A concise formula for generalized two-qubit Hilbert–Schmidt separability probabilities

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Abstract

We report major advances in the research program initiated in ‘Moment-based evidence for simple rational-valued Hilbert–Schmidt generic $2 \times 2$ separability probabilities’ (Slater and Dunkl 2012 J. Phys. A: Math. Theor. 45 095305). A highly succinct separability probability function $P(\alpha)$ is put forth, yielding for generic (nine-dimensional) two-rebit systems, $P(\frac{1}{2}) = \frac{29}{64}$, (15-dimensional) two-qubit systems, $P(1) = \frac{8}{33}$ and (27-dimensional) two-quater(nionic)bit systems, $P(2) = \frac{26}{323}$. This particular form of $P(\alpha)$ was obtained by Qing-Hu Hou by applying Zeilberger’s algorithm (‘creative telescoping’) to a fully equivalent—but considerably more complicated—expression containing six $\gamma F_3$ hypergeometric functions (all with argument $\frac{27}{64} = \left(\frac{3}{4}\right)^3$). That hypergeometric form itself had been obtained using systematic, high-accuracy probability-distribution-reconstruction computations. These employed 7501 determinantal moments of partially transposed $4 \times 4$ density matrices, parameterized by $\alpha = \frac{1}{2}, 1, \frac{3}{2}, 2, \ldots, 32$. From these computations, exact rational-valued separability probabilities were discernible. The (integral/half-integral) sequences of 32 rational values then served as input to the Mathematica FindSequenceFunction command, from which the initially obtained hypergeometric form of $P(\alpha)$ emerged.

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

1. Introduction

Our study will be devoted to addressing the fundamental quantum-information-theoretic problem, apparently first explicitly discussed by Życzkowski, Horodecki, Sanpera and Lewenstein (ZHSL) [1] in their highly-cited 1998 paper, ‘Volume of the set of separable states’ [1]. They gave ‘three main reasons of importance’—philosophical, practical and physical—for examining such problems (cf [2]). Specifically, we will address the problem raised in [1] of what proportion (that is, ‘separability probability’) of quantum states are
separable/disentangled [3]. We endow the (generalized two-qubit) states, to which we confine our attention here, with the Hilbert–Schmidt (Euclidean/flat) metric and its accompanying measure [4, 5]. It is certainly also of interest to study the problem posed by ZHSL in alternative—but perhaps analytically even more challenging—settings, in particular that of the Bures (minimal monotone) metric/measure [5–11].

We report an apparent resolution of the ZHSL separability probability problem in the generalized two-qubit Hilbert–Schmidt context, in terms of the titular ‘concise formula’, which we will denote by $P(\alpha)$. Though we still lack a fully rigorous argument for its validity, the formula strongly appears to fulfil the indicated role, while manifesting important mathematical (random matrix theory [12, 13], ...) and physical (quantum entanglement [1, 5, 13]) properties. Thus, we have

$$P(\alpha) = \sum_{i=0}^{\infty} f(\alpha + i),$$

where

$$f(\alpha) = P(\alpha) - P(\alpha + 1) = \frac{q(\alpha) 2^{-4\alpha-6} \Gamma(3\alpha + \frac{5}{2}) \Gamma(5\alpha + 2)}{3\Gamma(\alpha+1) \Gamma(2\alpha+3) \Gamma(5\alpha + \frac{11}{2})},$$

and

$$q(\alpha) = 185 000 \alpha^5 + 779 750 \alpha^4 + 1289 125 \alpha^3 + 1042 015 \alpha^2 + 410 694 \alpha + 63 000$$

$$= \alpha(5\alpha(25\alpha(740\alpha + 3119) + 10 313) + 208 403) + 410 694 \alpha + 63 000.$$  

A reader, equipped with any standard contemporary mathematical language programming package (Maple, Mathematica, Matlab, ...), can readily verify that (to arbitrarily high-precision [hundreds/thousands of digits]), quite remarkably (but not yet formally proven [14]), $P(0) = 1$, $P(\frac{1}{2}) = \frac{29}{64}$, $P(1) = \frac{8}{33}$ and $P(2) = \frac{26}{323}$ (figures 3 and 4). In terms of the physical implications of the formula, we find compelling evidence that $P(\alpha)$ yields the separability probability [1]—with respect to Hilbert–Schmidt measure—of generalized two-qubit states, where, in particular $\alpha = 0, \frac{1}{2}, 1, 2$ correspond to classical, rebit, qubit and quater(nionic)bit states, respectively.

We will indicate below the multistep procedure by which the particular concise form of $P(\alpha)$ presented above was obtained. This process depended upon, first, the derivation [15] of (hypergeometric-based) formulas for the moments of probability distributions over the determinants of partially transposed density matrices, followed by the estimation (using a certain Legendre-polynomial-based probability-distribution-reconstruction procedure [16]) from those moments of cumulative (over the separability interval) probabilities. Then, $\alpha$-parameterized sequences of these cumulative probabilities were analyzed to extract the underlying structure captured by $P(\alpha)$. This initially took a relatively complicated hypergeometric form (figure 3), from which the concise formula above was subsequently derived (figures 5 and 6) by Qing-Hu Hou using Zeilberger’s algorithm [17].

1.1. Background

The underpinning, predecessor paper [15]—addressing the relatively long-standing $2 \times 2$ separability probability question [1, 7, 8, 18–24] (cf [10, 25, 26])—consisted largely of two sets of analyses. The first set was concerned with establishing formulas for the bivariate determinantal product moments $\langle |\rho^{PT}| \rho| \rangle$, $k, n = 0, 1, 2, 3, \ldots$, with respect to Hilbert–Schmidt (Euclidean/flat) measure [5, section 14.3] [4], of generic (nine-dimensional) two-rebit and (15-dimensional) two-qubit density matrices $\rho$. Here $\rho^{PT}$ denotes the partial transpose of the $4 \times 4$ density matrix $\rho$. Nonnegativity of the determinant $|\rho^{PT}|$ is both a necessary and sufficient condition for separability in this $2 \times 2$ setting [27].
In the second set of primary analyses in [15], the univariate determinantal moments \( \langle |\rho_{PT}|^{n} \rangle \) and \( \langle (|\rho_{PT}| |\rho|)^{n} \rangle \), induced using the bivariate formulas, served as input to a Legendre-polynomial-based probability-distribution-reconstruction algorithm of Provost [16, section 2] (cf [28]). This yielded estimates of the desired separability probabilities. The reconstructed probability distributions based on \(|\rho_{PT}| \) are defined over the interval \(|\rho_{PT}| \in [-\frac{1}{16}, \frac{1}{256}] \), while the associated separability probabilities are the cumulative probabilities of these distributions over the nonnegative subinterval \(|\rho_{PT}| \in [0, \frac{1}{256}] \). We note that for the fully mixed (classical) state, \(|\rho_{PT}| = \frac{1}{256} \), while for a maximally entangled state, such as a Bell state, \(|\rho_{PT}| = -\frac{1}{16} \), thus, delimiting the range of \(|\rho_{PT}| \).

A highly intriguing aspect of the (not yet rigorously established) determinantal moment formulas obtained by C Dunkl in [15, appendix D.4] was that both the two-rebit (\( \alpha = \frac{1}{2} \)) and two-qubit (\( \alpha = 1 \)) cases could be encompassed by a single formula, with a Dyson-index-like parameter \( \alpha \) serving to distinguish the two cases. Additionally, the results of the formula for \( \alpha = 2 \) and \( n = 1 \) and 2 have recently been confirmed computationally by Dunkl using the ‘Moore determinant’ (quasideterminant) [30, 31] of \( 4 \times 4 \) quaternionic density matrices. (However, tentative efforts of ours to verify the \( \alpha = 4 \) [conjecturally, octonionic [32], problematical] case, have not proved successful.)

When the probability-distribution-reconstruction algorithm [16] was applied in [15] to the two-rebit case (\( \alpha = \frac{1}{2} \)), employing the first 3310 moments of \(|\rho_{PT}| \), a (lower-bound) estimate that was 0.999 955 times as large as \( 29_{64} \approx 0.453\,120 \) was obtained (cf [33, p 6]).

Analogously, in the two-qubit case (\( \alpha = 1 \)), using 2415 moments, an estimate that was 0.999 997 066 times as large as \( 8_{33} \approx 0.242\,424 \) was derived. This constitutes an appealingly simple rational value that had previously been conjectured in a quite different (non-moment-based) form of analysis, in which ‘separability functions’ had been the main tool employed [24]. (Note, however, that the two-rebit separability probability conjecture of \( \frac{8}{17} \), somewhat secondarily advanced in [24], has now been discarded in favor of \( \frac{29}{64} \).) Let us note, supportively, that in an extensive Monte Carlo analysis, Zhou, Chern, Fei and Joynt obtained an estimate for this two-qubit separability probability of 0.2424 ± 0.0002 [34, equation (B7)]. Additionally, in the very same context, Fonseca-Romero, Rincón and Viviescas report a compatible statistic of 24% [35, section 8].

Further, the determinantal moment formulas advanced in [15] were then applied with \( \alpha \) set equal to 2. This appears—as the indicated recent (Moore determinant) computations of Dunkl show—to correspond to the generic 27-dimensional set of quaternionic density matrices [36, 37]. Quite remarkably, a separability probability estimate, based on 2325 moments, that was 0.999 999 987 times as large as \( 26_{323} \approx 0.080\,4954 \) was found.

2. Outline of present study

In the present study, we extend these three (individually-conducted) moment-based analyses in a more systematic, thorough manner, jointly embracing the sixty-four integral and half-integral values \( \alpha = \frac{1}{2}, 1, \frac{3}{2}, 2, \ldots, 32 \). We do this by accelerating, for our specific purposes, the Mathematica probability-distribution-reconstruction program of Provost [16], in a number of ways. Most significantly, we make use of the three-term recurrence relations for the Legendre polynomials. Doing so obviates the need to compute each successive higher-degree Legendre polynomial \( ab\ initial \).

In this manner, we were able to obtain—using exact computer arithmetic throughout—‘generalized’ separability probability estimates based on 7501 moments for \( \alpha = \frac{1}{2}, 1, \frac{3}{2}, \ldots, 32 \). In figure 1 we plot the logarithms of the resultant sixty-four separability
probability estimates (cf [15, figure 8]), which fall close to the line $-0.946\,418\,1889\alpha$. In figure 2 we show the residuals from this linear fit.

In figure 3 we present a hypergeometric-function-based formula, together with striking supporting evidence for it, that appears to succeed in uncovering the functional relation $(P(\alpha))$ underlying the entirety of these sixty-four generalized separability probabilities. Further, in (6), and the immediately preceding text, we list a number of remarkable values yielded by this hypergeometric formula for values of $\alpha$ other than the basic sixty-four (half-integral and integral) values from which we have started.

Then, we are able to report—with the assistance of Qing-Hu Hou—a striking condensation of the lengthy expression presented in figure 3, that is, the titular 'concise formula' (equations (1)–(3)).

Some additional computational results of interest are presented in the appendix.

3. New results

3.1. The three basic (rebit, qubit, quaterbit) conjectures revisited

3.1.1. $\alpha = \frac{1}{2}$—the two-rebit case. In [15], a lower-bound estimate of the two-rebit separability probability was obtained, with the use of the first 3310 moments of $|\rho^{PT}|$. It was 0.9999 55 times
Hypergeometric formula $P(\alpha)$ for Hilbert–Schmidt generic $2 \times 2$ generalized separability probabilities and evidence that it reproduces the basic three (real $[\alpha = \frac{1}{2}]$, complex $[\alpha = 1]$ and quaternionic $[\alpha = 2]$) conjectures of $\frac{29}{27}$, $\frac{8}{3}$ and $\frac{26}{233}$.

Figure 3. Hypergeometric formula $P(\alpha)$ for Hilbert–Schmidt generic $2 \times 2$ generalized separability probabilities and evidence that it reproduces the basic three (real $[\alpha = \frac{1}{2}]$, complex $[\alpha = 1]$ and quaternionic $[\alpha = 2]$) conjectures of $\frac{29}{27}$, $\frac{8}{3}$ and $\frac{26}{233}$.

Figure 4. Generalized two-qubit separability probability function $P(\alpha)$, with $P(0) = 1$, $P(\frac{1}{2}) = \frac{29}{27}$, $P(1) = \frac{8}{3}$, $P(2) = \frac{26}{233}$ for generic classical four-level ($\alpha = 0$), two-rebit ($\alpha = \frac{1}{2}$), two-qubit ($\alpha = 1$) and two-quaterbit ($\alpha = 2$) systems, respectively.
as large as $29/64 \approx 0.453120$. With the indicated use now of 7501 moments, the figure increases to $0.999989567$. This outcome thus fortifies our previous conjecture.

3.1.2. $\alpha = 1$–the two-qubit case. In [15], a lower-bound estimate of the two-qubit separability probability was obtained, with the use of the first 2415 moments of $|\rho_{PT}|$, that...
Figure 6. Second Maple worksheet of Hou used in deriving concise form of hypergeometric formula (figure 3).
was 0.999 997 066 times as large as $\frac{8}{17} \approx 0.242 424$ (cf [34, equation (B7)]). Employing 7501 moments, this figure increases to 0.999 999 86.

3.1.3. $\alpha = 2$—the quaternionic case. In [15], a lower-bound estimate of the (presumptive) quaternionic separability probability was obtained that was 0.999 999 987 times as large as $\frac{26}{323} \approx 0.080 4954$, using the first 2325 moments of $|\rho_{PT}|$. Based on 7501 moments, this figure increases, quite remarkably still, to 0.999 999 993.

3.2. Generalized separability probability hypergeometric formula

A principal motivation in undertaking the analyses reported here—in addition to further scrutinizing the three specific conjectures reported in [15]—was to uncover the functional relation underlying the curve in figure 1 (and/or its original non-logarithmic counterpart).

Preliminarily, let us note that the zeroth-order approximation (being independent of the particular value of $\alpha$) provided by the Provost Legendre-polynomial-based probability-distribution-reconstruction algorithm is simply the uniform distribution over the interval $|\rho_{PT}| \in \left[ -\frac{1}{16}, \frac{1}{256} \right]$. The corresponding zeroth-order separability probability estimate is the cumulative probability of this distribution over the nonnegative subinterval $[0, \frac{1}{16}]$, that is, $\frac{\frac{1}{16}}{\frac{1}{16} + \frac{1}{256}} = \frac{1}{17} \approx 0.058 8235$. So, it certainly appears that speedier convergence (section 3.1) of the algorithm occurs for separability probabilities, the true values of which are initially close to $\frac{1}{17}$ (such as $\frac{26}{323} \approx 0.080 4954$ in the quaternionic case). Convergence also markedly increases as $\alpha$ increases.

It appeared, numerically, that the generalized separability probabilities for integral and half-integral values of $\alpha$ were rational values (not only $\frac{26}{323}, \frac{8}{17}, \frac{26}{323}$, for the three specific values $\alpha = \frac{1}{2}, 1, 2$ of original focus). With various computational tools and search strategies based upon emerging mathematical properties, we were able to advance additional, seemingly plausible conjectures as to the exact values for $\alpha = 3, 4, \ldots, 32$, as well. (We inserted many of our high-precision numerical estimates into the search box on the Wolfram Alpha website—which then indicated likely candidates for corresponding rational values.)

We fed this sequence of thirty-two conjectured rational numbers into the FindSequenceFunction command of Mathematica. (This command ’attempts to find a simple
function that yields the sequence \( a_n \) when given successive integer arguments,’ but apparently can succeed with rational arguments, as well.) To our considerable satisfaction, this produced a generating formula (incorporating a diversity of hypergeometric functions of the \( \,_pF_{p-1} \) type, \( p = 7, \ldots, 11 \), all with argument \( z = \frac{27}{46} = \left( \frac{3}{2} \right)^3 \) for the sequence (cf [38, equation (11)]). (Let us note that \( z^{-\frac{1}{2}} = \frac{46}{27} \) is the ‘residual entropy for square ice’ [39, p 412] (cf [40, equations(27), (28)]. An analogous appearance of \( \frac{27}{46} \) occurs in a hypergeometric ['Ramanujan-like'] summation for \( \frac{1657}{3} \) of Guillera [41]. In a private communication, he remarked that the value \( z = \frac{27}{46} \) appears to frequently occur in hypergeometric identities, and that this appears to have some modular or modular-like origin.). In fact, the Mathematica command succeeds using only the first 28 conjectured rational numbers, but no fewer—so it seems fortunate that our computations were so extensive.)

However, the formula produced by the Mathematica command was quite cumbersome in nature (extending over several pages of output). With its use, nevertheless, we were able to convincingly generate rational values for half-integral \( \alpha \) (including the two-rebit 29 conjecture), also fitting our corresponding half-integral thirty-two numerical estimates exceedingly well. (Let us strongly emphasize that the hypergeometric-based formula was initially generated using only the integral values of \( \alpha \). The process was fully reversible, and we could first employ the half-integral results to generate the formula—which then—seemingly perfectly fitted the integral values.)

At this point, for illustrative purposes, let us list the first ten half-integral and ten integral rational values (generalized separability probabilities), along with their approximate numerical values.

\[
\begin{align*}
\alpha &= \frac{1}{2}, \quad \frac{29}{62} = 0.453125 & \alpha &= 1, \quad \frac{3}{6} = 0.242424 \\
\alpha &= \frac{3}{4}, \quad \frac{36}{61} = 0.137562 & \alpha &= 2, \quad \frac{5}{6} = 0.8084954 \\
\alpha &= \frac{5}{2}, \quad \frac{51}{64} = 0.048083 & \alpha &= 3, \quad \frac{1999}{2208} = 0.029081 \\
\alpha &= \frac{7}{4}, \quad \frac{38}{51} = 0.079498 & \alpha &= 4, \quad \frac{6462}{7695} = 0.0108722 \\
\alpha &= \frac{9}{2}, \quad \frac{6531}{8581} = 0.0107152 & \alpha &= 5, \quad \frac{18014}{19999} = 0.0041701 \\
\alpha &= \frac{11}{4}, \quad \frac{7362}{9383} = 0.0025994 & \alpha &= 6, \quad \frac{179804}{200000} = 0.00162519 \\
\alpha &= \frac{13}{2}, \quad \frac{2137}{2560} = 0.0004408 & \alpha &= 7, \quad \frac{1911501}{2200000} = 0.00064309 \\
\alpha &= \frac{15}{4}, \quad \frac{124792}{153843} = 0.000403227 & \alpha &= 8, \quad \frac{131139}{1600000} = 0.000254391 \\
\alpha &= \frac{17}{2}, \quad \frac{40757}{512000} = 0.000160753 & \alpha &= 9, \quad \frac{74195}{8000000} = 0.000101729 \\
\alpha &= \frac{19}{4}, \quad \frac{113879}{143049} = 0.000064469 & \alpha &= 10, \quad \frac{738710}{9000000} = 0.0000408939
\end{align*}
\]

(4)

To simplify the cumbersome (several-page) output yielded by the Mathematica FindSequenceFunction command, we employed certain of the ‘contiguous rules’ for hypergeometric functions listed by Krattenthaler in his package HYP [42] (cf [43]). Multiple applications of the rules C14 and C18 there, together with certain gamma function simplifications suggested by C Dunkl, led to the rather more compact formula displayed in figure 3. This formula incorporates a six-member family \( (k = 1, \ldots, 6) \) of \( \gamma_6 \) hypergeometric functions, differing only in the first upper index \( k \),

\[
\gamma_6 \left( k, \alpha + \frac{2}{5}, \alpha + \frac{3}{5}, \alpha + \frac{4}{5}, \alpha + \frac{5}{6}, \alpha + \frac{7}{6}, \alpha + \frac{13}{10}, \alpha + \frac{3}{2}, \alpha + \frac{17}{10}, \alpha + \frac{19}{10}, \alpha + 2, \alpha + \frac{21}{10}, \frac{27}{64} \right).
\]

(5)
(The reader will note interesting sequences of upper and lower parameters (cf [44]).) In general, we are only able to evaluate the formula numerically, but then to arbitrarily high (hundred-, if not thousand-digit) precision, giving us strong confidence—despite the lack yet of a formal proof (cf [14])—in the validity of the exact generalized separability probabilities \( \frac{21}{2}, \frac{8}{3}, \frac{26}{33}, \ldots \), that we advance.

3.2.1. Additional interesting values yielded by the hypergeometric formula. Let us now apply the formula (figure 3) to values of \( \alpha \) other than the initial sixty-four studied. For \( \alpha = 0 \), the formula yields—as would be expected—the ‘classical separability probability’ of 1. Further, proceeding in a purely formal manner (since there appears to be no corresponding genuine probability distribution over \([ - \frac{1}{16}, \frac{1}{256} ]\), for the negative value \( \alpha = -\frac{1}{2} \), the formula yields \( \frac{1}{2} \). For \( \alpha = -\frac{1}{4} \), it yields \( -2 \). Remarkably still, for \( \alpha = \frac{1}{4} \), the result is clearly (to one thousand decimal places) equal to 2 minus \( \frac{34}{21\text{agm}(1, \sqrt{2})} \approx 2 - \frac{17\sqrt{\pi}}{21\pi} \approx 0.648 699 3992 \), where the arithmetic–geometric mean of 1 and \( \sqrt{2} \) is indicated. (The reciprocal of this mean is Gauss’s constant.) For \( \alpha = \frac{1}{2} \), the result equals \( 2 - \frac{69689\sqrt{3}}{4420\sqrt{6\pi}} \approx 0.327 968 4732 \), while for \( \alpha = -\frac{2}{3} \), we have
\[
\begin{align*}
\frac{128}{21\text{agm}(1, \sqrt{2})} &+ 2 = 2 + \frac{22\sqrt{\pi}}{21\pi} \approx 7.087 249 321. \\
\text{For } \alpha = \frac{2}{3}, \text{ the outcome is } 2 - \frac{288 \cdot 927\sqrt{\pi}}{344 \cdot 080\pi} \approx 0.364 248 974 56.
\end{align*}
\]
Results are presented in the table:

| \( \alpha \) | \( P(\alpha) \) | value |
|-------------|----------------|------|
| \( -\frac{1}{4} \) | \( 2 + \frac{32\sqrt{\pi}}{21\pi} \) | 7.087 25 |
| \( -\frac{1}{3} \) | \( 2 - \frac{8\pi}{3\sqrt{3}\pi} \) | 1.245 27 |
| \( \frac{1}{3} \) | \( \frac{2}{3} \) | 0.666 667 |
| \( \frac{1}{4} \) | \( \frac{2}{3} + \frac{3\pi}{4\pi} \) | 3.461 |
| \( \frac{1}{2} \) | 2 | 2 |
| \( \frac{1}{4} \) | \( 2 - \frac{17\sqrt{\pi}}{21\pi} \) | 0.648 699 |
| \( \frac{1}{3} \) | \( 2 - \frac{49\sqrt{\pi}}{9\pi} \) | 0.572 443 |
| \( \frac{2}{3} \) | \( 2 - \frac{288 \cdot 927\sqrt{\pi}}{344 \cdot 080\pi} \) | 0.364 249 |
| \( \frac{3}{4} \) | \( 2 - \frac{9689\sqrt{\pi}}{4420\sqrt{6\pi}} \) | 0.327 968 |

(Let us note that the term \( \frac{3\sqrt{\pi}}{4\pi} \approx 1.460 998 48 \) present in the result for \( \alpha = -\frac{1}{4} \) is ‘Baxter’s four-coloring constant’ for a triangular lattice [39, p 413].) Also, for \( \alpha = -1 \), we have \( \frac{\sqrt{2}}{2} \). For \( \alpha = -\frac{1}{2} \), the result is \( \frac{\sqrt{2}}{2} \).

4. Concise reformulation of \( \gamma F_6 \) hypergeometric expression (figure 3)

We had previously ourselves been unable to find an equivalent form of \( P(\alpha) \) with fewer than six hypergeometric functions (figure 3). Qing-Hu Hou of the Center for Combinatorics of Nankai University, however, was able to obtain the remarkably succinct and clearly correct results (1)–(3)—which he communicated to us in a few e-mail messages. (Accompanying them were two Maple worksheets indicating his calculations [figures 5 and 6].) Hou first observed that the hypergeometric-based formula for \( P(\alpha) \) could be expressed as an infinite summation.
Letting $P_l(\alpha)$ be the $l$-th such summand, application of Zeilberger’s algorithm \cite{17} (a method for producing combinatorial identities, also known as ‘creative telescoping’) yielded that

$$P_l(\alpha) - P_l(\alpha + 1) = -P_{l+1}(\alpha) + P_l(\alpha). \quad (7)$$

(The package APCI—available at http://www.combinatorics.net.cn/homepage/hou/—was employed. In a different quantum-information context, Datta employed the algorithm to ascertain that no closed form exists for a certain series, ‘retarding’ the evaluation of the ‘ratio of the negativity of random pure states to the maximal negativity for Haar-distributed states of $n$ qubits’ \cite[appendix A, table 1]{45}.) Summing over $l$ from 0 to $\infty$, Hou found that

$$P(\alpha) - P(\alpha + 1) = P_0(\alpha). \quad (8)$$

Letting $f(\alpha) = P_0(\alpha)$, the concise summation formula (1) is obtained. (C Krattenthaler indicated (Krattenthaler, private communication) that these results might equally well be derived without recourse to Zeilberger’s algorithm. Also, a referee expressed puzzlement at the peculiar (redundant) form of equation (7). This appears to be an artifact arising from the particular manner in which the algorithm is applied in the proving of hypergeometric identities.)

We certainly need to indicate, however, that if we do explicitly perform the infinite summation indicated in (1), then we revert to a (‘nonconcise’) form of $P(\alpha)$, again containing six hypergeometric functions. Further, it appears that we can only evaluate (1) numerically—but then easily to hundreds and even thousands of digits of precision—giving us extremely high confidence in the specific rational-valued Hilbert–Schmidt separability probabilities advanced.

5. Concluding remarks

There remain the important problems of formally verifying the formulas for $P(\alpha)$ (as well as the underlying determinantal moment formulas for $|\rho^{PT}|, \ldots$, in \cite{15}, employed in the probability-distribution-reconstruction process), and achieving a better understanding of what these results convey regarding the geometry of quantum states \cite{5, 46, 47}. Further, questions of the asymptotic behavior of the formula ($\alpha \to \infty$) and of possible Bures metric \cite{5–8, 18} counterparts to it, are under investigation \cite{11}.

We are currently engaged in attempting to determine further properties—in addition to the cumulative (separability) probabilities over $[0, \frac{1}{16}]$ obtained from the titular concise formula (equation (1)–(3))—of the probability distributions of $|\rho^{PT}|$ over $[-\frac{1}{16}, \frac{1}{256}]$, as a function of the Dyson-index-like parameter $\alpha$. As one such finding, it appears that the y-intercept (at which $|\rho^{PT}| = 0$, that is, the separability-entanglement boundary) in the presumed quaternionic case ($\alpha = 2$) is $\frac{7425}{216} = \frac{29 \times 3^2 \times 5 \times 11}{216} \approx 218.382$ \cite{48}. (The Legendre-polynomial-based probability-distribution-reconstruction algorithm of Provost \cite{16} yielded an estimate 0.999 999 997 42 times as large as $\frac{7425}{216}$, when implemented with 10 000 moments. Based also on 10 000 moments—but with inferior convergence properties—the two-qubit [$\alpha = 1$] and two-rebit [$\alpha = \frac{1}{2}$] y-intercepts were estimated as 389.995 (conjecturally equal to 390 = $2 \cdot 3 \cdot 5 \cdot 13$) and 502.964, respectively \cite{48}.)

The foundational paper of ZHSL, ‘Volume of the set of separable states’ \cite{1} (cf \cite{2}), did ask for volumes, not specifically probabilities. At least, for the two-rebit, two-qubit and two-quaterbit cases, $\alpha = \frac{1}{2} , 1$ and 2, we can readily, using the Hilbert–Schmidt volume formulas of Andai \cite[theorems 1–3]{36} (cf \cite{4, 5}), convert the corresponding separability probabilities to the separable volumes $\frac{3914156993718034944000000}{3914156993718034944000000} = \frac{29 \times 3^4 \times 5^7 \times 11^8 \times 17}{3914156993718034944000000}$ and $\frac{3914156993718034944000000}{3914156993718034944000000} = \frac{29 \times 3^4 \times 5^7 \times 11^8 \times 17}{3914156993718034944000000}$, respectively. The determination of
separable volumes—as opposed to probabilities—for other values of $\alpha$ than these fundamental three appears to be rather problematical, however.

Let us also note the relevance of the study of Szarek, Bengtsson and Życzkowski [49], in which they show that the convex set of separable mixed states of the $2 \times 2$ system is a body of constant height. Theorem 2 of that paper, in conjunction with the results here, allows one, it would seem, to immediately deduce that the separability probabilities of the generic minimally-degenerate/boundary 8-, 14-, and 26-dimensional two-rebit, two-qubit, and two-quaterbit states are one-half (that is, $\frac{29}{32}$, $\frac{4}{13}$ and $\frac{13}{323}$) the separability probabilities of their generic non-degenerate counterparts.

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Appendix. Exact values of derivatives of $P(\alpha)$

A.1. Successing derivatives at $\alpha = 0$

The first derivative of $P(\alpha)$ evaluated at (the classical case) $\alpha = 0$ is $-2$, while the second derivative is $40-20 \zeta(2) = 40 - \frac{10\pi^2}{3} \approx 7.10132$. (The third derivative was computed as $-43.7454236566749417600$.)

A.2. First derivatives at $\alpha = 1, 2, \ldots, \text{ et al}$

The first derivative of $P(\alpha)$ at $\alpha = -\frac{1}{2}$ is $-\frac{80}{3}$ and at $\alpha = \frac{1}{2}$ is $\frac{384}{917} (917-984 \log(2)) \approx 0.611831$, and $-2$ at $\alpha = 0$, as previously mentioned. We have also been able to determine rational values of $P(\alpha)$ for $\alpha = 1, 2, \ldots, 97$. We list the first seven of these. (The Mathematica command FindSequenceFunction, however, did not succeed in this instance in generating an underlying function for this sequence of 97 rational numbers—although, of course, one can be directly obtained from our explicit form of $P(\alpha)$.)

\[
\begin{bmatrix}
\alpha & P'(\alpha) \\
1 & -130.577 \\
2 & -3177.826 \\
3 & -3598.754 \\
4 & -9432.221 \\
5 & -7745.968 \\
6 & -16370.966 \\
7 & -12455.275 \\
\end{bmatrix}
\approx
\begin{bmatrix}
-0.285489 \\
-0.0845257 \\
-0.0289266 \\
-0.0105241 \\
-0.00395978 \\
-0.00152186 \\
-0.000593494 \\
\end{bmatrix}
\]  

\[\text{(A.1)}\]

References

[1] Życzkowski K, Horodecki P, Sanpera A and Lewenstein M 1998 Phys. Rev. A 58 883
[2] Singh R, Kunkwal R and Simon R 2013 arXiv:quant-ph/1307.1454
