Hilbert-Schmidt Orthogonality of $\det(\rho)$ and $\det(\rho^{PT})$ over the Two-Rebit Systems $\rho$ and Further Determinantal Moment Analyses

Paul B. Slater

ISBER, University of California, Santa Barbara, CA 93106

(Dated: April 1, 2011)

Abstract

A complete description of the multitudinous ways in which quantum particles can be entangled requires the use of high-dimensional abstract mathematical spaces. We report here a particularly interesting feature of the nine-dimensional convex set–endowed with Hilbert-Schmidt (Euclidean/flat) measure–composed of two-rebit ($4 \times 4$) density matrices ($\rho$). To each $\rho$ is assigned the product of its (nonnegative) determinant $|\rho|$ and the determinant of its partial transpose $|\rho^{PT}|$–negative values of which, by the results of Peres and Horodecki, signify the entanglement of $\rho$. Integrating this product, $|\rho||\rho^{PT}| = |\rho\rho^{PT}|$, over the nine-dimensional space, using the indicated (HS) measure, we obtain the result zero. The two determinants, thus, form a pair of multivariate orthogonal polynomials with respect to HS measure. However, orthogonality does not hold, we find, if the symmetry of the nine-dimensional two-rebit scenario is broken slightly, nor with the use of non-flat measures, such as the prominent Bures (minimal monotone) measure–nor in the full HS extension to the 15-dimensional convex set of two-qubit density matrices. We discuss relations–involving the HS moments of $|\rho^{PT}|$–to the long-standing problem of determining the probability that a generic pair of rebits/qubits is separable.

PACS numbers: Valid PACS 03.67.Mn, 02.30.Cj, 02.30.Zz, 02.50.Sk

*Electronic address: slater@kitp.ucsb.edu
I. INTRODUCTION AND STATEMENT OF MAIN RESULTS

The simplest form of finite-dimensional system capable of exhibiting the fundamental, holistic property of entanglement—"that feature of quantum formalism which makes it impossible to simulate quantum correlations within any classical formalism" [1]—is that composed of a pair of two-level systems (quantum bits or "qubits") [2]. The joint state of two qubits is describable \( (2 \times 2 = 4) \) by a \( 4 \times 4 \) density matrix \( \rho \), that is a Hermitian matrix (its transpose equalling its complex conjugate) having its four nonnegative diagonal entries (probabilities)–as well as its four nonnegative eigenvalues–summing to one [3]. The entirety of such \( 4 \times 4 \) density matrices with their entries restricted to real values—which will be our principal subject of analysis here–forms a nine-dimensional convex set. We note that \( 2 \times 2 \) density matrices with real entries have been termed "rebits" [4].

Endowing the nine-dimensional set of pairs of rebits with Hilbert-Schmidt (HS) (Euclidean/flat) measure [2, sec. 14.3] [5, 6], we arrive at the following trio of computational results [7]. The three are: (1) the average value or mean (first moment) of the (necessarily nonnegative) determinant of \( \rho \), denoted \( |\rho| (\equiv \det(\rho)) \), is \( \frac{1}{2288} = (2^4 \cdot 11 \cdot 13)^{-1} \); (2) the mean of the determinant \( |\rho^{PT}| \) of the partial transpose (PT) of \( \rho \)–negative values of which, by the celebrated results of Peres [8] and the Horodecki family [9], are fully equivalent (for qubit-qubit systems—as well as qubit-qutrit systems, representable by \( 6 \times 6 \) density matrices) to the entanglement/nonseparability of \( \rho \)—is \( -\frac{1}{858} = -(2 \cdot 3 \cdot 11 \cdot 13)^{-1} \); and (3) the mean of the product of these two determinants, that is \( |\rho||\rho^{PT}| \) \( (= |\rho\rho^{PT}| \) by the Cauchy-Binet [Gram’s] Theorem), is zero. (The partial transpose–identifiable with the antiunitary operation of time-reversal [10] (cf. [11, 12])—of a \( 4 \times 4 \) matrix can be obtained simply by transposing in place its four \( 2 \times 2 \) blocks.)

So, by assigning to each generic real \( 4 \times 4 \) density matrix \( \rho \), a value equal to this product of determinants, we find that the total (but yet undetermined, necessarily negative) value allotted to the entangled states exactly cancels the (necessarily nonnegative) value allotted to the disentangled/separable states. This result appears to be special to the HS measure, as the analogous trio of results using the well-known Bures (minimal monotone) measure [2, sec. 14.4] [14] is \( \frac{1}{8192} = 2^{-13} \) and, numerically, -0.0030959720 and -1.124478 \( \cdot 10^{-7} \). It is a natural hypothesis–but one apparently presenting substantial computational challenges to test–that this zero-mean (HS) result extends to the standard 15-dimensional
convex set of $4 \times 4$ density matrices with arbitrary complex off-diagonal entries \[^{13}\text{sec. 2}].\) We can not, however, unqualifiedly, straightforwardly extend the interpretation of the zero-product-mean hypothesis to bipartite quantum systems describable by density matrices of dimensions greater than four. Then, $\rho^{PT}$ can have more than one negative eigenvalue, with an even number of such eigenvalues yielding a positive value for the determinant $|\rho^{PT}|$ (cf. \[^5\]). Thus, a nonnegative value of $|\rho^{PT}|$ would not necessarily indicate that $\rho$ is separable.

The zero-product-mean HS result does not hold, in general, however, for arbitrary two-qubit scenarios. This can be seen by slightly modifying in each of three ways, our basic nine-dimensional two-rebit example—thereby diminishing its inherent symmetry. Firstly, if we set one off-diagonal pair of entries ($\rho_{34} = \rho_{43}$, say) of $\rho$ to zero, giving us an 8-dimensional convex set of density matrices, we obtain a mean of the probability distribution over $|\rho|$ of $\frac{1}{4752} = (2^4 \cdot 3^3 \cdot 11)^{-1} \approx 0.000210438$, for $|\rho^{PT}|$, a mean of $-\frac{13}{9504} = -13(2^5 \cdot 3^3 \cdot 11)^{-1} \approx -0.00136785$, and for the product of the two determinants, a nonzero mean of $\frac{1}{2196480} = (2^{10} \cdot 3 \cdot 5 \cdot 11 \cdot 13)^{-1} \approx 4.55274 \cdot 10^{-7}$. Secondly, if we increase the dimensionality from nine to ten by letting $\rho_{34}$ and $\rho_{43}$ be arbitrary complex conjugates of each other, then, the trio of means, numerically, is 0.000412154, -0.00082468, and (small, but apparently nonzero) $3.6035 \cdot 10^{-8}$. Thirdly, for the eight-dimensional set of $4 \times 4$ density matrices with real entries consisting of those minimally degenerate matrices having one eigenvalue zero—which constitute the boundary of the basic nine-dimensional set \[^{15}\]—the mean of the product of the three nonzero eigenvalues is $\frac{1}{66} \approx 0.0151515$, the mean of $|\rho^{PT}|$ is $-\frac{5}{2376} \approx -0.00210438$, while the mean of the product of $|\rho^{PT}|$ and the three nonzero eigenvalues is also nonzero, that is, $-\frac{1}{47520} \approx -0.0000210438$. (Of course, in this last minimally degenerate analysis, the determinant $|\rho|$, equalling the product of its four eigenvalues, is zero. So, we replace it, for our purposes, by the product of the three generically nonzero eigenvalues.) We, additionally, have found that no pair of principal ($4 \times 4$, $3 \times 3$, $2 \times 2$) minors, other than $|\rho|$ and $|\rho^{PT}|$—one minor of $\rho$ and the other of $\rho^{PT}$—are orthogonal over the nine-dimensional set with respect to HS measure.

Since both $|\rho|$ and $|\rho^{PT}|$ in the generic (two-rebit) nine-dimensional case are polynomials in nine variables, it is suggestive, at least, to consider these two determinants as a pair of multivariate orthogonal polynomials (MOPS)\[^{16-18}\] with respect to the HS measure. Grif-
Almost and Spanò have reviewed multivariate orthogonal polynomials with respect to weight measures given by Dirichlet distributions over simplices (such as that to be given below by (26) [6] over the 3-dimensional simplex formed by the diagonal entries of $4 \times 4$ density matrices [18]).

Let us also note, in our basic nine-dimensional scenario, that the expected value with respect to the Hilbert-Schmidt measure of the determinant of the commutator (appearing in the von Neumann equation for the time evolution of $\rho$), $[\rho, \rho^{PT}] = \rho \rho^{PT} - \rho^{PT} \rho$, is zero too. (Jarlskog found the the determinant of the commutator of mass matrices vanishes "if and only if there is no CP nonconservation" [19].) The analogous result was nonzero, that is $\frac{79}{27675648} \approx 2.8545 \cdot 10^{-6}$, when, once again, we broke the symmetry by setting $\rho_{34} = \rho_{43} = 0$.

The range of possible values of $|\rho|$ is $[0, 2^{-8}]$, that of $|\rho^{PT}|$ is $[-2^{-4}, 2^{-8}]$, while that of the product $|\rho||\rho^{PT}|$, in the nine-dimensional scenario, we find, is $[-2^{-12} \cdot 3^{-3}, 2^{-16}]$. This last upper limit is reached, clearly, by the fully mixed (classical) state—the diagonal density matrix with diagonal entries (probabilities) all equal to $\frac{1}{4}$. An instance of a density matrix attaining the last lower limit is

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

(1)

Now, the determinant $|\rho|$ is $\frac{1}{\sqrt{76}} (2\sqrt{3} - 3) \approx 0.0000805732$ and $|\rho^{PT}| = \frac{1}{\sqrt{76}} (-3 - 2\sqrt{3}) \approx -0.0112224$ (their product being the indicated lower limit $-\frac{1}{110992} \approx -9.04225 \cdot 10^{-6}$). Both $\rho$ and $\rho^{PT}$ have three identical eigenvalues ($\frac{1}{12} (3 - \sqrt{3}) \approx 0.105662$ for $\rho$, and $\frac{1}{12} (3 + \sqrt{3}) \approx 0.394338$ for $\rho^{PT}$). The isolated eigenvalue for $\rho$ is $\frac{1}{4} (1 + \sqrt{3}) \approx 0.683013$, and for $\rho^{PT}$, $\frac{1}{4} (1 - \sqrt{3}) \approx -0.183013$. The purity (index of coincidence [2, p. 56]), $\text{Tr}(\rho^2)$, of (1) equals $\frac{1}{2}$, so its inverse (the participation ratio [2, 20]) is 2.

A. Failure of Hilbert-Schmidt orthogonality in generic 15-dimensional two-qubit case

With the considerable computational (Mathematica) assistance of Michael Trott, we investigated the orthogonality hypothesis in the more demanding 15-dimensional generic two-qubit scenario, utilizing the Euler-angle parameterization of Tilma, Byrd and Sudarshan.
[57], together with the appropriate formulas of Žyczkowski and Sommers [5, eq. (3.11)]. For the expected value of $|\rho||\rho^{PT}|$, we obtained the nonzero value of $-\frac{1}{4576264} \approx -2.18519 \cdot 10^{-7}$, and for the mean of $|\rho^{PT}|$, the more negative value, $-\frac{7}{3876} \approx -0.00180599$. (Normalizing the two quantitates $|\rho|$ and $|\rho^{PT}|$ to have unit length [the latter numerically], we find that their inner product is approximately -0.07. This translates into an angle of 94 degrees, close to orthogonality.) are, since it appears to be even more computationally challenging to normalize $|\rho^{PT}|$ so that its average HS length is unity.) (However, we are not presently able to evaluate how close to orthogonality the determinants $|\rho|$ and $|\rho^{PT}|$ are, since it appears to be even more computationally challenging to normalize $|\rho^{PT}|$ so that its average HS length is unity.) The mean of $|\rho|$ is known [5, eq. (3.11)] to be $\frac{1}{3876} = (2^2 \cdot 3 \cdot 17 \cdot 19)^{-1} \approx 0.000257998$.

### B. Separability probabilities

It has been a relatively long-standing problem of "philosophical, practical and physical" significance [20] (in the recently-burgeoning field of quantum information [21]) to determine the probability (with respect to a number of measures, such as the HS and Bures) that a pair of qubits is separable [20, 22, 25, 31]. In this regard, it would be of interest to, in some manner, combine (to achieve a fuller understanding of the "geometry of quantum states" [2]) the trio of HS (first) moment (mean) results given above with two theorems (apparently the only ones yet developed) pertaining to entanglement in terms of the Hilbert-Schmidt measure (cf. [31]).

#### 1. Existing theorems

One of these theorems states that the probability that a generic bipartite state (of arbitrary dimension) has a positive partial transpose (PPT) is twice the probability that a generic boundary (minimally degenerate [one eigenvalue zero]) state has a PPT. (For the proof, it was established that the convex set of mixed PPT states is "pyramid-decomposable and hence is a body of constant height" [15].) The other (but now dimension-specific) theorem—derived by enforcing the nonnegativity of pairs of principal 3 $\times$ 3 minors of $\rho^{PT}$—is that the probability that a generic real 4 $\times$ 4 density matrix has a PPT (or, equivalently, by the Peres-Horodecki results, is separable) is no greater than $\frac{1129}{2100} \approx 0.537619$, nor no less
(using the concept of *absolute* separability \[23\] and the important Verstraete-Audenaert-de Moor bound \[24\]) than \(\frac{6928-2205\pi}{29/2} \approx 0.0348338 \[25\]. (An absolutely separable state is one that can not be entangled by any unitary transformation.) From these two theorems together, one easily obtains the corollary that the HS separability probability of a generic two-rebit minimally degenerate state is no greater than \(\frac{1129}{4200} \approx 0.26881\).

C. Higher-order moments

In addition to the trio of HS means (*first* moments) given above, we have been able to compute exactly several higher-order moments, as well, for the nine-dimensional scenario. The corresponding trio of *second* (raw/non-central) moments is

\[
\frac{1}{2489344} = (2^{10} \cdot 11 \cdot 13 \cdot 17)^{-1} \approx 4.01712 \cdot 10^{-7}, \quad \frac{27}{2489344} = \frac{3^3}{2^{10} \cdot 11 \cdot 13 \cdot 17} \approx 0.0000108462, \quad \text{and} \quad \frac{7}{5696345244800} = \frac{7}{2^{15} \cdot 3^2 \cdot 5 \cdot 13 \cdot 17 \cdot 19 \cdot 23} \approx 1.2288585 \cdot 10^{-12}. \]

From our several results, we can deduce that the generic two-rebit Hilbert-Schmidt correlation between \(|\rho|\) and \(|\rho^{PT}|\) is positive, that is \(\frac{\zeta'}{\text{real}} = 945 \frac{4^{3-2m} \Gamma(2m+2) \Gamma(2m+4)}{\Gamma(4m+10)} \approx 0.360291\).

Further, making use of the generalized normalization constants \[5, \text{eq. (4.3)}\], we obtain that the \(m\)-th moment of the probability distribution over \(|\rho|\) is

\[
\zeta'_{m/\text{real}} = 945 \frac{4^{3-2m} \Gamma(2m+2) \Gamma(2m+4)}{\Gamma(4m+10)}.
\]  

(2)

Let us also note that the counterpart of this result for the 15-dimensional generic complex two-qubit states is

\[
\zeta'_{m/\text{complex}} = 10897286400 \frac{\Gamma(m+1) \Gamma(m+2) \Gamma(m+3) \Gamma(m+4)}{\Gamma(4(m+4))}.
\]  

(3)

1. Application of Chebyshev inequality

The skewness \((\gamma_1)\) of the Hilbert-Schmidt probability distribution over \(|\rho^{PT}|\) is negative (as well as all odd moments \([m = 1, 3, 5, 7, 9]\) so far computed), that is, -3.13228–so, the left tail of the distribution is more pronounced than the right tail–while its kurtosis \((\gamma_2)\), a measure of ”peakedness” is quite high, 17.6316. (Higher kurtosis indicates that more of the variance is the result of infrequent extreme deviations than frequent modestly sized deviations.) From the first two moments, we obtain the variance

\[
\sigma^2 = \frac{30397}{3203785728} \approx 9.487838 \cdot 10^{-6}.
\]  

(4)
Application of the standard-form one-sided Chebyshev inequality \[26\] (we perform a linear transformation, so that negative values of \(|\rho|\) are mapped to \([0,1]\)), then, yields an upper bound on the Hilbert-Schmidt separability probability of the two-rebit density matrices of \(\frac{3087}{34749} \approx 0.874759\). This is a substantially weaker upper bound, however, than that of \(\frac{1129}{2100} \approx 0.537619\) established in \[25\], by enforcing the nonnegativity of pairs of \(3 \times 3\) principal minors of the partial transpose, and even weaker than \(\frac{1024}{135\pi^2} \approx 0.76854\), obtained by requiring the nonnegativity of all six \(2 \times 2\) principal minors of the partial transpose \[25\].

D. Fits of probability distributions to computed moments

1. Beta distribution fit to first two moments

Further, we linearly mapped \(|\rho|\) ∈ \([-\frac{1}{16}, \frac{1}{256}]\) to \(y\), so that \(y \in [0,1]\), and transformed its exact first nine moments accordingly. Then we exactly fit the first and second such moments to a basic (two-parameter) beta distribution, giving us a probability distribution of the form (Fig. [1]),

\[
P|\rho|\rho^T|(y) = \frac{y^{(a-1)}(1-y)^{(b-1)}}{B(a,b)}; \quad a = \frac{15171156}{516749} \approx 29.3588, \quad b = \frac{5018013}{2066996} \approx 2.42768, \quad (5)
\]

where \(B(a,b)\) is the beta function. The ratios of the next six transformed moments \((m = 3, \ldots, 8)\) to the corresponding moments of this beta distribution all rather remarkably lie between 0.99 and 1 (with the ratio of the ninth moments being 0.986) (Fig. [2]). Integrating the distribution (5) over the interval \(y \in [\frac{16}{17}, 1]\), we obtain an associated separability probability estimate of 0.4183149.

We did similarly linearly transform the product of \(|\rho|\) and \(|\rho|\rho^T|\) to lie in the unit interval \([0,1]\), and exactly fit to the so-transformed first two moments, a beta distribution of the form (cf. (5))

\[
P|\rho||\rho^T|(y) = \frac{y^{(a-1)}(1-y)^{(b-1)}}{B(a,b)}; \quad a = \frac{2392921}{57792} \approx 41.4057, \quad b = \frac{21536289}{308224} \approx 68.8722. \quad (6)
\]

The associated probability (over the separability domain \([\frac{16}{43}, 1]\)) was computed as 0.49331935. Using numerical methods, we found that the (transformed) third moment of the distribution of the product \(|\rho||\rho^T|\) was approximately 99.84% as large as the third moment of (6), but the fourth moment was only 62.25% as large. So, this fit to a beta distribution
certainly appears to be inferior to the earlier one (5) (Figs. 1 and 2) based on fitting the
first two moments of $|\rho^{PT}|$.

2. Use of two general moment-fitting procedures

One can use the calculated exact nine moments of $|\rho^{PT}|$ in certain formulas for cumu-
lative distribution functions, in order to approximate the desired, specific (separability)
probability that $|\rho^{PT}|$ is greater than zero [27, 28, eq. (2)] (cf. [30]). In Fig. 3 we display
together one such set of nine (greater) separability probability estimates based on the non-
parametric (stable approximant) reconstruction approach of Mnatsakanov [27], along with
the analogous first nine (lesser) estimates using the orthogonal-polynomial-based method-
ology of Provost and Ha [28, eq. (3.5)]. (In the latter approach, we used the well-fitting
beta distribution (5) as a "baseline" density that is adjusted by associated modified Jacobi
orthogonal polynomials.) It is clear that additional (exact) moments ($m > 9$) are certainly
needed to more satisfactorily sharpen the generic two-rebit separability probability estimates
in Fig. 3. Then, one might be able to obtain convincing evidence–in the absence of the
desired, but highly challenging exact symbolic computation–for the true (hypothetically ex-
act [22, 25, 31]) value of the separability probability. (Perhaps, somewhat relatedly, Gurvits
has shown "that the weak membership problem for the convex set of separable normalized
bipartite density matrices is NP-hard" [32].)

II. METHODOLOGIES EMPLOYED

A. Density Matrix Parameterizations

Our analysis proceeds in the framework of the Bloore (or correlation coefficient) param-
eterization [29, 33, 34] of the $4 \times 4$ density matrices ($\rho$) which allows us (in the generic
two-rebit case of immediate interest here) to work primarily in seven dimensions, rather
than the nine naively expected. Also, in our computations, we still further reparametrize
three ($z_{13}, z_{14}, z_{24}$) of the six correlations

$$z_{ij} = \frac{\rho_{ij}}{\sqrt{\rho_{ii}\rho_{jj}}}, \quad 1 \leq i < j \leq 4, \quad z_{ij} \in [-1, 1] \quad (7)$$
in terms of partial correlations [34], allowing certain requisite integrations to be performed simply over six-dimensional hypercubes, rather than more complicated domains [25]. (Alternatively, and reasonably computationally competitively, one may utilize the cylindrical algebraic decomposition [35] to define the integration limits [as indicated in [29, sec. II]] that specify the domain of feasible density matrices, directly within the Bloore-type framework, without transforming to partial correlations.)

The computation of the $m$-th Hilbert-Schmidt moment over $|\rho^{PT}|$ is carried out in two stages. (The moments of the distribution of purity $P(\rho) = \text{Tr}\rho^2$ for quantum states with respect to the Bures measure have recently been determined by Osipov, Sommers and Życzkowski [36], while Giraud has investigated the Hilbert-Schmidt counterparts [37, 38].) In the first stage, we perform an integration over the six-dimensional hypercube $[-1,1]^6$ of the $m$-th power of a (transformed) polynomial ($\tilde{P}$)–proportional to $|\rho^{PT}|$–in seven variables ([29, eq. (7)]). (The proportionality factor is $(\rho_{22}\rho_{33})^{2m}$.) The free (unintegrated) variable is of the form

$$\mu = \sqrt{\frac{\rho_{11}\rho_{44}}{\rho_{22}\rho_{33}}},$$

(8)

where the $\rho_{ii}$’s are the diagonal entries of $\rho$. (In the related study [29], $\nu = \mu^2$ was used as the principal variable, and in [25], $\xi = \log \mu$.) We have that (before the transformation to partial correlations, yielding $\tilde{P}$) the multivariate polynomial (proportional to $|\rho^{PT}|$)

$$P = -z_{14}^2\mu^4 + 2z_{14} (z_{12}z_{13} + z_{24}z_{34}) \mu^2 + (V + W) \mu^2 + 2z_{23} (z_{12}z_{24} + z_{13}z_{34}) \mu - z_{23}^2,$$

(9)

where

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

and

$$W = -2z_{13}z_{14}z_{23}z_{24} + z_{13}^2 (z_{24}^2 - 1) + 1.$$

The transformation of the three correlations $z_{13}, z_{14}, z_{24}$ to partial correlations (denoted $Z_{13,2}, Z_{24,3}, Z_{14,23}$) takes the form [34]

$$z_{14} \rightarrow z_{12}z_{23}z_{34} + \sqrt{z_{12}^2 - 1} \sqrt{z_{23}^2 - 1} z_{13,2}z_{34} + z_{12} \sqrt{z_{23}^2 - 1} \sqrt{z_{34}^2 - 1} z_{24,3} +$$

$$\sqrt{z_{12}^2 - 1} \sqrt{z_{34}^2 - 1} z_{13,2} - 1 \sqrt{z_{23}^2 - 1} z_{14,23} + \sqrt{z_{12}^2 - 1} \sqrt{z_{23}^2 - 1} z_{13,2}z_{24,3},$$

$$z_{13} \rightarrow z_{12}z_{23} + \sqrt{z_{12}^2 - 1} \sqrt{z_{23}^2 - 1} z_{13,2}, z_{24} \rightarrow z_{23}z_{34} + \sqrt{z_{23}^2 - 1} \sqrt{z_{34}^2 - 1} z_{24,3}. $$

9
The jacobian for this transformation is (note that one of the six variables [or three partial correlations]–\(z_{14,23}\)–is absent)

\[ J(z_{12}, z_{23}, z_{34}, z_{13,2}, z_{24,3}) = (z_{12}^2 - 1) (z_{23}^2 - 1) (z_{34}^2 - 1) \sqrt{z_{13,2}^2} - 1 \sqrt{z_{24,3}^2} - 1. \]  

(11)

**B. Intermediate functions/polynomials and their coefficients**

For the \(m\)-th moment (\(\text{Moment}_m \equiv \zeta_m^\prime\)), the indicated six-dimensional integration of \(P_m\) in now reparameterized (partial correlation) form \(\tilde{P}_m\) over the hypercube defined by \(z_{12}, z_{23}, z_{34}, z_{13,2}, z_{24,3}, z_{14,23} \in [-1, 1]\) takes the form—including a normalization factor of \(\frac{27}{32\pi^2}\)–the ("intermediate function") result

\[ I_m(\mu) = \frac{27}{32\pi^2} \int_{-1}^{1} \int_{-1}^{1} \int_{-1}^{1} \int_{-1}^{1} \int_{-1}^{1} \int_{-1}^{1} J(z_{12}, z_{23}, z_{34}, z_{13,2}, z_{24,3}, z_{14,23}) \tilde{P}_m(z_{12}, z_{23}, z_{34}, z_{13,2}, z_{24,3}, z_{14,23})^m dz_{12}dz_{23}dz_{34}dz_{13,2}dz_{24,3}dz_{14,23}. \]

(12)

For the first \((m = 1)\) moment, we have the result (Fig. 4)

\[ I_1(\mu) = -\frac{\mu^4}{5} + \frac{34\mu^2}{125} - \frac{1}{5}, \]

(13)

for the second moment \((m = 2)\),

\[ I_2(\mu) = \frac{3\mu^8}{35} - \frac{12\mu^6}{875} + \frac{20898\mu^4}{42875} - \frac{12\mu^2}{875} + \frac{3}{35}, \]

(14)

and for the third \((m = 3)\),

\[ I_3(\mu) = -\frac{\mu^{12}}{21} - \frac{54\mu^{10}}{875} - \frac{27873\mu^8}{42875} - \frac{466876\mu^6}{157625} - \frac{27873\mu^4}{42875} - \frac{54\mu^2}{875} - \frac{1}{21}. \]

(15)

At this point, we omit terms of lower order \(2j\) than \(2m\), since their coefficients—in a symmetrical manner—match the coefficients \(C_{4m-2j}(m)\). Then,

\[ I_4(\mu) = \frac{\mu^{16}}{33} + \frac{584\mu^{14}}{5775} + \frac{278884\mu^{12}}{282975} + \frac{8984\mu^{10}}{4851} + \frac{65788454\mu^8}{20543985} + \ldots, \]

(16)

\[ I_5(\mu) = -\frac{3\mu^{20}}{143} - \frac{18\mu^{18}}{49049} - \frac{70881\mu^{16}}{44141} - \frac{2178728\mu^{14}}{485851} - \frac{59472398\mu^{12}}{273546273} + \ldots, \]

(17)

\[ I_6(\mu) = \frac{\mu^{24}}{65} + \frac{2556\mu^{22}}{17875} + \frac{5454\mu^{20}}{2695} + \frac{3359372\mu^{18}}{315315} + \frac{3273117\mu^{16}}{86515} + \frac{597414184\mu^{14}}{7872865} + \frac{173821048732\mu^{12}}{1771394625} + \ldots, \]

(18)
\[ I_7(\mu) = \frac{\mu^{28}}{85} - \frac{4298\mu^{26}}{27625} - \frac{826637\mu^{24}}{303875} - \frac{165865636\mu^{22}}{8204625} - \frac{71226035\mu^{20}}{722007} - \frac{1947049760374\mu^{18}}{6711055065} \]
\[ + \frac{9337320181911\mu^{16}}{16776376625} - \frac{3322566596617765\mu^{14}}{48487372844625} - \cdots \]
\[ I_8(\mu) = \frac{3\mu^{32}}{323} + \frac{6672\mu^{30}}{40375} + \frac{12986136\mu^{28}}{3674125} + \frac{4250871568\mu^{26}}{121246125} + \frac{3319251741068\mu^{24}}{14670781125} + \cdots \]
\[ + \frac{2024301386770232\mu^{20}}{826454003375} + \frac{6510285844520752\mu^{18}}{14049718057375} + \frac{385343531016220966\mu^{16}}{724560431244625} + \cdots \]

For the nine cases \((m = 1, \ldots, 9)\) we have so far been able–with considerable computational expense–to explicitly compute, the coefficients of the corresponding \(4m\)-degree even polynomials \(I_m(\mu)\) are, as already indicated, symmetric–for reasons not immediately apparent–around the \(\mu^{2m}\) term.

1. Formulas for the coefficients of the intermediate functions and their root and pole structure

The constant terms (which equal the coefficients of the \(\mu^{4m}\) term) of the intermediate functions, used in the computation of the moments of \(|\rho^{PT}|\), are expressible as

\[ C_0(m) = C_{4m}(m) = \frac{3(-1)^m}{4 (m + \frac{1}{2}) (m + \frac{3}{2})}. \]  

(22)

Additionally, the coefficients of the second and \((4m - 2)\) terms are

\[ C_2(m) = C_{4m-2}(m) = \frac{3(-1)^m m(2m(4m - 5) - 15)}{100 (m - \frac{1}{2}) (m + \frac{1}{2}) (m + \frac{3}{2})}. \]  

(23)

Further, the coefficients of the fourth and \((4m - 4)\) terms are

\[ C_4(m) = C_{4m-4}(m) = \frac{3(-1)^m m(2m(2m(8m(6m - 7) + 155) - 13) - 1017) - 315)}{19600 (m - \frac{3}{2}) (m - \frac{1}{2}) (m + \frac{1}{2}) (m + \frac{3}{2})}. \]  

(24)

These results were obtained using the "rate", guessing program of C. Krattenthaler. Then further, M. Trott was able to obtain the result (using the FindSequenceFunction command of Mathematica, which searches for a possible rational form)

\[ C_6(m) = C_{4m-6}(m) = \]  

(25)
\[
(-1)^m(m - 1)m(4m(2m(4m(4m(20m(4m - 11) + 173) - 4303) + 4733) + 14911) - 9165) - 4725
\]
\[
529200 (m - \frac{5}{2}) (m - \frac{3}{2}) (m - \frac{1}{2}) (m + \frac{1}{2}) (m + \frac{3}{2})
\]

From the formulas for these coefficients, it is clear that the numerator of the coefficient 
\[C_{2j}(m) = C_{4m-2j}(m)\] of \(\mu^{2j}\) is a polynomial of degree \(3j\), and the denominator is a polynomial of degree \(j + 2\). (The denominators are very simple in structure \([30]\)–as evidenced above.) For \(j = 0\), the roots are \(-\frac{3}{2}\) and \(-\frac{1}{2}\), and as \(j\) increases by 1, an additional root 1 larger in value than the previous smallest is added. Thus, poles occur at the coefficient functions at such half-integers.

2. Asymptotic convergence of dominant roots to half-integers

Utilizing this observation, we were then able to move on to obtaining the coefficients \(C_8(m) = C_{4m-8}(m)\), \(C_{10}(m) = C_{4m-10}(m)\) \(C_{12}(m) = C_{4m-12}(m)\), \(C_{14}(m) = C_{4m-14}(m)\) and \(C_{16}(m) = C_{4m-16}(m)\)–but not yet higher. In studying the (nontrivial) roots of these functions, we have detected one quite interesting feature. That is, as \(j\) increases, the dominant roots of \(C_{2j}(m)\) show very strong evidence of converging to \(j - \frac{1}{2}\), the subdominant roots to \(j - \frac{3}{2}\)…For instance, for \(j = 8\), the dominant roots of \(C_{16}(m) = C_{4m-16}(m)\) are 7.49999796, 6.4999352, 5.4980028, 4.493216, while for \(j = 7\), they are 6.5000204, 5.500556, 4.515944. Such roots would then come increasingly close to canceling the near-to-matching poles in the denominators in \(C_{2j}(m)\) as \(j\) increases. (This behavior suggests an intimate connection with the theory of angular momentum and its [semiclassical] asymptotics \([40]\).)

C. Use of the intermediate functions \(I_{m}(\mu)\) to compute the \(m\)-th moment of \(|\rho^{PT}|\)

In the second stage of our procedure to compute the \(m\)-th Hilbert-Schmidt moment, we reverse the substitution \([8]\) in these \(4m\)-degree polynomials, multiply the result by the necessarily nonnegative factor \((\rho_{22}\rho_{33})^{2m}\) (the factor \((\rho_{22}\rho_{33})^2\) had been removed, as previously indicated, in forming the polynomial \(P\) in seven variables, proportional to \(|\rho^{PT}|\)) and also by the jacobian corresponding to the transformation to Bloore (correlation) variables for the two-rebit density matrices \([6]\)

\[
\text{jac} = (\rho_{11}\rho_{22}\rho_{33}\rho_{44})^{\frac{3}{2}}, \quad \beta = 3.
\]

(26)
\( \beta = 6 \), for the two-qubit case, and \( \beta = 12 \) for the corresponding quaternionic scenario, in accordance with random matrix theory results.) The result of the indicated multiplications is, then, integrated over the unit three-dimensional simplex,

\[
\rho_{11} + \rho_{22} + \rho_{33} + \rho_{44} = 1, \quad \rho_{ii} \geq 0, \quad i = 1, \ldots, 4
\]  

(27)
to obtain the \( m \)-th moment \(( \zeta'_m )\). In other words (taking into account the appropriate normalization factor), and setting \( \rho_{44} = 1 - \rho_{11} - \rho_{22} - \rho_{33} \), the computation takes the form

\[
\text{Moment}_m \equiv \zeta'_m = \frac{1146880}{\pi^2} \int_0^1 \int_0^{1-\rho_{11}} \int_0^{1-\rho_{11}-\rho_{22}} (\rho_{22}\rho_{33})^{2m} (\rho_{11}\rho_{22}\rho_{33}\rho_{44})^{\frac{3}{2}} I_m \left( \sqrt{\frac{\rho_{11}\rho_{44}}{\rho_{22}\rho_{33}}} \right) d\rho_{33} d\rho_{22} d\rho_{11}.
\]  

(28)

We are, in fact, able to perform the indicated \textit{symbolic} integration, obtaining thereby (using an index \( i \equiv 2j \))

\[
\text{Moment}_m = \zeta'_m = \frac{1146880}{\pi^2 \Gamma(4m+10)} \sum_{i=0,2,4}^{4m} \Gamma \left( \frac{i+5}{2} \right)^2 \Gamma \left( \frac{-i}{2} + 2m + \frac{5}{2} \right)^2 C_i(m)
\]  

(29)

\[
= \frac{2293760}{\pi^2 \Gamma(4m+10)} \left( \sum_{i=0,2,4}^{2m-2} \Gamma \left( \frac{i+5}{2} \right)^2 \Gamma \left( \frac{-i}{2} + 2m + \frac{5}{2} \right)^2 C_i(m) \right) + \frac{1146880}{\pi^2 \Gamma(4m+10)} \Gamma \left( m + \frac{5}{2} \right)^4 C_{2m}(m),
\]

where the \( C_i(m) \)’s are our previously-indicated rational coefficient functions ((22)-(25)), symmetric about \( 2m \). These (rational functions) \( C_i(m) \)’s themselves–as discussed above–are the ratios of polynomials in \( m \) of degree \( \frac{3i}{2} \) divided by the term (using the Pochhammer symbol, as well as rising factorials for gamma functions with half-integer arguments)

\[
\text{denominator}(C_i(m)) = \left( \frac{1-i}{2} + m \right)^{\frac{i+2}{2}} = \frac{\Gamma \left( m + \frac{5}{2} \right)}{\Gamma \left( \frac{-i}{2} + m + \frac{1}{2} \right)} = \frac{2^{\frac{i+2}{2}}(2m+3)!!}{(-i+2m-1)!!}
\]

(30)

\[
= \prod_{k=-2,0,\ldots}^{i} \left( m + \frac{1-k}{2} \right).
\]

For \( i = 4 \), by way of example, this gives us the denominator of (24),

\[
\left( m - \frac{3}{2} \right) \left( m - \frac{1}{2} \right) \left( m + \frac{1}{2} \right) \left( m + \frac{3}{2} \right).
\]  

(31)

On the other hand, the \textit{numerators} of the \( C_i(m) \)’s for \( m > 0 \) have zero as a trivial root, and for \( m > 4n \), trivial roots \( 0, \ldots n \).
Again, converting gamma functions with half-integer arguments to rising factorials, we have, equivalently to (29), that

\[ \text{Moment}_m = \zeta'_m = \]

\[
\frac{2^{7-4m}}{\Gamma[4m + 10]} (2m + 3)! \left[ C_{2m}(m) + 2\sum_{i=0,3,...}^{(3+i)!} \left( 3 - i + 4m \right) C_i(m) \right].
\]

Pursuant to these formulas, the first moment (mean) of the Hilbert-Schmidt probability distribution of \( |\rho_{PT}| \) over the interval \([-\frac{1}{16}, \frac{1}{256}]\) was found to be

\[ \zeta'_1 = -\frac{1}{858} = -\frac{1}{2 \cdot 3 \cdot 11 \cdot 13} \approx -0.0011655, \]

falling within the [negative] region (\( |\rho_{PT}| < 0 \)) of entanglement. (We were also able to compute this result using the alternative Euler-angle parameterization of the real density matrices \[39\], but only after correcting a typographical error in the associated Haar measure \[39, \text{eq. (48)}\], in which the factor \( \sin x \) had to be replaced by its square. Also, we depart from the standard convention of denoting moments by \( \mu \), since that symbol has been employed in our earlier studies \[25, 29\] and above \[8\].) Then, successively, the (necessarily decreasing in absolute value) raw (non-central) moments are

\[ \zeta'_3 = -\frac{3^3}{2^{10} \cdot 11 \cdot 13 \cdot 17} \approx 0.0000108462, \]

\[ \zeta'_4 = -\frac{2^{13} \cdot 5^2 \cdot 7 \cdot 11 \cdot 13 \cdot 17 \cdot 19}{21859} \approx -1.2629773 \cdot 10^{-7}, \]

\[ \zeta'_5 = -\frac{2^{18} \cdot 3 \cdot 5 \cdot 7^2 \cdot 13 \cdot 17 \cdot 19 \cdot 23 \cdot 29}{23071} \approx -4.27531 \cdot 10^{-11}, \]

\[ \zeta'_6 = -\frac{2^{28} \cdot 3 \cdot 5 \cdot 11^2 \cdot 17 \cdot 19 \cdot 23 \cdot 29 \cdot 31}{3253917653076541440} \approx 1.01949 \cdot 10^{-12}, \]

\[ \zeta'_7 = -\frac{419856257}{43 \cdot 2179 \cdot 4481} \approx -2.73223 \cdot 10^{-14}, \]

\[ \zeta'_8 = -\frac{21117403349591928832000}{109 \cdot 155461} \approx 8.02431 \cdot 10^{-16}, \]

and (requiring four days of Mathematica computation on a MacMini machine)

\[ \zeta'_9 = -\frac{6102620963}{240565904621616585139814400} \approx \]
\[
\frac{19 \cdot 199 \cdot 1614023}{2^{37} \cdot 3 \cdot 5^2 \cdot 11^3 \cdot 13 \cdot 23 \cdot 29 \cdot 31 \cdot 37 \cdot 41 \cdot 43} \approx -2.53678 \cdot 10^{-17}.
\]

(After four weeks of uninterrupted computation, we did not succeed, however, in determining \(\zeta'_10\).)

Interestingly, the sequence of denominators immediately above (in apparent contrast to that of the numerators) appears to be ”nice” in that the number of their prime factors do not grow rapidly, but rather linearly. This is a strong indication of the possible existence of a ”closed form”, that is an expression which is built by forming products and quotients of factorials [41, fn. 12].

D. Use of moments to estimate the probability distribution over \(|\rho^{PT}|\)

In Fig. 5 we display a (naive) fit of a simple power series in \(|\rho|^{PT}\) of degree nine to the computed first nine moments ((33)-(41)) (cf. [37, Figs. 1, 2]) of the Hilbert-Schmidt probability distribution over \(|\rho^{PT}|\), where \(\rho\) is a generic two-rebit density matrix. No nonnegativity constraints were, however, imposed and considerable incursions into negative regions result. (Such negativity can be obviated through the use of maximum-entropy, spline-fitting and other methodologies [27, 28, 30, 44, 46, 47], and we do explore such directions.)

The Hilbert-Schmidt separability probability predicted by the curve in Fig. 5—that is the ”probability mass” (the resultant of both positive and negative values) lying within the interval \([0, \frac{1}{256}]\)—is 0.39648, while our previous studies [25], indicate that the actual value is somewhat higher, \(\approx 0.45\)—a discrepancy the use of additional higher-order moments should ameliorate.

Since the plotted distribution (Fig. 5) appears to be unimodal, one can presumably use the computations of the first and second moments above to isolate the mode of the distribution within the interval [43, eq. (13)]

\[
\left\{-\frac{1}{858} - \frac{\sqrt{50397}}{4576}, \frac{\sqrt{50397}}{4576} - \frac{1}{858}\right\} = \{-0.00650062, 0.00416962\}, \tag{42}
\]

containing the value \(|\rho^{PT}| = 0\). Narrower intervals containing the mode can be obtained using higher-order moments and the associated Hankel determinants [43, Thm. 3.2].
E. Numerical computations of higher-order intermediate functions \((j \geq 9)\)

It is clear that it would be of considerable utility to have available exact values for still higher-order \((than m = 9)\) moments—and for the coefficients \(C_{2j}(m) \equiv C_{i}(m)\) of the terms in the intermediate functions/polynomials \(I_{m}(\mu)\)—but the associated computational demands seem quite considerable.

Our only current recourse, in this regard, then, appeared to be a numerical one. We employed a quasi-Monte Carlo (Tezuka-Faure [48, 49]) procedure (using 18,870,000 [low-discrepancy] points) to estimate the values of \(C_{2j}(m)\) for \(j \geq 9\) and \(m \geq 10\), for \(m = 10, \ldots, 50\). (Actually, by the evident symmetry around the \(2m\)-th power of the coefficients of the intermediate functions, we were able to obtain two values [which we averaged] for each point.) Coupling these approximate results with the exact formulas for the intermediate functions obtained above for \(j < 9\) (sec. II B), we obtained estimates of the first fifty moments. (We investigated the possibility of using these additional numerical results to infer the desired further exact formulas for the \(C_{2j}(m)\)'s, but this seemed too demanding a task, given the ordinary machine precision of our quasi-Monte Carlo simulations and the evident high [multi-digit] complexity of the exact coefficients.)

1. Cumulative distribution function calculations

We then used these values (the first nine moments being exact, and the remaining "semi-exact" forty-one, being sums of exact and numerical terms) in the procedure of Mnatsakanov for approximating the "moment-determinate cumulative distribution function (cdf) from its moments". The relevant formula for the cdf (at the separable/nonseparable boundary of principal interest to us) based on the first \(K = m\) moments (linearly mapping \(|\rho^{PT}|\) to lie in [0,1], and the moments accordingly) is of the form [27, eq. (2)] [50, eq. (1.3)]

\[
F_{K,\zeta'} = \sum_{k=0}^{K_{p}} \sum_{j=k}^{K} (-1)^{j-k} \binom{K}{j} \binom{j}{k} \zeta'_j, \tag{43}
\]

(We have to subtract this [entangled probability estimate] from 1 to get the [complementary] separability probability estimate, to be plotted as a function of the number of moments \(K\).)

In Fig. 6 we show estimates of this value based on increasingly large numbers of moments. (For more than thirty-six moments, the results turn negative. If we just employ in this same reconstruction procedure, the known exact formulas for the coefficients of the intermediate
functions—effectively setting the supplementary/corrective numerical terms to zero—then the two sets of results are quite close up to twenty moments, but then become considerably more ill-behaved when none of our supplementary numerical results is included [Fig. 7]. In a recent interesting study, Gzyl and Tagliani concluded that thirty-two was "the maximum allowable moments before incurring numerical instability, unless one conducts the calculation with high accuracy [50]. They also assert that "the additional information introduced by using the \((M + 1)\)-order moment is ‘visible’ only after the 0.6\(M\)-th decimal digit". In this regard, let us note that the quasi-Monte Carlo calculations used to complement the exact results here were conducted with only ordinary machine precision.)

It would appear that the wide range and lack of stability of estimates is reflective of the ill-posedness of the Hausdorff moment (inverse) problem (stemming ultimately from the lack of orthogonality of the sequence \(1, x, \ldots, x^n, \ldots\) [50]). In Fig. 8 we show the ratio of the exact (but incomplete for \(m > 9\)) moment computations to that (semi-exact one) based on the exact and complementary numerical results.

F. Libby-Novick (three-parameter) probability distribution

We have explored the use of extensions of the (two-parameter) beta distribution [51, chap. 5] [52] to better fit the nine exact moments than found, as presented above (sec. ID1), with the particular distribution [53] that had been fit to the first two moments of \(|\rho^{PT}|\). Doing so, we were able to obtain a three-parameter Libby-Novick (LN) distribution of the form [53] [51, eq. (IX.1)],

\[
P_{LN}(y) = \frac{\lambda^a y^{a-1}(1 - y)^{b-1}}{B(a, b)(1 - (1 - \lambda)y)^{a+b}},
\]

\[a \approx 3.7141606, b \approx 359.577737, \lambda \approx 0.00064805.
\]

This gave us a further considerably improved fit over that of [53] to the first nine exact moments. (The ninth moment was now predicted within 99.6%—as opposed to within 98.6%—and the preceding moments better still—in a monotonically declining goodness-of-fit manner from the first to the ninth.) The estimated separability probability now increased to 0.429121.

To arrive at the probability distribution (44), we started with the beta distribution fit [5] that exactly reproduced the first two moments, now trying to fit the first three moments. This involved a very long (slowly converging) iterative process, which at each stage, appealingly,
seemed to improve the fit to all our computed fifty (nine exact and forty-one, "semi-exact")
moments. Additionally, the estimated separability probability seemed to increase at each step, which we found to better accord with our earlier extensive numerical investigations
[22, sec. IX.A] [29, sec. V.A.2] [25].

One can employ the Libby-Novick distribution (44) as a "baseline density", in the manner
below using the beta distribution, following the methodology of Ha and Provost [28, eq. (3.5)], to generate estimates of the HS separability probability.

G. Moments based on lesser principal minors of $\rho^{PT}$ than its determinant

A necessary, but not sufficient condition that a two-qubit density matrix be separable is
that any $3 \times 3$ principal minor of its partial transpose be nonnegative [25]. So, we can select
one such minor, say (cf. (9)),

$$\text{minor}_{3 \times 3} = \frac{\rho_{11}^2 \rho_{44}^2}{\mu^2} (\mu^2 z_{14}^2 - 2 \mu z_{12} z_{13} z_{14} + z_{13}^2 + z_{12}^2 - 1), \quad (45)$$

expressed in terms of the Bloore parameterization, and compute the associated moments.
(Enforcing the nonnegativity of such a minor yields an upper bound of $\frac{22}{35} \approx 0.628571$ on the
Hilbert-Schmidt probability of separability of generic two-rebit systems [25].) We have been
able to compute exactly the first forty-five such moments of the probability distribution
over the interval $[-\frac{1}{8}, \frac{1}{27}]$, following very much the same scheme as we pursued for the first
nine moments of $|\rho^{PT}|$. The first two moments are $-\frac{1}{264}$ and $\frac{7}{74880}$, while remarkably, the
(raw) third moment is identically zero (cf. [54]). The form the corresponding "intermediate
functions" now took for these first three cases were (cf. (13)-(15))

$$I_1(\mu) = \frac{1}{5} (\mu^2 - 3), \quad (46)$$
$$I_2(\mu) = \frac{1}{875} \left(75 \mu^4 - 182 \mu^2 + 395\right)$$

and

$$I_3(\mu) = \frac{125 \mu^6 - 297 \mu^4 + 675 \mu^2 - 935}{2625}.$$  

General formulas could now also be obtained for the coefficients of the $2j$-th powers of
the intermediate functions. These involved the Mathematica functions LerchPhi or Differ-
enceRoot (cf. (22)-(25)). However, we were unable to find a general formula for the $m$-th
moment, even based on the availability of the first fifty-eight moments.
III. MOMENTS OF THE PRODUCT OF $|\rho|^PT$ AND $|\rho|$

The main foci of our initial analyses had been, firstly, the moments of the determinant $|\rho^{PT}|$ of the partial transpose of generic two-rebit density matrices, and, secondarily, the moments of the (necessarily nonnegative) determinant $|\rho|$ of the underlying density matrix itself—the moments of the latter determinant being more computationally amenable, it is clear, to exact analyses.

Now, in this context, it is not unnatural to ask the question of the nature of the moments of the product of these two determinants, $|\rho||\rho^{PT}| = |\rho \rho^{PT}|$ (cf. [55, p. 564]). This approach potentially contributes insight into the separability probability question, since a value of the product less than zero still indicates the presence of an entangled state, and a value greater than zero, a separable state. (It would appear that the argument in [3] of Augusiak, Horodecki and Demianowicz could be adapted, so that the value of the product could be construed as that obtainable from a single certain observable measurement.)

In undertaking the associated analysis of moments, we immediately encountered a most interesting result. The first moment or mean of the normalized product $|\rho||\rho^{PT}|$ is zero, that is

$$\zeta_1' = 0,$$

(47)

the associated "intermediate function" being (cf. [13])

$$I_1(\mu) = -\frac{24\mu^4}{875} + \frac{3888\mu^2}{42875} - \frac{24}{875}. \quad (48)$$

(Numerically, the first moment of the absolute value of the normalized product is $5.86519 \cdot 10^{-7}$. This is close to the absolute value, $\frac{1}{1963104} \approx 5.09397 \cdot 10^{-7}$, of the product of the mean of $|\rho|$, that is, $\frac{1}{2288}$, and the mean of $|\rho^{PT}|$, $-\frac{1}{858}$.) The second moment (cf. (34)) is

$$\zeta_2' = \frac{7}{5696343244800} \approx 1.2288585 \cdot 10^{-12} \quad (49)$$

(so, the corresponding standard deviation is the square root of this, that is $\sqrt{0.0007} \approx 1.10854 \cdot 10^{-6}$) with the associated intermediate function being (cf. [14])

$$I_2(\mu) = \frac{192\mu^8}{94325} - \frac{12032\mu^6}{1528065} + \frac{5561984\mu^4}{184895865} - \frac{12032\mu^2}{1528065} + \frac{192}{94325}. \quad (50)$$

(To compute the $m$-th moment of the probability distribution of the product, using the new set of intermediate functions, we employ the same formula as (28), but for the replacement
of the exponent $\frac{3}{2}$ by $\frac{3}{2} + m$.) We see that the coefficients of the constant (and highest power of $\mu$) terms in the first and second intermediate functions immediately above (48), (50) are $-\frac{24}{875}$ and $\frac{192}{94325}$. The next four such constant coefficients ($m = 3, 4, 5, 6$) have been found to be $-\frac{1024}{472925}, \frac{16384}{58683245}, -\frac{393216}{9670250577}$ and $\frac{1048576}{163136611875}$. However, we have yet to obtain a general formula, parallel to (22), in light of the increased computational burden, encompassing these six values.

The third to the sixth moments are

\begin{align*}
\zeta_3' &= \frac{1}{677899511057612800} = \frac{7}{2^{18} \cdot 3^2 \cdot 5^2 \cdot 13 \cdot 17 \cdot 19 \cdot 23} \approx 1.2288585 \cdot 10^{-12} \quad (51) \\
\zeta_4' &= \frac{1}{4597329480920227840000} = \frac{7}{2^{18} \cdot 3^2 \cdot 5^2 \cdot 13 \cdot 17 \cdot 19 \cdot 23} \approx 1.2288585 \cdot 10^{-12} \quad (52) \\
\zeta_5' &= \frac{1}{1166268080340730283953257280} = \frac{7}{2^{18} \cdot 3^2 \cdot 5^2 \cdot 13 \cdot 17 \cdot 19 \cdot 23} \approx 1.2288585 \cdot 10^{-12} \quad (53)
\end{align*}

and

\begin{align*}
\zeta_6' &= \frac{3929}{4158654163938276392103553381781471232} = \frac{7}{2^{18} \cdot 3^2 \cdot 5^2 \cdot 13 \cdot 17 \cdot 19 \cdot 23} \approx 1.2288585 \cdot 10^{-12}. \quad (54)
\end{align*}

Despite their lengthy digital descriptions, the ratios of these six moments to the HS moments of $|\rho|^2 k$—given by (2) are rather remarkably simple, that is,

\begin{align*}
\{0, \frac{77}{54}, \frac{24}{55}, \frac{209}{175}, \frac{598}{833}, \frac{3929}{3724}\} \quad (55)
\end{align*}

We have only so far been able to compute the two-qubit analogue of the first (zero) of the six ratios above—it turning out quite remarkably to be $\frac{3}{2}/. Since these ratios are so simple, it suggested to us that we might be more able to progress in our series of analyses, by making our initial goal the computation of these (unknown) but apparently well-behaved ratios—for higher-order moments—rather than the very small values of these moments themselves.

**IV. SUMMARY**

We have studied here the moments of probability distributions generated by certain determinantal functions of generic two-qubit density matrices ($\rho$) with real entries ("rebits") over the associated nine-dimensional convex domain, assigned Hilbert-Schmidt measure. It
was found that the mean of the (nonnegative) determinant $|\rho|$ is $\frac{1}{2288}$, the mean of the determinant of the partial transpose $|\rho^{PT}|$—negative values indicating entanglement—is $-\frac{1}{858}$, while the mean of the product of these two determinants, $|\rho||\rho^{PT}| = |\rho\rho^{PT}|$, is zero. We determined the exact values—also rational numbers—of the succeeding eight moments of $|\rho^{PT}|$. At intermediate steps in the derivation of the $m$-th moment of $|\rho^{PT}|$, rational functions $C_{2j}(m)$ emerge, yielding the coefficients of the $2j$-th power of even polynomials ("intermediate functions" $I_m(\mu)$) of total degree $4m$. These functions possess poles at finite series of consecutive half-integers ($m = -\frac{3}{2}, -\frac{5}{2}, \ldots, \frac{2j-1}{2}$), and certain (trivial) roots at finite series of consecutive natural numbers ($m = 0, \ldots, \lfloor \frac{m}{2} \rfloor$). The (nontrivial) dominant roots of $C_{2j}(m)$ appear to converge, as $j$ increases, to the same half-integer values ($m = \ldots, \frac{2j-3}{2}, \frac{2j-1}{2}, \ldots$). If formulas for $C_{2j}(m)$ could be developed for arbitrary $j$—we do possess them already for $j < 9$—then, the desired Hilbert-Schmidt separability probability would be computable to high accuracy.

We reproduced the (linearly transformed) first nine moments of $|\rho^{PT}|$ quite closely by a certain (two-parameter) beta distribution, and still more closely by a three-parameter (Libby-Novick) extension of it. The first two moments of $|\rho^{PT}|$—when employed in the one-sided Chebyshev inequality—gave an upper bound of $\frac{20097}{34749} \approx 0.874759$ on the Hilbert-Schmidt separability probability of two-rebit density matrices. We ascertained by numerical methods that the orthogonality established of $|\rho|$ and $|\rho^{PT}|$ with respect to Hilbert-Schmidt measure does not hold with respect to the Bures (minimal monotone) measure, nor if we slightly distort the symmetry of our basic nine-dimensional generic two-rebit scenario.

**Acknowledgments**

I would like to express appreciation to the Kavli Institute for Theoretical Physics (KITP) for computational support in this research, to Michael Trott for lending his Mathematica expertise, and Christian Krattenthaler, Mihai Putinar, Robert Mnatsakanov, Mark Coffey and Charles Dunkl for general discussions and insights.

[1] R. Horodecki, P. Horodecki, M. Horodecki, and K. Horodecki, Rev. Mod. Phys. 81, 865 (2009).

[2] I. Bengtsson and K. Życzkowski, *Geometry of Quantum States* (Cambridge, Cambridge, 2006).

[3] R. Augusiak, R. Horodecki, and M. Demianowicz, Phys. Rev. 77, 030301(R) (2008).
FIG. 1: The (two-parameter) beta probability distribution that closely (within $98.6\%$) reproduces the (linearly transformed to the interval $[0,1]$) first exact nine moments of $|\rho^{PT}|$. The vertical axis corresponds to the separable-entangled boundary ($y = 16/17 \approx 0.941176$), so the mode of the distribution (located at $y = 0.95206948$, corresponding to $|\rho^{PT}| = 0.000723364$) lies within the separable region.

[4] C. M. Caves, C. A. Fuchs, and P. Rungta, Found. Phys. Letts. 14, 199 (2001).
[5] K. Życzkowski and H.-J. Sommers, J. Phys. A 36, 10115 (2003).
[6] A. Andai, J. Phys. A 39, 13641 (2006).
[7] P. B. Slater, arXiv:1007.4805.
[8] A. Peres, Phys. Rev. Lett. 77, 1413 (1996).
[9] M. Horodecki, P. Horodecki, and R. Horodecki, Phys. Lett. A 223, 1 (1996).
[10] D. Bruss and C. Macchiavello, Found. Phys. 35, 1921 (2005).
[11] J. E. Avron, G. Bisker, and O. Kenneth, J. Math. Phys. 48, 102107 (2007).
[12] D. Bruss and C. Macchiavello, Found. Phys. 35, 1921 (2005).
FIG. 2: Ratios of the $m$-th exact moment of $|\rho^{PT}|$ (linearly transformed to the interval $[0,1]$) to the $m$-th moment of the beta probability distribution fitted to the first and second moments.

[13] K. Życzkowski, J. Phys. A 41, 355302 (2008).
[14] J. E. Avron and O. Kenneth, Ann. Phys. 324, 470 (2009).
[15] S. Szarek, I. Bengtsson, and K. Życzkowski, J. Phys. A 39, L119 (2006).
[16] I. Dumitriu, A. Edelman, and G. Shuman, J. Symb. Comp. 42, 587 (2007).
[17] C. Dunkl and Y. Xu, *Orthogonal Polynomials in Several Variables* (Cambridge, Cambridge, 2001).
[18] R. C. Griffiths and D. Spanò, arXiv:0809.1431.
[19] C. Jarlskog, Phys. Rev. Lett. 55, 1039 (1985).
[20] K. Życzkowski, P. Horodecki, A. Sanpera, and M. Lewenstein, Phys. Rev. A 58, 883 (1998).
[21] M. A. Nielsen and I. L. Chuang, *Quantum computation and quantum information* (Cambridge, Cambridge, 2000).
[22] P. B. Slater, J. Phys. A 40, 14279 (2007).
[23] M. Kuś and K. Życzkowski, Phys. Rev. A 63, 032307 (2000).
[24] F. Verstraete, K. Audenaert, and B. D. Moor, Phys. Rev. A 64, 012316 (2001).
[25] P. B. Slater, J. Phys. A 43, 195302 (2010).
[26] A. W. Marshall and I. Olkin, Ann. Math. Statist. 31, 488 (1960).
FIG. 3: Separability probability estimates for the generic real $4 \times 4$ density matrices based on differing numbers ($m = 1, \ldots, 9$) of exact moments of $|\rho^{PT}|$, using the nonparametric reconstruction procedures of Mnatsakanov [27]—giving the higher (blue) set of nine points—and the polynomial adjustment of the baseline density methodology of Ha and Provost [28]. The horizontal axis is drawn to intercept the vertical at $\frac{1129}{2100} \approx 0.537619$, the least upper bound so far established [25].

[27] R. M. Mnatsakanov, Statist. Prob. Lett. 78, 1612 (2008).
[28] H.-T. Ha and S. B. Provost, Commun. Stat.–Simul. Comput. 36, 1135 (2007).
[29] P. B. Slater, Phys. Rev. A 75, 032326 (2007).
[30] D. Bertsimas and I. Popescu, SIAM J. Optim. 15, 780 (2005).
[31] P. B. Slater, J. Geom. Phys. 58, 1101 (2008).
[32] Pentney W, Meila M (2003) Classical deterministic complexity of Edmond’s problem and quantum entanglement. Proc. Thirty-Fifth ACM Symp. Theory Comput.
[33] F. J. Bloore, J. Phys. A 9, 2059 (1976).
[34] H. Joe, J. Multiv. Anal. 97, 2177 (2006).
[35] C. W. Brown, J. Symbolic Comput. 31, 521 (2001).
[36] V. A. Osipov, H.-J. Sommers, and K. Życzkowski, J. Phys. A 43, 055302 (2010).
[37] O. Giraud, J. Phys. A 40, 2793 (2007).
[38] O. Giraud, J. Phys. A 40, F1053 (2007).
FIG. 4: The six intermediate functions $I_m(\mu), m = 1, \ldots, 6$. The curves for even $m$ curve upward, for odd $m$ downward, with the steepness of the curves increasing with $m$.

[39] P. B. Slater, J. Geom. Phys. 59, 17 (2009).

[40] M. Ragni, A. C. P. Bitencourt, C. D. S. Ferreira, V. Aquilanti, R. W. Anderson, and R. G. Littlejohn, Intl. J. Quant. Chem. 110, 731 (2009).

[41] C. Krattenthaler, Sém. Lothar. Combin. 42, B42q (1999).

[42] P. N. Gavriliadis and G. A. Athanassoulis, Probabilistic Engineering Mech. 8, 329 (2003).

[43] P. N. Gavriliadis, Commun. Statist.-Theor. Meth. 37, 671 (2008).

[44] V. John, I. Angelov, A. A. Öncüll, and D. Thévenin, Chem. Eng. Sci. 62, 2890 (2007).

[45] H. Dette and W. J. Studden, The theory of canonical moments with applications in statistics, probability, and analysis (John Wiley, New York, 1997).

[46] R. M. Mnatsakanov, Statist. Prob. Lett. 78, 1869 (2008).

[47] I. Popescu, Math. Oper. Res. 30, 1 (2005).

[48] G. Ökten, MATHEMATICA in Educ. Res. 8, 52 (1999).

[49] H. Faure and S. Tezuka, in Monte Carlo and Quasi-Monte Carlo Methods 2000 (Hong Kong),
FIG. 5: Fit—without nonnegativity constraints imposed—of a nine-degree polynomial to the first nine exactly-computed moments of the Hilbert-Schmidt probability distribution over $|\rho^{PT}|$, where $\rho$ is a generic two-rebit density matrix. The domain of separability is $|\rho^{PT}| > 0$.

[50] H. Gzyl and A. Tagliani, Appl. Math. Comput. 216, 3319 (2010).
[51] A. K. Gupta and S. Nadarajah, Handbook of Beta Distribution and Its Applications (Marcel Dekker, New York, 2004).
[52] M. B. Gordy, Comput. Econ. 12, 61 (1998).
[53] D. L. Libby and M. R. Novick, J. Educ. Statist. 7, 271 (1982).
[54] J. M. Elkin, Amer. Math. Monthly 62, 37 (1955).
[55] Y. V. Fyodorov and B. A. Khoruzhenko, Commun. Math. Phys. 273, 561 (2007).
[56] J. Batle, A. R. Plastino, M. Casas, and A. Plastino, Phys. Lett. A 298, 301 (2002).
[57] T. Tilma, M. Byrd, and E. C. G. Sudarshan, J. Phys. A 35, 10445 (2002).
FIG. 6: Separability probability estimates based on differing numbers (exact for $m \leq 9$ and "semi-exact" for $m > 9$) of moments, using the reconstruction procedure of Mnatsakanov [27]. The horizontal axis is drawn to intercept the vertical at $\frac{1129}{2100} \approx 0.537619$, the least upper bound so far established [25].
FIG. 7: Separability probability estimates, without any complementary numerical (quasi-MonteCarlo) input (for $m > 9$), using the reconstruction procedure of Mnatsakanov \[27\]. The horizontal axis intercepts the vertical at $\frac{1129}{2100} \approx 0.537619$, the least upper bound so far established \[25\].
FIG. 8: Ratios of moments computed using the exact and complementary numerical (for $m > 9$) results to those based only on the exact, but incomplete (for $m > 9$) results.