 282 & 278478 \\
- & - & 27 & 50991 \\
- & - & 1 & 7542 \\
- & - & - & 749 \\
- & - & - & 42 \\
- & - & - & 1
\end{pmatrix}. \quad (24)
\]

We observe that the leading coefficients \(C_{3n-i}\) of all four numerators are 1, so they are monic in character, while the next-to-leading coefficients fit the pattern \(C_{3n} = 3n(n + 3)/2\).

It is evident at this point, in striking analogy to the general two-rebit formula (14), that in the two-qubit scenario,

\[
\langle |\rho|^k \rangle_{\text{two-qubit/HS}} = \frac{\hat{A}_n}{3^n} \langle |\rho|^k \rangle_{\text{two-qubit/HS}}, \quad (25)
\]
where, again, both the numerator $\hat{A}_n$ and the denominator $\hat{B}_n$ are 3\(n\)-degree polynomials in \(k\), and (cf (15))

\[
\hat{B}_n = 2^{6n}(k + \frac{9}{2})_n(2k + \frac{13}{2})_{2n}.
\]

### 6. Determinantal product moment formulas for 6 \(\times\) 6 density matrices

Of course, one may also consider issues analogous to those discussed above for bipartite quantum systems of higher dimensionality. To begin such a course of analysis, we have found for the generic real 6 \(\times\) 6 (‘rebit–retrit’) density matrices (occupying a 20-dimensional space) the result

\[
\langle |\rho| k |\rho_{PT} | \rangle_{\text{rebit–retrit}} / \text{HS} = \frac{4k^5 + 40k^4 + 95k^3 - 220k^2 - 1149k - 1170}{576(k + 4)(3k + 11)(3k + 13)(6k + 23)(6k + 25)}
\times \langle |\rho| k \rangle_{\text{rebit–retrit}} / \text{HS}.
\] (26)

Increasing the exponential parameter \(n\) from 1 to 2, we obtained that the rational function adjustment factor for \(\langle |\rho| k |\rho_{PT} | ^2 \rangle_{\text{rebit–retrit}} / \text{HS}\) is the ratio of

\[
16k^9 + 336k^8 + 2616k^7 + 8496k^6 + 12069k^5 + 101979k^4 + 903539k^3 + 3316809k^2 + 5620320k + 3715740
\]

\[
\times (6k + 25)(6k + 29)(6k + 31).
\] (27)

Additionally, for the generic complex 6 \(\times\) 6 (qubit–qutrit) density matrices (occupying a 35-dimensional space), we have obtained the result

\[
\langle |\rho| k |\rho_{PT} | ^n \rangle_{\text{qubit–qutrit}} / \text{HS} = \frac{k^5 + 15k^4 + 37k^3 - 423k^2 - 2558k - 3840}{72(2k + 13)(3k + 19)(3k + 20)(6k + 37)(6k + 41)}
\times \langle |\rho| k \rangle_{\text{qubit–qutrit}} / \text{HS}.
\] (28)

It should be pointed out, however, that in contrast to the 4 \(\times\) 4 density-matrix case, the nonnegativity of the determinant of the corresponding partial transpose of a 6 \(\times\) 6 density matrix does not guarantee separability, since possibly two eigenvalues of the partial transpose could be negative, indicative of entanglement, while still yielding a nonnegative determinant (cf [17]).

### 7. Minimally degenerate two-rebit density matrices

For the eight-dimensional manifold composed of generic minimally degenerate two-rebit systems (corresponding to the density matrices \(\rho\) with at least one eigenvalue zero), forming the boundary of the nine-dimensional manifold of generic two-rebit systems, we have computed the HS moments of \(|\rho_{PT}^n|, n = 1, \ldots, 10\). (For such systems, \(|\rho_{PT}^n| \in [-\frac{1}{16}, \frac{1}{16}]\).) These results are given in appendix C. (One of us (CD) was able to find rational functions of \(k\) for \(n = 1, 2, 3\)—but not yet further—which yielded these moments when \(k\) was set to zero.)

We note that as a particular case of results of Szarek, Bengtsson and Życzkowski [28], the HS probability that a generic two-rebit system is separable is twice the HS probability that a generic minimally degenerate two-rebit system is separable.
8. Estimation of separability probabilities, using conjectured formulas

8.1. Two-rebit case ($\alpha = \frac{1}{2}$)

We now utilize the conjectured formulas (appendix D.6)—developed at an intermediate stage in our research effort—with the Dyson-index-type parameter $\alpha$ set to $\frac{1}{2}$, corresponding to the two-rebit case. In figure 4, we display the corresponding HS separability-probability estimates obtained by application of the Legendre-polynomial-based probability-density reconstruction (Mathematica) procedure of Provost [29, equation (15)]—yielding least-squares approximating polynomials—to the sequence of the first 3310 moments of $(|\rho||\rho^{PT}|)^n$ (upper blue curve) and to the sequence of the first 3310 moments of $|\rho^{PT}|^n$ (lower red curve). (All our computations here and below were conducted with 48-digit accuracy. A uniform ‘baseline density’ was, in effect, assumed, while the use in this capacity of a beta distribution, fitted to the first two moments, and Jacobi polynomials yielded highly erratic estimates when the corresponding Mathematica algorithm of Provost [29, pp 750–2] was applied.)

In figure 4, the last/highest pair of estimates is $\{0.453\,104\,500, 0.454\,543\,513\}$, so it certainly appears that the true (common) separability probability for the two variables must lie within this interval. The convergence properties of the two sequences of estimates display parallel (increasing–decreasing) behavior in the two-qubit case. (In appendix D.5, we develop a distinct/alternative probability-distribution reconstruction approach of interest—which is applied to considerably fewer moments than 3310—to the two-rebit separability-probability estimation problem.)

Our 2007 hypothesis [2, section X.A] that the HS separability probability of generic two-rebit systems is $\frac{5}{27} \approx 0.470\,588$ can, thus, be decisively rejected (figure 4), since it clearly lies outside the confining interval. We will here note that in the later 2010 study [7, p 7], a numerical estimate of 0.452 8427, substantially different from $\frac{5}{27}$, was reported, and it was additionally observed that in [2, section V.A.2], the best numerical estimate of the two-rebit separability probability obtained there had been 0.453 8838. A possible exact value of $\frac{5}{27} = 0.453\,125$—which does lie within the confining interval in figure 4—was, in fact, suggested in [7, p 6]. Use
of linear algebraic principles did allow us in [7] to establish an upper bound on the generic two-rebit HS separability probability of \( \frac{1129}{2100} \approx 0.537619 \).

We note, importantly, that the lower bound of the confining interval 0.4531014500 is 0.999955 times as large as \( \frac{29}{64} \).

8.2. Two-qubit case \((\alpha = 1)\)

In figure 5, we similarly show—for the two-qubit case \((\alpha = 1)\)—the estimates obtained by the application of the probability-distribution reconstruction procedure of Provost [29, equation (15)] to sequences of 2415 moments of \((|\rho||\rho^{PT}|)^n\) (upper blue curve) and \(|\rho^{PT}|^n\) (lower red curve). We, of course, note that the lower bound obtained of 0.2424235313 seems to support well our 2007 hypothesis [2, section X.B] that the HS separability probability of generic two-qubit systems is \( \frac{233}{833} \approx 0.242424 \). (The ratio of this lower bound to that based on 2414 moments is 1.0000006779, indicative of strong convergence. The analogous ratio for the upper estimate was 0.99999153401—somewhat less strong.)

Zyczkowski, Horodecki, Sanpera and Lewenstein, in their foundational paper [1, equation (36)], provided a numerical estimate—0.632 \( \pm \) 0.002—of the generic two-qubit separability probability, using as a measure the product of the uniform distribution on the 3-simplex of eigenvalues and the Haar measure on the 15-dimensional \( 4 \times 4 \) unitary matrices. (The \( 4 \times 4 \) density matrices were, then, in a sense, over-parameterized. The authors were ‘surprised’ that the probability exceeded 50%.) They also advanced [1, equation (35)] certain analytical arguments that the probability was in the interval [0.302, 0.863]. While these studies are of great conceptual interest, they did not specifically employ as measures those defined by the volume elements of metrics of interest (such as the HS, Bures, ...) over the quantum states.

8.3. Reconstructed probability distributions

In figures 6 and 7, we show (based on 200 moments, using now the procedure of Mnatsakanov [30]), rather than that of Provost [29], the reconstructed HS two-rebit and two-qubit probability
Figure 6. Reconstructed—and linearly transformed to [0,1]—HS two-rebit probability distributions based on 200 moments of $|\rho|\rho^{PT}$ (blue, lower peaked curve) and $|\rho^{PT}|$ (red, higher peaked curve).

Figure 7. Reconstructed—and linearly transformed to [0,1]—HS two-qubit probability distributions based on 200 moments of $|\rho|\rho^{PT}$ (blue, lower peaked curve) and $|\rho^{PT}|$ (red, higher peaked curve).

distributions for both sets of moments, all distributions linearly transformed to the interval [0,1].

8.4. $\alpha$ as a free parameter

As an exercise of interest, let us consider the Dyson-index-like parameter $\alpha$ in appendix D.6, with the values $\frac{1}{4}$ and 1 conjecturally corresponding to the two-rebit and two-qubit moments, respectively, as a free/continuous parameter (cf [31]), and perform our standard separability-probability calculations using the Provost algorithm [29]—taking the same ranges as before for the determinantal moment variables. Based on 96 moments, we obtain figure 8.

8.5. $\alpha = 2$ (quaternionic?)

In figure 9, we show—for the $\alpha = 2$ (presumptively quaternionic) case (appendix D.6)—the estimates obtained by application of the procedure of Provost [29, equation (15)] to the
Figure 8. Separability-probability estimates as a function of the parameter $\alpha$ (appendix D.6). The upper curve is based on 96 moments of $|\rho||\rho_{PT}|$ and the lower curve on 96 moments of $|\rho_{PT}|$. Also included as horizontal lines are the two-rebit ($\alpha = \frac{1}{2}$), two-qubit ($\alpha = 1$) and two-‘quaterbit’ ($\alpha = 2$) and ‘classical’ ($\alpha = 0$) conjectures of Andai [16, theorem 4], in the quaternionic case, for the (univariate) moments of $|\rho|$ (cf [32]). Also, there is the issue of whether or not the nonnegativity of the determinant of the partial transpose is equivalent to separability, as it is known to be in the two-rebit and two-qubit cases [17].) The lower estimate based on 2325 moments is 0.080 495 355 (which is 1.000 000 000 049 times the corresponding estimate based on 2324 moments). This

sequences of moments of $|\rho||\rho_{PT}|^n$ (upper blue curve) and $|\rho_{PT}|^n$ (lower red curve). (We use the term ‘presumptively’, precisely, because we have performed no explicit calculations—as we certainly have done in the two-rebit ($\alpha = \frac{1}{2}$) and two-qubit cases ($\alpha = 1$)—involving $4 \times 4$ quaternionic density matrices. We are, thus, proceeding under the assumption that we can extrapolate our formula to the case $\alpha = 2$. We note, however, that this formula does agree with that of Andai [16, theorem 4], in the quaternionic case, for the (univariate) moments of $|\rho|$ (cf [32]). Also, there is the issue of whether or not the nonnegativity of the determinant of the partial transpose is equivalent to separability, as it is known to be in the two-rebit and two-qubit cases [17].) The lower estimate based on 2325 moments is 0.080 495 355 (which is 1.000 000 000 049 times the corresponding estimate based on 2324 moments). This
Figure 10. Two sets of estimates of the (octonionic?) HS separability probability. The upper (blue) decreasing curve is based on our conjectured formulas—using \( \alpha = 4 \)—for the expected values of \((|\rho|^n|\rho^{PT}|)^n\) and the lower (red) curve, similarly for \(|\rho^{PT}|^n\). The true value appears to be constrained to lie within [0.010 872 2086, 0.026 439 6063]. 2125 moments were employed.

2325-moment estimate can be truly remarkably well fitted by the relatively simple fraction \( \frac{26}{323} \approx 0.0804953560 \).

In the framework of [2, section IX], the ‘scaling factor’ used to obtain the \( \frac{26}{323} \) result would be \( \frac{19 \, 136 \pm 12}{152 \, 809 \, 335} \), where \( 19 \, 136 = 2^6 \times 13 \times 23 \) and \( 152 \, 809 \, 335 = 3^6 \times 5 \times 7 \times 53 \times 113 \). (In these calculations, we took the total HS quaternionic volume to be equal to the product of that volume given by Andai in [16] and the normalization factor of \( 2^{13} \) indicated there—thus, giving us the HS volume in the Zyczkowski–Sommer framework [3] that we have employed throughout.) For our two other conjectures, the associated scaling factors would be \( (\alpha = \frac{1}{2}, \text{two-rebit}) \frac{1452^4}{729^2} \times \frac{5}{863} \approx 0.0108722086 \) times as large as the estimated separability probability. Convergence is comparatively very strong in this instance and definitely seems to improve, in general, as the Dyson-index-like parameter \( \alpha \) increases.

8.6. \( \alpha = 4 \) (octonionic?)

In figure 10, we show—for the \( \alpha = 4 \) (octonionic? (cf [9, 10, 33])) case—the estimates obtained by application of the procedure of Provost [29, equation (15)] to sequences of 2125 moments of \((|\rho|^n|\rho^{PT}|)^n\) (upper blue curve) and \(|\rho^{PT}|^n\) (lower red curve). The fraction \( \frac{26}{323} \approx 0.010 \, 872 \, 2086 \) is 0.999 999 9981 times as large as the estimated separability probability. Convergence is comparatively very strong in this instance and definitely seems to improve, in general, as the Dyson-index-like parameter \( \alpha \) increases.

8.7. \( \alpha = 0 \) (classical?)

If we set \( \alpha = 0 \) in (appendix D.6) for the (mixed-moments) case \( n = k \), we obtain the simplification

\[
(|\rho|^n|\rho^{PT}|)^n = \frac{4096^{-\alpha}\Gamma(2n + 1)^3}{\left(\frac{2}{3}\right)^{2n}\binom{3}{2n} n!}.
\]  

(31)
Figure 11. Two sets of estimates of the (classical?) HS separability probability, using \( \alpha = 0 \). The upper (red) decreasing curve is based on our conjectured formula (appendix D.6) for the expected values of \( |\rho^{PT}| \) —and the lower (blue) curve, similarly for \( (|\rho||\rho^{PT}|) \) —given by the simplified formula (31). 1650 moments were employed, with the last pair of estimates being \{0.96238936, 0.99445741\}.

In figure 11, we plot our standard pair of two estimates (although now the roles of upper and lower curves are reversed). It appears that there is convergence to 1, that is, \( \alpha = 0 \) corresponds, in some sense, to a classical scenario, in which no entanglement is present. In regard to setting \( \alpha = 0 \), we remark that doing so assigns measure zero to the off-diagonal entries of the Cholesky factor. The determinant and PT determinant are identical as far as the measure is concerned, and the probability distribution is the same as that of the product \( t_1 t_2 t_3 t_4 \) on the simplex in 3-space \((t_1, t_2, t_3 \geq 0, t_4 = 1 - t_1 - t_2 - t_3 \text{ and } t_4 \geq 0)\). The attempt to reconstruct the underlying probability distribution yields an inelegant integral of a hypergeometric series.

8.8. Other values of \( \alpha \)

We also have conducted Legendre-polynomial reconstruction analyses for a number of other values of \( \alpha \), which we summarize in the form (cf figure 8)

\[
\begin{pmatrix}
\frac{1}{4} & 850 & [0.64744667, 0.63955009] \\
\frac{3}{4} & 525 & [0.34299437, 0.32784144] \\
\frac{3}{4} & 1600 & [0.13756171, 0.14950325] \\
3 & 1075 & [0.029008076, 0.055230359] \\
8 & 850 & [0.000254391328, 0.055713576]
\end{pmatrix}
\]

(32)

The first two columns give the value of \( \alpha \) and the number of moments employed, and the last the confining interval for the associated separability probabilities, with the first value being based on the moments of \( |\rho^{PT}| \) and the second on the moments of \( (|\rho||\rho^{PT}|) \). Convergence of the probability-distribution reconstruction algorithm, based on the moments of \( |\rho^{PT}| \), appears to greatly increase as \( \alpha \) increases. (An extremely close fractional fit to the lower bound for \( \alpha = 8 \) is \( \frac{81}{318407} \approx 0.0002543913215 \).)
8.9. Specialized lower dimensional ('non-generic') cases

In [2, section II.A], we considered classes of $4 \times 4$ real, complex and quaternionic density matrices, where—as usual—the diagonal entries were allowed to take values in the 3-simplex, but now five of the six pairs of off-diagonal entries were nullified, leaving only the $(2,3)$ and $(3,2)$ pair as free. (The associated separability probabilities were found to be $\frac{5\pi}{16}$, $\frac{1}{3}$ and $\frac{1}{10}$.) We (appendix D.7) have now been able to prove formulas for the bivariate moments in these specialized scenarios.

9. HS and Bures probability distributions over $|\rho|$ 

In the course of this work, one of us (CD) developed a result (following his joint work with Życzkowski reported in [34], where ‘the machinery for producing densities from moments of Pochhammer type’ was developed) giving the univariate probability distribution over $t \in [0, 1]$ that reproduces the HS moments of $t = 2^{8}|\rho|$, where $\rho$ is a generic two-rebit density matrix. (If we set $n = 0$ in our general (bivariate) determinantal moment framework above, we obtain the (univariate) moments of $|\rho|$.) This probability distribution took the form (cf [15, equation (4.3)])

$$
\frac{63}{8}\left(\sqrt{1 - \sqrt{t}}(-8t - 9\sqrt{t} + 2) + 15t\log(\sqrt{1 - \sqrt{t}} + 1) - \frac{15}{2}t\log(t)\right)
$$

(33)

(see appendix D.2 below for further details). CD was also able to derive, in similar fashion, the Bures metric [4, 26] counterpart of this HS result (33). It took the form (appendix D.3)

$$
-4\sqrt{t} - t(2\sqrt{t} + 13) + 3\pi(4\sqrt{t} + 1) + 2(12\sqrt{t} + 3)\sin^{-1}(1 - 2\sqrt{t})
\pi \sqrt{t}
$$

(34)

In figure 12, we display these two (HS and Bures) probability distributions.

\begin{figure}
\centering
\includegraphics[width=\textwidth]{figure12}
\caption{Probability distributions (33) and (34) over $t = 2^{8}|\rho|$ ($t \in [0, 1]$). The HS (red) curve dominates the Bures curve above $t = 0.021702$.}
\end{figure}
10. Discussion

10.1. Background

A basic linear-algebraic criterion that a Hermitian matrix be nonnegative definite, that is, has all its eigenvalues nonnegative, is that all its principal minors be nonnegative. In [7], we were able to implement this criterion, in part, making use of the $3 \times 3$ minors, establishing thereby that the HS probability that a generic two-rebit system is separable is bounded above by $1129 \approx 0.537619$. (The absolute separability probability of $6928 \approx 0.0348338$ provided the best exact lower bound established in this specific setting [7], it appeared. The set of absolutely separable two-qubit states are described in figures 1–5 in [35] (cf [36–38]). No immediate application of the moment-based approach adopted in this study to the description of the absolutely separable states is apparent.) That study [7] was a continuation of a series of papers of ours (including [2, 39–46]) in which we examined the separability-probability question—for the HS as well as various monotone (such as the Bures) metrics—from a variety of mathematical perspectives, employing a number of density-matrix parameterizations. A major motivation in undertaking the moment-related analyses reported above was to further sharpen our separability-probability estimates, perhaps even being able to arrive at an estimate accurate to several decimal places, and possibly obtain thereby convincing evidence for a particular true value.

Despite the considerable computational efforts expended in calculating high-order moments, the goal of high accuracy nevertheless appeared remote—that is, until the apparent advances (appendix D) that we have sought to subsequently exploit above. This somewhat pessimistic viewpoint had been based on a continuing series of attempts by us—using a wide variety of probability-density reconstruction methodologies—to isolate the two-rebit separability probability on the basis of the initially computed (limited number of) 13 moments. As an example (cf appendix D.5), use of the nonparametric procedure of Mnatsakanov [30] yielded HS generic two-rebit separability-probability estimates of 0.458 2596, 0.429 704 96 and 0.403 212 91 based on the first 11, 12 and 13 moments of $|\rho_{PT}|$ (appendix A), so no convergence was apparent, at least, with these few moments. The corresponding estimates were 0.541 4052, 0.392 3661 and 0.479 2091 based on 11, 12 and 13 moments of $|\rho||\rho_{PT}|$ (appendix B). Use of the first ten moments in a certain maximum-entropy reconstruction methodology [47] gave an estimate of 0.409 858. Additionally, incorporation of the first 12 moments into an adaptive spline-based algorithm [48] gave 0.450 2338. The semiparametric Legendre-polynomial-based reconstruction approach of Provost [29]—our chief computational procedure in the main body of this paper—gave estimates of 0.385 6787 and 0.484 6628 based on the first 13 moments of $|\rho_{PT}|$ and $|\rho||\rho_{PT}|$, respectively.

We had, thus, before the general formula, encountered evident difficulties in ascertaining to high accuracy the values of separability probabilities. These difficulties, it seemed, perhaps manifested the NP-hardness of the problem of distinguishing separable quantum states from entangled ones [49–51]. As possible evidence for such a contention, if one knew all the generic HS two-rebit moments of $|\rho_{PT}|$, then presumably one could determine the associated separability probability to arbitrarily high accuracy. But to know all these moments, it appeared that one would have to know an indefinitely large number of the functions $C_{n-i}$ ((20)–(23)), from which the needed constant terms could be extracted. In the apparent absence of a generating rule for these increasingly high-order functions (but see appendix D), an indefinitely large amount of computation appeared to be required. (‘Although [quantum entanglement] is usually fragile to the environment, it is robust against conceptual and mathematical tools, the task of which is to decipher its rich structure’ [52, p 865].) In
[19, section II.B], an earlier study of ours of the moments for two-rebit systems, we encountered a somewhat analogous rather intractable state of affairs, employing the Bloore (correlation-coefficient) parameterization of density matrices (and not the Cholesky decomposition parameterization, as in this study). There, a general formula for the denominators of certain important “intermediate functions” could be discerned, but only explicit results obtained for an initial set \(\{m = 2, 4, 6, \ldots, 16\}\) of the corresponding numerators. So higher order moments—and, thus, high accuracy—appeared out of reach there (but certainly in light of the apparent progress—but not yet rigorously established—the matters there might also be readdressed).

10.2. Results

In this paper, we have advanced four specific conjectures \((\alpha = 0, \frac{1}{2}, 1, 2)\) (figure 8). The reader might have been somewhat skeptical of our strong predisposition to conjecture rational values for the various separability probabilities under consideration. A basis for this inclination had been established in [2], where a pattern of rational separability probabilities appeared through the application of exact methods to lower dimensional non-generic (but more easily computed) quantum scenarios (section 8.9).

In regard to the conjecture [2, section IX.B] that the HS separability probability of generic (15-dimensional) two-qubit systems is \(\frac{83}{33}\), Życzkowski informally wrote: ‘It would be amazing if such a simple number occurs to be true! I wonder then if it is likely that this result may be derived analytically (by a clever integration), or perhaps even ‘guessed’ from some symmetry arguments (which are still missing)’. From the first author’s viewpoint, perhaps one of the chief hurdles here is simply the exceptionally high-dimensionality and quartic (separability) constraints that need to be addressed in any integration (‘clever’ or otherwise). Possibly with the advent of more powerful symbolic (quantum?) computational systems, this obstacle might be directly overcome. Also, in terms of symmetry principles, the (Keplerian) concept of ‘stella octangula’ [53, 54] has proved useful in studying separability, and might conceivably do so (in some higher dimensional realization) in the future. Certain interesting aspects of convexity were applied in [28] to obtain theorems pertaining to HS separability probabilities.

The general formulas remain formally unproven. However, our confidence in their validity is certainly enhanced by the reasonableness and non-anomalous behavior (figures 4–10) of our various (separability) probability estimation procedures, for various values of \(\alpha\), which rely upon them. If the formulas did not, in fact, yield genuine moments of probability distributions, we would certainly expect that to be manifested, in some overt manner (negative probabilities, probabilities greater than unity, non-convergent behavior, ...) in our reconstruction efforts.

It is interesting to note that of our three basic (two-rebit, -qubit, -‘quaterbit’ [11]) separability-probability conjectures—\(\frac{29}{61}, \frac{8}{33}, \frac{26}{323}\)—the two-qubit is the simplest, in the sense of having the smallest denominator (and numerator). The two-qubit systems exist conceptually in the framework of (standard/conventional/phenomenological) complex quantum mechanics [32, 10, section 2].

A further observation is that although in random matrix theory, a (Dyson-index) parameter \(\beta = 1\) (the dimension of the corresponding division algebra [10]) is typically assigned to the real systems, in the (Cholesky decomposition-based) analysis (appendix D), the use, instead, of \(\alpha = \frac{1}{2}\) appears to be natural—since one-halves repeatedly arise in the integration over the real sphere in \(\mathbb{R}^{10}\).
Knowledge of all the moments of $|\rho^{PT}|$ and $|\rho||\rho^{PT}|$ theoretically determines the complete probability distributions of these two variables (since the ranges of these two variables are bounded). In some sense, this constitutes more information than it might seem one should require to determine the single (separability) probability of primary, motivational interest [1]. So, if at some point in time, the separability-probability questions can be resolved by some more direct methods, then it may appear that the analytical moment-based approach pursued here was more than that, in fact, truly required for the task at hand. Nevertheless, in the interim, this approach has clearly greatly advanced our knowledge of the ranges within which the separability probabilities must lie—even if not helping to pinpoint their conjectured exact (simple rational) values.

10.3. Bures analyses

In a naive exercise, we investigated whether or not the bivariate moment formulas presented here might further hold—at least up to proportionality—if one were to simply replace the expectation with respect to the HS metric in them by expectation with respect to the Bures (minimal monotone) metric [4, 16, 26, 39, 42]. However, such a possible relationship appeared to be quite emphatically ruled out, at least with the one specific example, formula (5) above, we numerically studied in these regards.

In [39, equation (16)], we had—based on extensive quasi-Monte Carlo numerical integrations—advanced the hypothesis that the two-qubit Bures separability probability took the form (with the ‘silver mean’, $\sigma_{Ag} = \sqrt{2} - 1$)

$$P_{\text{sep}}^{\text{Bures}} = \frac{1}{\pi^8} \approx 0.073 \, 338 \, 937 \, 67$$

(35)

(which we do note is obviously irrational—in contrast to our HS conjectures). We have recently begun to re-examine the results of that 2005 study, particularly in light of the later (2009) development, making use of Ginibre ensembles, of a ‘simple and efficient algorithm to generate at random, density matrices distributed according to the Bures measure’ [55] (cf [56, equation (22)]). In an ongoing calculation, employing extended-precision-independent normal random variables, we have obtained (using the normal approximation to the binomial distribution)—based on 281 350 000 realizations (20 627 508 being separable, giving a probability of 0.073 3162)—a 95% confidence interval

$$[0.073 \, 285 \, 72, \ 0.073 \, 346 \, 64].$$

We note that this interval does contain the conjectured value (35) for the true Bures two-qubit separability probability. (Consistently with these analyses, if we introduce our HS two-qubit separability-probability conjecture of $8^8$ into the inequality of Ye [57, mid. p 7], we obtain 0.003 738 82 as a lower bound on the Bures two-qubit separability probability. Application of the very next inequality of Ye appears to yield 599 089, obviously greater than 1, as an upper bound on this probability.)

Acknowledgments

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Appendix A. Two-rebit HS moments $\langle |\rho^{PT}|^{n}\rangle_{\text{two-rebit/HS}}, n = 1, \ldots, 13$

\[
\begin{pmatrix}
1 & -0.001655 \\
2 & -0.0000108462 \\
3 & 1.6298 \times 10^{-7} \\
4 & 2.0931 \times 10^{-9} \\
5 & -4.27531 \times 10^{-11} \\
6 & 1.01949 \times 10^{-12} \\
7 & -2.73223 \times 10^{-14} \\
8 & -5.23678 \times 10^{-17} \\
9 & 8.52025 \times 10^{-19} \\
10 & -3.01039 \times 10^{-20} \\
11 & 1.11038 \times 10^{-21} \\
12 & -4.24992 \times 10^{-23}
\end{pmatrix}.
\]

(A.1)

Appendix B. Two-rebit HS moments $\langle (|\rho| |\rho^{PT}|)^{n}\rangle_{\text{two-rebit/HS}}, n = 1, \ldots, 13$

\[
\begin{pmatrix}
1 & 0 \\
2 & 0.0000108462 \\
3 & 2.0931 \times 10^{-9} \\
4 & 4.27531 \times 10^{-11} \\
5 & 1.01949 \times 10^{-12} \\
6 & 2.73223 \times 10^{-14} \\
7 & 5.23678 \times 10^{-17} \\
8 & 8.52025 \times 10^{-19} \\
9 & -3.01039 \times 10^{-20} \\
10 & 1.11038 \times 10^{-21} \\
11 & -4.24992 \times 10^{-23}
\end{pmatrix}.
\]

(B.1)
Appendix C. Moments of $|\rho^{PT}|^n$, $n = 1, \ldots, 10$, for minimally degenerate pairs of rebits

$$
\begin{pmatrix}
1 & -5/2776 & -0.002 104 38 \\
2 & 270/1006 & 0.000 018 4133 \\
3 & -9/34777 600 & -2.587 87 \times 10^{-7} \\
4 & 89 942 261 760/463 & 4.925 38 \times 10^{-9} \\
5 & -4032 782 401 536/2445 & -1.143 13 \times 10^{-10} \\
6 & 17 856 064 542 223 808/631 & 3.055 91 \times 10^{-12} \\
7 & -6 948 198 442 598 400/474 047 & -9.081 49 \times 10^{-14} \\
8 & 16 176 381 160 115 404 800/4003 573 & 2.930 3 \times 10^{-15} \\
9 & -39 643 007 353 595 550 220 800/3397 & -1.090 86 \times 10^{-16} \\
10 & 9 248 892 257 224 397 600 & 3.672 86 \times 10^{-18}
\end{pmatrix}
$$

(C.1)

Appendix D. Two-rebit and two-qubit moments

Let $\Omega$ denote the set of $4 \times 4$ (symmetric) real positive definite matrices and $\Omega_1$ denote the matrices of trace 1 in $\Omega$. Recall that $\langle X \rangle$ denotes the expectation of the random variable $X$, with the associated probability density being implicit from the text. Furthermore, $|\rho|$ denotes $\det \rho$.

D.1. Construction of density functions

We describe the tools used to determine densities whose moment sequence is given in Pochhammer form. Here we restrict to densities supported on $[0, 1]$. Let $f(x)$ be defined on $0 \leq x \leq 1$, such that $f(x) \geq 0$, $f$ is continuous on $0 < x < 1$ and $\int_0^1 f(x) \, dx = 1$. There is an associated random variable $X$, with $\Pr[a < X < b] = \int_a^b f(x) \, dx$. The moment sequence is $\langle X^n \rangle = \int_0^1 x^n f(x) \, dx$, $n = 0, 1, 2, \ldots$. Observe that the moment sequence uniquely defines the density because the support is a bounded interval.

First, we consider a beta-type distribution: let $\alpha, \beta > 0$, and

$$f(x) = \frac{1}{B(\alpha, \beta)} x^{\alpha-1} (1-x)^{\beta-1}, \quad 0 < x < 1,$n = 0, 1, 2, \ldots.
$$

(Recall $B(\alpha, \beta) = \Gamma(\alpha) \Gamma(\beta)/\Gamma(\alpha + \beta)$.) This uses the identity $\Gamma(\alpha+n)/\Gamma(\alpha) = (\alpha)_n := \prod_{i=1}^n (\alpha+i-1)$, the Pochhammer symbol.

**Lemma D.1.** Suppose $X_1, X_2$ are independent random variables on $[0, 1]$ with densities $f_i$, $i = 1, 2$. Then the density for $X_1 X_2$ is

$$f(x) := \int_0^1 f_1(t) f_2 \left( \frac{x}{t} \right) \frac{1}{t} \, dt.$$

If the moments of $X_1, X_2$ are $\mu^{(i)} = \langle X_i^n \rangle = \int_0^1 x^n f_i(x) \, dx$, then $\langle X_1^n X_2^n \rangle = \mu^{(1)} \cdot \mu^{(2)}$, $n = 0, 1, 2, \ldots$, that is,

$$\int_0^1 x^n f(x) \, dx = \mu^{(1)} \cdot \mu^{(2)}, \quad n = 0, 1, 2, \ldots.$$
The lemma was stated and used in [34, p 123521]. Also we use the duplication formulas for Pochhammer symbols,
\[(\alpha)_{2n} = 2^{2n} \left(\frac{\alpha}{2}\right)_n \left(\frac{\alpha + 1}{2}\right)_n,\]
\[(2n)! = (1)_{2n} = 2^{2n} n! \left(\frac{1}{2}\right)_n,\]
\[(2n + 1)! = (2)_{2n} = 2^{2n} n! \left(\frac{3}{2}\right)_n.\]

**D.2. Density of the determinant under the HS metric**

The ten-dimensional cone \(\Omega\) is equipped with the measure \(\prod_{1 \leq i, j \leq 4} d\rho_{ij}\) (where \(\rho = (\rho_{ij})_{i,j=1}^4\) is the generic matrix). The probability distribution on \(\Omega\) is the (nine-dimensional) restriction of this measure.

The following lemma applies to \(N \times N\) positive-definite matrices for any \(N = 2, 3, \ldots\). Each such matrix \(\rho\) has a Cholesky decomposition:
\[\rho = CC^t,\]
where \(C\) is upper triangular with entries \(c_{ij}\), \(c_{ij} = 0\) for \(i > j\) and \(c_{ii} \geq 0\) for all \(i\). The entries of \(\rho\) are \(\rho_{ij} = \sum_{k=1}^N c_{ik}c_{kj} = \sum_{k=1}^{\min(i,j)} c_{ik}c_{kj}\). Consider the Jacobian matrix \(\frac{\partial \rho}{\partial c}\) where the dependent variables are \(\rho_{ij}, i \leq j\).

**Lemma D.2.** Suppose \(\rho = CC^t\); then
\[\det \frac{\partial \rho}{\partial c} = 2^N \prod_{i=1}^N c_{ii}^{N+1-i}.\]

**Proof.** We use the following simple fact: suppose \(y_i = f_i(x_1, x_2, \ldots, x_i), 1 \leq i \leq N;\) then the matrix \(\left(\frac{\partial f_i}{\partial x_j}\right)\) is lower triangular (0 for \(j > i\)) and \(\det \left(\frac{\partial f_i}{\partial x_j}\right) = \prod_{i=1}^N \frac{\partial f_i}{\partial x_i}\). Now order the following (independent) variables: \(c_{11}, c_{12}, \ldots, c_{1N}, c_{21}, c_{22}, \ldots, c_{2N}, c_{33}, \ldots, c_{N-1,N-1}, c_{N-1,N}, c_{NN}\). For \(i \leq j\), \(\rho_{ij} = \sum_{k=1}^{i-1} c_{ik}c_{kj} + c_{ii}c_{ij}\) and thus
\[\left|\det \frac{\partial \rho}{\partial c}\right| = \prod_{i=1}^N \prod_{j=i+1}^N \frac{\partial \rho_{ij}}{\partial c_{ij}} = \prod_{i=1}^N (2c_{ii}^{N-i+1}).\]

Now set \(N = 4\). The preimage \(S\) of \(\Omega\) (for the map \(C \mapsto C^tC\)) is a modified octant of the unit sphere in \(\mathbb{R}^{10}\), because \(\text{Tr}(C^tC) = \sum_{1 \leq i, j \leq 4} c_{ij}^2\). Recall the condition \(c_{ii} \geq 0\), but the other entries can have arbitrary signs. The surface measure \(dm\) on \(S\) is essentially a Dirichlet measure: consider a monomial on \(S\), that is,
\[f(C) := \prod_{1 \leq i, j \leq 3} c_{ij}^{n_{ij}},\]
then

1. if \(n_{ij}\) is odd for some \(i < j\), then \(\int_S f(C) dm(C) = 0\);
2. if \(n_{ij}\) is even for each \(i < j\), then
\[\int_S f(C) dm(C) = \frac{\Gamma(5)}{\Gamma\left(\frac{1}{2}\right)^4} \frac{1}{\Gamma\left(5 + \frac{1}{2} \sum_{1 \leq i, j \leq 4} n_{ij}\right)} \prod_{1 \leq i, j \leq 4} \Gamma\left(\frac{1}{2} + n_{ij}\right);\]
We know that the range of previous results, consider $X$ thus, $\int \mathcal{S}\, \text{d}m(\mathcal{C}) = \frac{1}{(5)^N} \prod_{1 \leq i \leq j \leq 4} \left( \frac{1}{2} \right)^{n_{ij}/2}.$

In our usage, either case 1 or case 3 applies. Combining the Jacobian and the fact $|\rho| = c_1^2 c_2^2 c_3^2 c_4^2$, we obtain (for the normalized measure, that is, $\gamma \int_{\mathcal{S}} \frac{\partial \rho}{\partial \mathcal{C}} \text{d}m(\mathcal{C}) = 1$, $k = 0, 1, 2, \ldots)$.

(1) if $n_{ij}$ is odd for some $i < j$, then $\int_{\mathcal{S}} |\rho|^k \, f(\mathcal{C}) \, \text{d}m(\mathcal{C}) = 0$;
(2) if $n_{ij}$ is even for each $i \leq j$, and $N := \sum_{1 \leq i \leq j \leq 4} n_{ij}$, then
\[
\gamma \int_{\mathcal{S}} |\rho|^k \, f(\mathcal{C}) \, \text{d}m(\mathcal{C}) = \frac{1}{(10)^{nk}} \prod_{1 \leq i < j \leq 4} \left( \frac{1}{2} \right)^{n_{ij}/2}.
\]

The special case $f(\mathcal{C}) = 1$ provides the moments of the random variable $\langle \rho \rangle$; indeed
\[
\gamma \int_{\mathcal{S}} |\rho|^k \, \text{d}m(\mathcal{C}) = \frac{1}{(10)^{nk}} \prod_{1 \leq i < j \leq 4} \left( \frac{1}{2} \right)^{n_{ij}/2}.
\]

We know that the range of $|\rho|$ is $[0, \frac{1}{\sqrt{2}}]$ (the maximum is achieved at $\rho = \frac{1}{\sqrt{2}}$); to use the previous results, consider $X = 2^k |\rho|$. Then
\[
\langle X^n \rangle = 2^{2n} \left( \frac{3}{2} \right)_n \left( \frac{5}{2} \right)_n \left( \frac{7}{2} \right)_n \left( \frac{9}{2} \right)_n \left( \frac{11}{2} \right)_n = 2^{2n} \frac{2^{2n} (4)_{2n} 2^{-2n} (2)_{2n}}{(5)_{2n} \left( \frac{11}{2} \right)_{2n}} = \frac{(4)_{2n}}{(5)_{2n} \left( \frac{11}{2} \right)_{2n}}.
\]

Thus, $X$ is (equidistributed as) the product of two independent random variables $X_1, X_2$ with
\[
\langle X_1^n \rangle = \frac{(4)_{2n}}{(5)_{2n}} = \frac{4}{4 + 2n} = \frac{2}{2 + n},
\]
\[
\langle X_2^n \rangle = \frac{(2)_{2n}}{\left( \frac{11}{2} \right)_{2n}}.
\]

Clearly $X_1$ has the density $f_1(t) = 2t, 0 \leq t \leq 1$. The density of $X_2$ is
\[
f_2(t) = \frac{1}{2B \left( 2, \frac{7}{2} \right)} (1 - \sqrt{t})^{5/2},
\]

because
\[
\int_0^1 t^n f_2(t) \, dt = \frac{1}{2B \left( 2, \frac{7}{2} \right)} \int_0^1 t^n (1 - \sqrt{t})^{5/2} \, dt = \frac{1}{B \left( 2, \frac{7}{2} \right)} \int_0^1 s^{2n} (1 - s)^{5/2} \, ds = \frac{(2)_{2n}}{\left( \frac{11}{2} \right)_{2n}}.
\]

The density $f(x)$ of $X$ is given by
\[
f(t) = \int_{-\infty}^t f_1 \left( \frac{x}{s} \right) f_2(s) \, ds = \frac{2}{2B \left( 2, \frac{7}{2} \right)} \int_{-\infty}^1 \frac{x}{s} (1 - \sqrt{t})^{5/2} \, ds.
\]
Using the Bures metric, one obtains

\[ D.3. \text{Density of the determinant under the Bures metric} \]

Using the Bures metric, one obtains

\[ \langle |\rho|^n \rangle = \frac{1}{2^n n!} \int_0^1 x^n f(x) dx = \frac{1}{(n+1)(2n+1)} \frac{(\frac{3}{2})_{2n}}{(4)_{2n}}, \]

for \( n = 0, 1, 2, \ldots \). As above we consider the random variable \( X = 2^k |\rho| \).

The density \( f(x) \) of \( X \), for \( 0 < x \leq 1 \), satisfies

\[ \int_0^1 x^n f(x) dx = \frac{1}{(n+1)(2n+1)} \frac{(\frac{3}{2})_{2n}}{(4)_{2n}}, \quad n = 0, 1, 2, \ldots \]

We express \( X \) as the product of two random variables.

Let

\[ f_1(t) = t^{-1/2} - 1, \quad 0 < t \leq 1; \]

then

\[ \int_0^1 t^n f_1(t) dt = \frac{1}{(n+1)(2n+1)}, \quad n = 0, 1, 2, \ldots \]

Next observe (from equation D.1)

\[ \frac{\Gamma(4)}{\Gamma(\frac{3}{2}) \Gamma(\frac{3}{2})} \int_0^1 s^{3/2} (1-s)^{3/2} ds = \frac{(\frac{3}{2})_{2n}}{(4)_{2n}}, \]

so set \( s = t^{1/2} \) (and note \( \frac{\Gamma(4)}{\Gamma(\frac{3}{2}) \Gamma(\frac{3}{2})} = \frac{16}{\pi} \)) to obtain

\[ \frac{8}{\pi} \int_0^1 t^{2n+1/2} (1-t^{1/2})^{3/2} dt = \frac{(\frac{3}{2})_{2n}}{(4)_{2n}}, \quad n = 0, 1, 2, \ldots \]

Let

\[ f_2(t) = \frac{8}{\pi} t^{-1/4} (1-t^{1/2})^{3/2}, \quad 0 < t \leq 1. \]
By lemma D.1, the desired density function is
\[ f(x) = \int_{x}^{1} f_{1}(\frac{x}{t}) f_{2}(t) \frac{dt}{t} \]
\[ = \frac{8}{\pi} \int_{x}^{1} \left( \left( \frac{t}{x} \right)^{1/2} - 1 \right) t^{-1/4} (1 - t^{1/2})^{3/2} \, dt \]
\[ = \frac{8}{\pi \sqrt{x}} \int_{x}^{1} (t^{1/2} - x^{1/2}) t^{-1/4} (1 - t^{1/2})^{3/2} \, dt. \]
Substitute \( t = s^2 \); then
\[ f(x) = \frac{16}{\pi \sqrt{x}} \int_{x}^{1} (s - \sqrt{x}) s^{3/2} (1 - s)^{3/2} \, ds, \]
an elementary integral; indeed
\[ f(x) = \frac{1}{\pi \sqrt{x}} \left[ 3\pi (4\sqrt{x} + 1) - 4(13 + 2\sqrt{x}) \sqrt{x - x - 2(12\sqrt{x} + 3) \arcsin(2\sqrt{x} - 1)) \right]. \]
As with the HS metric, \( f(x) = O((1 - x)^{7/2}) \) near \( x = 1 \).

**D.4. The joint moments of \(|\rho|\) and \(|\rho^{PT}|\)**

The partial transpose \( \rho^{PT} \) of \( \rho \) is obtained by interchanging the values of \( \rho_{14} \) and \( \rho_{23} \) (and \( \rho_{41} \) and \( \rho_{32} \)). In this section, we introduce a conjecture for
\[ \langle |\rho^{PT}|^{n}|\rho|^{k} \rangle, \quad k, n = 0, 1, 2, 3, \ldots, \]
using the density on \( \Omega_1 \) coming from the HS metric.

For the upper triangular matrix \( C \) and \( \rho = C^* C \), we find
\[ |\rho^{PT}| = c_{11}^2 c_{22}^2 c_{33}^2 c_{44}^2 + 2c_{11}c_{22}(c_{11}c_{14} - c_{12}c_{13} - c_{22}c_{23}) \]
\[ \times \left( -c_{11}c_{23}c_{24} - c_{23}c_{34}c_{11} + c_{11}c_{33}c_{44} + c_{23}c_{33}c_{14} \right) \]
\[ - c_{22}c_{33}c_{34} - c_{12}c_{33}c_{44} + c_{23}c_{33}c_{14} \]
\[ = (c_{11}c_{14} - c_{12}c_{13} - c_{22}c_{23})^2 \]
\[ \times \left( 4c_{23}c_{14}c_{14} + c_{11}^2 c_{24} + c_{11}^2 c_{24} - 2c_{11}c_{14}c_{24} - 2c_{11}c_{12}c_{33}c_{34} \right) \]
\[ - 2c_{11}c_{12}c_{23}c_{24} + 2c_{22}c_{13}c_{24} + 2c_{22}c_{13}c_{24} + 2c_{22}c_{13}c_{24} + 2c_{22}c_{13}c_{24} \]
\[ = (c_{11}c_{14} - c_{12}c_{13} - c_{22}c_{23})^4. \]
Of course, \( |\rho| = c_{11}^2 c_{22}^2 c_{33}^2 c_{44}^2 \). We introduce some utility functions (throughout \( n, k = 0, 1, 2, \ldots \)). For a rational function \( F(k) = \frac{p(k)}{q(k)} \) of \( k \), define the degree to be \( \deg (p) - \deg (q) \):
\[ F_0(k) = \langle |\rho|^{k} \rangle = \frac{(11)(\frac{3}{2})_k(\frac{3}{2})_k}{(10)_4}, \]
\[ F_1(n, k) = \langle |\rho^{PT}|^{-n}|\rho|^{k} \rangle, \]
\[ F_2(n, k) = \langle |\rho|^{k} (|\rho^{PT}| - |\rho|)^{n} \rangle, \]
\[ R(n, k) = F_0(n + k)/F_0(k) = \frac{(k + 1)_n (k + \frac{3}{2})_n (k + 2)_n (k + \frac{5}{2})_n}{(4k + 10)_4}. \]
(Note \( F_2(0, 0) = 1 = R(0, k) \).) The goal is to find (and prove) a closed form for \( F_1(n, k) \), that is, a general formula. Direct computation for \( n = 1, 2, 3 \) shows that \( F_1(n, k) \) is rational in \( k \) of degree 0, and at first glance, does not have an obvious formula (for the numerator). Some
experimentation leads to the observation that \( F_1(n, k) - R(n, k) \) is of degree \(-2\) (verified only for small \( n \)). This motivates the investigation of the decomposition

\[
|\rho^{PT}|^n = \sum_{j=0}^{n} \binom{n}{j} |\rho|^{n-j} (|\rho^{PT}| - |\rho|)^j
\]

\[
F_1(n, k) = \sum_{j=0}^{n} \binom{n}{j} F_2(j, k + n - j) R(n - j, k).
\]

For \( n = 1 \), we compute

\[
F_1(1, k) = R(1, k) - \frac{1}{16(4k + 13)(k + 3)};
\]

this is an encouraging result, and it implies \( F_2(1, k) = \frac{1}{16(4k + 13)(k + 3)} \), of degree \(-2\). From the known value of \( F_1(2, k) \) and the equation

\[
F_1(2, k) = R(2, k) + 2F_2(1, k + 1) R(1, k) + F_2(2, k),
\]

we find

\[
F_2(2, k) = \frac{(k + 12)(2k + 7)}{256(k + 3)(k + 4)(4k + 11)(4k + 13)(4k + 17)}.
\]

This is of degree \(-3\), rather than the hoped-for \(-4\), and the factor \((k + 12)\) is not of the ‘good’ type, a divisor of \((k + 1)\). So we try to modify \( F_2(2, k) \) by adding a bit of \( F_2(1, k + 1) R(1, k) \); in fact

\[
F_2(2, k) + \frac{2}{k + 1} F_2(1, k + 1) R(1, k) = \frac{3}{128(k + 3)(k + 4)(4k + 11)(4k + 17)},
\]

of degree \(-4\). We now have a ‘good’ expansion of \( F_1(2, k) \), namely

\[
R(2, k) + \frac{2k}{k + 1} F_2(1, k + 1) R(1, k) + \left( F_2(2, k) + \frac{2}{k + 1} F_2(1, k + 1) R(1, k) \right).
\]

The terms are of degree \(0, -2, -4\) and each is an expression in linear factors. Next we consider \( F_2(3, k) \). This turns out to be of degree \(-5\) (rather than \(-6\)). Some effort leads to the satisfactory result:

\[
F_2(3, k) + \frac{6}{k + 1} F_2(2, k + 1) R(1, k) + \frac{12}{(k + 1)(k + 2)} F_2(1, k + 2) R(2, k)
\]

\[
= -\frac{3(k + 1)}{2048(k + 3)(k + 4)(k + 5)(4k + 11)(4k + 13)(4k + 21)},
\]

\[
= \frac{3(k - 1)}{16(k + 1)(k + 2)} F_2(2, k + 1) R(1, k) + \frac{6(k - 1)}{(k + 1)(k + 2)} F_2(1, k + 2) R(2, k)
\]

\[
= \frac{9(k - 1)(k + 2)(2k + 3)}{4096(k + 3)(k + 4)(k + 5)(4k + 11)(4k + 13)(4k + 15)(4k + 21)}.
\]

At this point, there are enough examples to try to fit a formula to these expansions. Indeed, for \( 0 \leq j \leq n \), let

\[
c_j(n, k) = \frac{1}{2^n(n + 1)(2k + 11/2)^{2n}}
\]

\[
\times \binom{4n!}{n-j} \binom{1/2}{n-j} \left( \frac{-2k - 2n - 3/2}{j} \right) (k - j + 1)(n-j) \binom{3/2}{n-j} (k + j)(n-j); \]

then

\[
F_1(n, k) = \sum_{j=0}^{n} c_j(n, k) \quad (D.2)
\]
is the conjectured formula. The degree of \( c_j(n, k) \) is \(-2j\). We use the descending Pochhammer symbol \((a)_{(n)} = \prod_{i=1}^{n} (a + 1 - i) = (-1)^n (-a)_n\). If the conjecture is valid, then for \(1 \leq j \leq n\),

\[
c_j(n, k) = \frac{(n)_j (j)_j}{j! (n + k - 1)_{(j-1)}} \times \sum_{i=0}^{j-1} \frac{1}{i!} (n + k - 1)_{(j-1-i)} (i + j - 1)_{(j-1-i)} \Gamma(j - i, n + k + i - j) R(n + i - j, k).
\]

This generalizes the examples found above. For generic \(k\), there is the expression

\[
F_1(n, k) = \frac{(k + 1)_n (k + \frac{3}{2})_n (k + 2)_n}{2^{\delta(n)} (k + 1)_n (2k + \frac{11}{2})_{2n}} \times {}_sF_4\left(\begin{array}{c}
-n, 1, \frac{1}{2}, -k, -2k - 2n - \frac{7}{2} \\
-k - n - 1, -k - n - \frac{1}{2}, k + n, k + n - 1 - \frac{1}{2}
\end{array} ; \frac{1}{2}, \frac{1}{2}, \frac{3}{2}, 1 \right).
\] (D.3)

This sum is a terminating balanced hypergeometric series. (The term ‘balanced’ means the sum of the numerator parameters + 1 equals the sum of the denominator parameters.) However, the \(sF_4\)-sum is symmetric in \((n, k)\) and the summation range is \(0 \leq j \leq \min(n, k)\). When \(0 \leq k < n\), this omits the terms in the first formula for the range \(0 \leq n - j < \frac{n-k}{2}\). For this case, the best way is to use equation (D.2) (or else use (D.3) with generic \(k\) to compute the rational function, and then substitute the desired integer value for \(k\).

The special case \(k = 0\) is

\[
F_1(n, 0) = \frac{2(2n + 1)!}{2^{\delta(n)} (n + 2) \left(\frac{1}{2}\right)_{2n}} + \frac{(2n)! \left(-2n - \frac{1}{2}\right)_n}{2^{\delta(n)} (3n) \left(\frac{1}{2}\right)_{2n}} \times {}_4F_3\left(\begin{array}{c}
-n - 2, -n - 1, 2, 3 \\
1, -n, 1 - n, 9, 2 + n
\end{array} ; 1 \right).
\]

Another interesting special case is \(k = n\):

\[
\langle |\rho|^{\nu} |\rho|^n \rangle = F_1(n, n) F_3(n) = \frac{(2n)! \left(\frac{1}{2}\right)_{2n}}{2^{\delta(n)} (n + 1)} \times {}_4F_3\left(\begin{array}{c}
-n, 1, \frac{1}{2}, -4n - \frac{1}{2} \\
-2n - 1, -2n - \frac{1}{2}, \frac{1}{2} - n
\end{array} ; 1 \right).
\]

The conjecture for \(F_1(n, k)\) has been checked by computer-aided symbolic algebra up to \(n = 13\).

D.5. Gaussian quadrature

The method of Gaussian quadrature based on orthogonal polynomials can be applied to the density problem (see [58, theorem 3.4.2, p 48]). Suppose that \(\mu\) is a probability measure supported on a bounded interval \([a, b]\) and the moments are \(\mu_j := \int_a^b x^j d\mu(x)\). The orthogonal polynomials \(\{P_n(x) : n = 0, 1, 2, \ldots\}\) for \(\mu\) (where \(P_n\) is of degree \(n\) and \(\int_a^b x^n P_n(x) d\mu(x) = 0\) for \(0 \leq j < n\)) are determined by the moment sequence. Solve the linear system

\[
\sum_{i=0}^{n-1} a_i \mu_{j+i} = -\mu_{j+n}, \quad 0 \leq j \leq n - 1,
\]

to obtain the coefficients \(a_i\) for the monic orthogonal polynomial

\[
P_n(x) = x^n + \sum_{i=0}^{n-1} a_i x^i.
\]
Then $P_n$ has $n$ distinct zeros $\lambda_1 < \lambda_2 < \ldots < \lambda_n$, contained in $(a, b)$. The structural constant $h_n = \int_a^b P_n(x)^2 \, d\mu(x) = \sum_{i=0}^{n-1} a_i \mu_{i+n} + \mu_{2n}$. The Gaussian quadrature rule with $n$ nodes is

$$G_n(p) = \sum_{i=1}^n w_{n,i} p(\lambda_i),$$

$$w_{n,i} = \frac{h_{n-1}}{P_n'(\lambda_i)P_{n-1}(\lambda_i)}, \quad 1 \leq i \leq n.$$

Then $G_n(p) = \int_a^b p \, d\mu$ for all polynomials $p$ of degree $\leq 2n - 1$. The sequence of discrete measures $\{G_n : n = 2, 3, \ldots\}$ converges weak-* in the dual space of $C[a, b]$ to the measure $\mu$. The piecewise linear graph formed by consecutively joining $[a, 0], \left[\frac{1}{2}(\lambda_1 + \lambda_2), w_1\right], \left[\frac{1}{2}(\lambda_2 + \lambda_3), w_1 + w_2\right], \ldots, \left[\frac{1}{2}(\lambda_i + \lambda_{i+1}), \sum_{j=1}^i w_j\right], \ldots, [b, 1]$ is an approximation to the cumulative distribution function (cdf) of $\mu$. (Consider this as a sort of mid-point integration rule.)

The orthonormal polynomials satisfy the three-term recurrence

$$x p_n(x) = \alpha_n p_{n+1}(x) + \beta_n p_n(x) + \alpha_{n-1} p_{n-1}(x), \quad p_{-1} = 0, \quad p_1 = 1.$$  

The most common approach to the computations is to find the coefficients $[\alpha_i, \beta_i]$ directly from the moments. This is known to be a numerically ill-conditioned problem, so a relatively large number of significant digits must be used in the calculation. The algorithm of [59, p 476] with 30-digit floating-point arithmetic was used here. The computed values were checked for accuracy by evaluating the errors

$$\varepsilon_j = \mu_j - \sum_{i=1}^n w_{n,i} \lambda_i^j, \quad 0 \leq j \leq 2n - 1.$$  

For the moments of $16 \|\rho^{PT}\|$ and $n = 20$, we obtain

$$\begin{bmatrix}
\lambda & -9501 & -9081 & -8587 & -8024 & -7402 \\
\lambda & -6734 & -6032 & -5309 & -4581 & -3860 \\
\lambda & -3160 & -2495 & -1877 & -1317 & -0824 \\
\lambda & -0410 & -008293 & -01040 & -02973 & -04698 \\
\lambda & 01372 & 03467 & 03440 & 04894 & 01194 \times 10^{-2}
\end{bmatrix}.$$  

One observes that a majority of the zeros are in $[-1, 0]$ and most of the mass is contained in $[-0.05, 0.05]$. With $n = 30$, we find four zeros in $(0, \frac{1}{16})$; the linear interpolation of the cdf gives $Pr(\|\rho^{PT}\| > 0) \simeq 0.429$.

The distribution of $2^{16} |\rho|^{\rho^{PT}}$ is somewhat more spread out over the interval. For $n = 30$, we find 17 zeros in $(0, 1)$, and linear interpolation yields $Pr(\|\rho^{PT}\| > 0) \simeq 0.461$.

**D.6. Conjectures for the complex case**

Here we consider the question of moments of $|q^{PT}|$ when $\rho$ is a $4 \times 4$ Hermitian positive-definite matrix of trace 1. The conjectured formulas have been verified for $n = 1, 2, 3, 4$ (see the previous sections). The conjecture was arrived at by inspecting the real case and using an analogous approach to the computed examples. It is interesting that the real and complex conjectured formulas can be combined into one formula with a parameter $\alpha$. Set $\alpha = \frac{1}{2}$ for
the real case and $\alpha = 1$ for the complex case. One could speculate whether $\alpha = 2$ is related to a quaternionic or symplectic version [16, 32, 33]. The general formulas are

$$|\langle \rho | = \frac{k!(\alpha + 1)_k(2\alpha + 1)_k}{2^{2\alpha}(3\alpha + \frac{3}{2})_k(6\alpha + \frac{3}{2})_k}$$

$$\frac{|\langle \rho^{|PT} |\rho |^k}_{/|\langle \rho |^k} = \frac{1}{2^{2\alpha}(k + 3\alpha + \frac{3}{2})_n(2k + 6\alpha + \frac{3}{2})_2n} \times \sum_{j=0}^{n} 4^j \binom{n}{j} (\alpha)_j (\alpha + \frac{1}{2})_j (k - j + 1)_{n-j} \times (-2k - 2n - 1 - 5\alpha)_{n-j}(k + 2 + \alpha)_{n-j}.$$

For generic $k$, this formula can be written as

$$|\langle \rho^{|PT} |\rho |^k}_{/|\langle \rho |^k} = \frac{(k + 1)_n(k + 1 + \alpha)_n(k + 1 + 2\alpha)_n}{2^{2\alpha}(k + 3\alpha + \frac{3}{2})_n(2k + 6\alpha + \frac{3}{2})_2n} \times sF_3 \left( \begin{array}{c} -n, -k, \alpha + \frac{1}{2}, -2k - 2n - 1 - 5\alpha \\ -k - n - \alpha, -k - n - 2\alpha, -\frac{k + n}{2}, -\frac{k + n - 1}{2} \end{array} ; 1 \right).$$

The special case $n = k$ is

$$|\langle \rho |^n_{\langle \rho^{|PT} \rangle^n} = \frac{(2n)! (1 + \alpha)_{2n}(1 + 2\alpha)_{2n}}{2^{12n}(3\alpha + \frac{3}{2})_{2n}(6\alpha + \frac{3}{2})_{2n}} sF_3 \left( \begin{array}{c} -n, \alpha + \frac{1}{2}, -4n - 1 - 5\alpha \\ -2n - \alpha, -2n - 2\alpha, -\frac{1}{2} - n \end{array} ; 1 \right).$$

For $k = 0$, we have

$$|\langle \rho^{|PT} |\rho |^k}_{/|\langle \rho |^k} = \frac{n!(\alpha + 1)_n(2\alpha + 1)_n}{2^{2\alpha}(3\alpha + \frac{3}{2})_n(6\alpha + \frac{3}{2})_n} + \frac{(-2n - 1 - 5\alpha)_{n}(\alpha + \frac{1}{2})_{n}}{2^{2\alpha}(3\alpha + \frac{3}{2})_n(6\alpha + \frac{3}{2})_2n} \times sF_3 \left( \begin{array}{c} -n - 2, -n - 1, 2\alpha + 1 \\ -n - 2, -n - 1, 2\alpha + 1 \end{array} ; 1 \right);$$

because of the denominator parameter $1 - n$, it is necessary to replace the $sF_3$-sum by 1 to obtain the correct value when $n = 1$.

### D.7. Lower dimensional (‘non-generic’) case study

In the Cholesky method, set five of the off-diagonal entries to zero; the positive matrix $\rho$ is

$$\begin{bmatrix}
0 & 0 & 0 & 0 \\
0 & x_2 & x_2 & x_2 \\
0 & x_2x_5 & x_5 & 0 \\
0 & 0 & 0 & x_5^2
\end{bmatrix}
$$

where $x_i \geq 0$, $1 \leq i \leq 4$, and $x_5$ comes from $\mathbb{R}^\beta$, equipped with an algebra structure including conjugation and a norm, e.g., $\beta = 2$, $C$.

Then $|\rho | = x_2^2x_5^2 + x_2^2$ and $|\rho^{|PT} |^2 = x_2^2(x_5^2 + x_2x_5)\left(x_2^2x_5^2 - x_2^2x_5^2\right).$ Consider $\rho$ as an element of $\mathbb{R}^{\beta+1}$; then the Jacobian for the map $C \mapsto C^*C$ is $J = 16x_1x_2^2x_5x_2^2$. Write $x_2x_5 = |x_5|^2$. With the usual Dirichlet integral techniques, integrating over the unit sphere
\[ \sum_{i=1}^{n} x_i^2 + |x|^2 = 1, \] we obtain the normalized integral

\[ \int x_1^{2m_1} x_2^{2m_2} x_3^{2m_3} x_4^{2m_4} |x|^2 \, d\mu = \frac{(k + 1)m_1}{(4 + \beta + 4k)m_1} \delta(k), \]

where \(|m| = \sum_{i=1}^{n} m_i\), and

\[ \delta(k) := \int (|\rho|)^k J(x) \, d\mu = \frac{k!^3 (1 + \frac{\beta}{2})^3}{(4 + \beta)^3}. \]

Then

\[ \int (|\rho|)^n (|\rho|)^k J(x) \, d\mu = \delta(k) \frac{(k + 1)^2 (k + 1 + \frac{\beta}{2})^2}{(4 + \beta + 4k)n} \times {}_4F_3 \left( \begin{array}{c} -n, k + 1 + \frac{\beta}{2} + n, k + 1 + \frac{\beta}{2} + n, \frac{\beta}{2} + 1 \\ -k - n, -k - n, k + 1 + \frac{\beta}{2} \end{array} \right). \]

Proof: Expand

\[ (|\rho|)^n = x_1^2 \left( x_2^2 + |x|^2 \right)^n \left( x_3^2 x_4^2 - x_2^2 |x|^2 \right)^n = \sum_{i=0}^{n} \binom{n}{i} \binom{n}{j} (-1)^i x_1^{2n-2i} x_2^{2n-2i} x_3^{2n-2j} x_4^{2n-2j} |x|^2. \]

Now integrate with the above formula (value divided by \( \delta(k) \)) to obtain

\[ \frac{1}{(4 + \beta + 4k)n} \sum_{i=0}^{n} \binom{n}{i} \binom{n}{j} (-1)^i (k + 1)^2 \frac{\beta}{2} \right)_n \frac{\beta}{2} \right)_j \frac{\beta}{2} \right)_j \times \sum_{i=0}^{n} \binom{n}{i} \frac{\beta}{2} \right)_j \frac{\beta}{2} \right)_j \]

by the Chu–Vandermonde sum, the second line equals \((k + 1 + \frac{\beta}{2} + j)_n\). Use the substitutions

\[ (k + 1)_{n-j} = (-1)^j \frac{(k + 1)_n}{(-k - n)_j}, \]

\[ \left( k + 1 + \frac{\beta}{2} + j \right)_n = \frac{(k + 1 + \frac{\beta}{2} + n)_j}{(k + 1 + \frac{\beta}{2} + j)_n}, \]

\[ \binom{n}{j} (-1)^j = \frac{(-n)_j}{j!}, \]

in the \( j \)-sum to produce the stated formula.
Example:

\[
\int (|\rho^T||\rho|^2 f(x) \, d\mu = \frac{\delta(k)}{(4+\beta+4k)^4} \times \frac{1}{4}(2k+2+\beta) \left\{(k+1)^2(2k+2+\beta) - \frac{1}{4}\beta(2k+4+\beta)^2\right\}
\]

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