Invariance of Bipartite Separability and PPT-Probabilities over Casimir Invariants of Reduced States

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Milz and Strunz (J. Phys. A: 48 [2015] 035306) recently studied the probabilities that two-qubit and qubit-qutrit states, randomly generated with respect to Hilbert-Schmidt (Euclidean/flat) measure, are separable. They concluded that in both cases, the separability probabilities (apparently exactly $\frac{8}{27}$ in the two-qubit scenario) hold constant over the Bloch radii ($r$) of the single-qubit subsystems, jumping to 1 at the pure state boundaries ($r = 1$). Here, firstly, we present evidence that in the qubit-qutrit case, the separability probability is uniformly distributed, as well, over the generalized Bloch radius ($R$) of the qutrit subsystem. While the qubit (standard) Bloch vector is positioned in three-dimensional space, the qutrit generalized Bloch vector lives in eight-dimensional space. The radii variables $r$ and $R$ themselves are the lengths/norms (being square roots of quadratic Casimir invariants) of these (“coherence”) vectors. Additionally, we find that not only are the qubit-qutrit separability probabilities invariant over the quadratic Casimir invariant of the qutrit subsystem, but apparently also over the cubic one—and similarly the case, more generally, with the use of random induced measure. We also investigate two-qutrit ($3 \times 3$) and qubit-qudit ($2 \times 4$) systems—with seemingly analogous positive-partial-transpose-probability invariances holding over what have been termed by Altafini, the partial Casimir invariants of these systems.

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I. INTRODUCTION

The separable quantum states are embedded in the set of all (separable and entangled) states [1]. The nature of this embedding and its magnitude, in terms of various measures of quantum-theoretic interest [2, 3], are fundamental (“philosophical,...practical,...physical” [4]) issues [2, 5]. We present below apparent relations between these issues and Casimir invariants [6]—distinguished elements of the center of the universal enveloping algebra of a Lie algebra. In the simplest, lowest-dimensional case exhibiting entanglement, that of two qubits, this invariant is the square of the familiar Bloch radius of either qubit subsystem. For a system with a three-state (qutrit) subsystem, one of the two Casimir invariants is the square of the corresponding “generalized Bloch radius” [7, 9], and similarly for higher-dimensional (qudit) subsystems.

In such regards, a diverse body of evidence—though yet no formal proof—has been developed, strongly indicating that the probability that a two-qubit state is separable/disentangled/classically correlated, that is, expressible as the convex sum of products of qubit states [10], is $\frac{8}{27} \approx 0.296296$. The measure employed in the underlying computations was the familiar Hilbert-Schmidt (Euclidean/flat) one [2, 13], while the integration of this measure was conducted over the standard 15-dimensional convex set of $4 \times 4$ (Hermitian) density matrices. (The separability probability is computed as the ratio of the Hilbert-Schmidt volume of separable states to the volume of all states [3].)

Let us also note—though they will not be further discussed here—that still other simple exact rational-valued separability probabilities appear to hold in related scenarios, with the use of Hilbert-Schmidt measure—as well as its generalization to random-induced measures [16]. Notable examples are the 9-dimensional two-re[al]bit and 27-dimensional two-quater[ionic]bit density matrices.

Relatedly, a “concise” infinite summation formula

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

of this embedding and its magnitude, in terms of various measures of quantum-theoretic interest [2, 3], are fundamental (“philosophical,...practical,...physical” [4]) issues [2, 5]. We present below apparent relations between these issues and Casimir invariants [6]—distinguished elements of the center of the universal enveloping algebra of a Lie algebra. In the simplest, lowest-dimensional case exhibiting entanglement, that of two qubits, this invariant is the square of the familiar Bloch radius of either qubit subsystem. For a system with a three-state (qutrit) subsystem, one of the two Casimir invariants is the square of the corresponding “generalized Bloch radius” [7, 9], and similarly for higher-dimensional (qudit) subsystems.

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I. INTRODUCTION

The separable quantum states are embedded in the set of all (separable and entangled) states [1]. The nature
where

\[ f(\alpha) = P(\alpha) - P(\alpha + 1) = \] (2)

\[ \frac{q(\alpha)2^{-4\alpha-6}\Gamma(3\alpha + \frac{5}{2})\Gamma(5\alpha + 2)}{3\Gamma(\alpha + 1)\Gamma(2\alpha + 3)\Gamma(5\alpha + \frac{15}{2})}, \] (3)

and

\[ q(\alpha) = 185000\alpha^5 + 779750\alpha^4 + 1289125\alpha^3 + 1042015\alpha^2 + 410694\alpha + 63000, \]

appears to apply in the Hilbert-Schmidt instances [13]. (The formula was constructed through an application by Qing-Hu Hou of the famous procedure of “creative telescoping” of Doron Zeilberger [17] to a lengthy hypergeometric-based expression.) Here, \(\alpha\) functions as a Dyson-index-like parameter of random matrix theory (cf. [18]). The formula yields \(P(_4) = \frac{29\pi^6}{264}\) in the two-rebit case, \(P(_2) = \frac{26\pi^2}{3\pi^2}\) in the two-querterbit scenario, as well as (apparently even more simply) the mentioned \(P(1) = \frac{\pi}{2}\) in the (standard) two-qubit case [14].

A. Contribution of Milz and Strunz

A further interesting contribution to this general area of separability-probability research (originating in the seminal paper of Życzkowski, Horodecki, Sanpera and Lewenstein [4]) was recently made by Milz and Strunz [19]. They studied cases of random (with respect to Hilbert-Schmidt measure) \(2 \times n\) \((n = 2, 3, 4)\) Hermitian density matrices. They found evidence that the putative (overall) separability probability of \(\frac{\pi}{2}\) appeared remarkably to hold constant along the Bloch radii \(r\) of the qubit subsystems in the \(n = 2\) case [19, eq. (31)], and also constant (but with smaller probabilities—cf. [20] eqs. (3)-(5)—in the \(n = 3, 4\) cases). In the \(n = 4\) qubit-qudit setting, the probability employed was that of having a positive partial transpose (PPT). (These uniformities do appear to hold in the half-open interval \(r \in [0, 1)\), jumping to 1 at the pure state boundary, that is, \(r = 1\).)

“The Bloch sphere provides a simple representation for the state space of the most primitive quantum unit—the qubit—resulting in geometric intuitions that are invaluable in countless fundamental information-processing scenarios” [21].

B. Repulsion phenomenon in joint two-qubit separability probabilities

Motivated by this recent work of Milz and Strunz, we were led to examine [22] in the specific \(n = 2\) two-qubit case the nature of the bivariate (joint) separability probability over the pair of Bloch radii \(r_A, r_B\)—that is, the norms/lengths of the Bloch/coherence [23] vectors of the induced single-qubit subsystems \((A, B)\). A certain repulsion phenomenon was uncovered.

That is, separability probabilities tended to be smaller, the closer in length that their two Bloch radii were to each other. (It appears to be an interesting research question of in what manner such observations are related to findings, pertaining to the use of the Ky Fan norm, in [24].) There, de Vicente asserts that “Theorem 1 has a clear physical meaning: there is an upper bound (emphasis added) to the correlations contained in a separable state.” The exact nature of the (now, clearly nonuniform) bivariate distribution over the pair of Bloch radii [22, Fig. 5], however, remains to be determined in this two-qubit and related (real, quaternionic, induced measure, …) cases.

II. QUBIT-QUTRIT ANALYSIS

We begin our series of analyses here by further examining the qubit-qutrit case, that is the \(2 \times n\) scenario with \(n = 3\). Presumably, by the analyses of Milz and Strunz [19, Fig. 4], the Hilbert-Schmidt separability probability holds constant over the Bloch radius \(r\) of the single-qubit subsystem.

Now, we investigate, additionally, the variation of the separability probability over the generalized Bloch radius \(R\) of the induced single-qutrit subsystem [21 eqs. (7), (15)] [3, 4] (the Bloch vector now being situated in 8-dimensional space). (“In place of the three Pauli matrices we now need the . . . eight Gell-Mann \(A\)-matrices to describe a generalization of the Bloch ball representation of qubit to the case of three-level system or qutrit . . . These matrices are familiar as generators of the unimodular unitary group SU(3) in its defining representation. Just like the Pauli matrices these form a complete set of hermitian, traceless, trace-orthogonal matrices”) [7].)

Accordingly, we generated \(N_{\text{tot}} = 10^8\) (one hundred million) qubit-qutrit density matrices, randomly with respect to Hilbert-Schmidt measure, employing the Ginibre ensemble methodology [25, eq. (15)]. Each such state was tested for its separability—that is, whether or not the six eigenvalues of the partial transpose (PT) of the density matrix were all nonnegative [26, 27]. The Bloch radii \((r \text{ and } R)\) were found for its reduced single-spin qubit and qutrit subsystems.

The number of separable density matrices found was \(N_{\text{sep}} = 2,699,590\), with the qubit-qutrit separability probability estimate accordingly being 0.0269059. We note that the associated 99.9% confidence interval of \(\{0.0269426, 0.0270492\}\) does not include a previously conjectured value of \(\frac{32}{1199} \approx 0.026688[11, \text{sec. 10.2}].\) (This conjecture had been arrived at in 2007 with the use of quasi-Monte Carlo sampling methods, rather than the now preferable Ginibre ensemble approach [25, eq. (15)], employed in this current study.) Milz and Strunz themselves did report an estimate of 0.02700±0.00016 [19, eq.
FIG. 1. Distributions (histograms) of sampled qubit-qutrit states over the Bloch radii, with the more sharply-peaked distribution corresponding to the qutrit generalized Bloch radius $R$. (We report a second, independent estimate—which we pool with this one—in sec. IV A.)

The values recorded of $r$ and $R$, ranging from zero to one (having been appropriately scaled in the qutrit case [23, eq. 6] [eq. (12)]), were discretized into intervals of length $1/100$. Thus, we generated two data matrices of dimensions $100 \times 100$, one corresponding to the one hundred million random $6 \times 6$ density matrices generated, and one for the subset of separable density matrices.

In Fig. 1 we show the distributions (that is, the numbers recorded) of the $N_{\text{tot}}$ sampled states with respect to each of the Bloch radii, and in Fig. 2 similarly only the $N_{\text{sep}}$ separable states. The distribution over the qutrit radial variable $R$ is more sharply peaked in each instance—and, of course and highly importantly, we note the very strong similarity in distributional shapes between these first two (total and separable) figures.

A. Modeling of the qutrit $R$-curves

Milz and Strunz [19, Fig. 3, eq. (27)] conjectured that the (qubit) $r$-curve in Fig. 1 would be proportional to $r^2(1 - r^2)^{16}$ (as well as $r^2(1 - r^2)^{2(m^2 - 1)}$, more generally for $2 \times m$ systems)—and their proposal was very well supported by our corresponding plot.

We, now, attempted a comparable fit to the $R$-curve in Fig. 1 and found that a scaled version of $R^7(1 - R^2)^{32}$ succeeded fairly well over the half interval $R \in [0, 1/2]$ (Fig. 3). ("Thus the boundary [of the spin-1 states] can never stray into the interior of the eight-dimensional solid sphere of radius $1/2$ contained in [the spin-1 states]" [7, p. 4].)

B. $r$- and $R$-invariances of separability probabilities

We take the ratios of the number of sampled separable states $N_{\text{sep}}$ to the number of all sampled states $N_{\text{tot}}$ in both $(r,R)$ cases for each subinterval of length $1/100$, giving us the desired univariate separability probability estimates over the pair of $[0,1]$ intervals. In Fig. 4 we show the counterpart to Fig. 5 in [19], manifesting the same constancy/invariance over $r$ as observed by Milz and Strunz (which served as the initial motivation for our further study here and in [22]).
FIG. 5. Separability probability estimates given by the ratio of the (qutrit) $R$-curve in Fig. 2 to the (qutrit) $R$-curve in Fig. 1.

Now, we newly present the $R$-counterpart (Fig. 5) to Fig. 1 being essentially indistinguishable in its flat character. (We can see from Figs. 1 and 2 that the number of sampled qubit-qutrit states declines in both tails of the distributions, leading naturally to more scatter in the tails of the two flat-like separability probability figures. It would be of interest to incorporate confidence intervals into these and certain of the succeeding figures—see employed in [22].) Let us note the availability of formal statistical tests for the equality of a collection of binomial proportions [28].

Thus, it now strongly appears that the qubit-qutrit Hilbert-Schmidt separability probabilities hold constant (except at the pure states), not only over the the qubit (standard) Bloch radius $r$, as Milz and Strunz interestingly indicated, but also over the qutrit generalized Bloch radius $R$. These parallel results are somewhat intuitive, given our first two plots (Figs. 1 and 2), since the shapes of the two curves in both plots appear essentially identical to one another.

C. Joint qubit-qutrit separability probability

In Fig. 6 we show our estimate of the bivariate (joint) qubit-qutrit separability probability distribution (cf. [22] Fig. 5) for the two-qubit counterpart.

III. HIGHER-DIMENSIONAL ANALYSES

It is of obvious interest to extend this form of analysis to further $m \times n$ systems, where now $mn > 6$, using the corresponding $(m^2 - 1)$ and $(n^2 - 1)$-dimensional forms of Bloch (coherence) vectors [25]. In such analyses, it would appear that the concept of positive partial transpose (PPT) probability is the appropriate one to replace that of separability probability. Conjecturally, then, such PPT-probabilities would continue to be found to hold constant along the (generalized) Bloch radii of the induced subsystems. This will appear to be the case in the further analyses below.

A. Two-qutrit analysis

We generated 100 million $9 \times 9$ density matrices, once again of a random nature with respect to Hilbert-Schmidt measure. Regarding them as two-qutrit systems (cf. [29, 30]), only 10,218 of them had positive partial transposes (PPT), leading to an associated PPT-probability of 0.00010218. (Having a PPT is now a necessary, but not sufficient, condition for separability. The 95% confidence interval for the true probability was $\{0.000100199, 0.000104161\}$ [cf. [31]].) We plotted these PPT-probabilities as a function of $R$ (Fig. 7)—presumably the function is of the same nature for a choice of $R = R_A$ or $R_B$—again having divided the interval $R \in [0, 1]$ into one hundred bins. (We had initially symmetrized the underlying $100 \times 100$ data matrix for added stability.)
The resulting two-qutrit plot (Fig. 7) appears to be not inconsistent with a hypothesis of constancy of PPT-probabilities along the generalized Bloch radius $R$. This figure had been obtained by taking the ratio of the Fig. 8 histogram to (the similarly shaped, again) Fig. 9 histogram. (No density matrices with $R > \frac{29}{50}$ were randomly generated, reflecting the relative rarity of states in this domain. The zero probabilities appearing near $R = 0$ should not be troubling, since presumably the estimated $R$-invariant probability is so small [0.000101481] that—given the corresponding sample sizes—zero outcomes are, in fact, the most likely ones here.)

**IV. HIGHER-ORDER (CUBIC) CASIMIR INVARIANTS**

Viewing the (generalized) Bloch radii in terms of quadratic Casimir invariants [23, 32], perhaps it might be insightful to employ the squares of the radii (that is, $r^2, R^2, \ldots$) as principal variables themselves, rather than simply $r, R, \ldots$ Further, the possibility that invariance of separability (PPT-)probabilities continues to hold with respect to other (non-quadratic, cubic, \ldots) Casimir invariants seems a topic well worthy of investigation, that we now pursue.

**A. Second qubit-qutrit analysis**

We undertook a qubit-qutrit analysis parallel to that reported above (employing again, as in sec. II a [new] sample of one hundred million random density matrices, of which 2,701,081 were separable.). But rather than plotting (as in Fig. 5) the separability probabilities as a function of the qutrit Bloch radius $R$ (the square root of the corresponding quadratic Casimir invariant $c_2$), we utilized the corresponding cubic Casimir invariant $c_3$ [23, eq. (35)] [7, eq. (11)] [6, eq. (20)],

$$c_3 = \overrightarrow{n} \times \overrightarrow{n} \cdot \overrightarrow{n}, \tag{4}$$

where $\overrightarrow{n}$ is the Bloch 8-vector (and $c_2 = \overrightarrow{n} \cdot \overrightarrow{n}$ is the square of the Bloch radius $R$). The resulting plot is Fig. 11 (Again, we apparently see noisy scatter in the extreme upper and lower tails, having relatively low numbers of sampled density matrices.)
we obtain a Hilbert-Schmidt qubit-qutrit separability probability estimate of 0.027003355, centered in the 95% confidence interval (0.0269609, 0.0270258).

V. POLYNOMIAL INVARIANTS IN TWO-QUBIT CASE

Byrd and Khaneja [23] had observed that the number of polynomial invariants [33] under unitary transformations is larger than the number of Casimir invariants, which are included as a subset. So, we might pose the further question of whether uniformity of separability (PPT-)probabilities holds too for any of the larger set of polynomial invariants.

Khvedelidze and Rogojin have listed (up to the fourth order) an “integrity basis of SU(2) \( \otimes \) SU(2) invariants in the enveloping algebra \( U(\mathfrak{su}(n)) \).” They, first, give three invariants of the second degree [34, eq. (34)] (also [35, eq. (29)]). The first two (\( C^{(200)} \), \( C^{(020)} \), in the notation of Quesne that they adopt), of the three, are simply equivalent to the squares of the Bloch radii \((r_A^2, r_B^2)\)—that is, the quadratic Casimir invariants.

So, we presumably know by the analyses of Milz and Strunz [19], and the supporting evidence in [22, Fig. 10] that the Hilbert-Schmidt two-qubit separability probability is uniformly distributed at apparently \( \approx \frac{8}{33} \) over these two second-degree invariants. We are now interested in whether the separability probability is also uniform over the third of their (now, non-local) second-degree polynomial invariants, namely

\[
C^{(002)} = c_{ij}c_{ij} = \sum_{i=1,j=1}^{3} c_{ij}c_{ij}. \tag{5}
\]

The \( c_{ij} \)'s are the entries of the \( 3 \times 3 \) “correlation matrix” in the well-known Fano decomposition of a two-qubit state [34, eq. (29)] (they “contain information on interactions between parts of a composite system” [34]). We have performed an analysis based on twenty million \( 4 \times 4 \) density matrices, randomly drawn with respect to Hilbert-Schmidt measure—with 4,843,346 of them being separable, yielding a separability probability estimate of 0.2421673. The corresponding plot is Fig. 12 (cf. [22, Fig. 52]).

Obviously, this plot constitutes, in general, compelling evidence against the invariance of separability probabilities over (non-local) polynomial invariants, less specific than the partial/local Casimir ones. Of course, it would be possible to similarly analyze the other (third- and fourth-degree, non-Casimir) invariant polynomials [34, eqs. (35)-(39)], but we have no particular expectations that any single one might lead to uniformity of separability probabilities.

VI. QUBIT-QUTRIT ANALYSES WITH RANDOM INDUCED MEASURE

One might additionally investigate—motivated by results of other recent studies [20, 30]—the issue of whether invariances such as those apparently observed above, continue to hold when, more generally, random induced measures [16], other than the specific (symmetric) Hilbert-Schmidt form of such measures are imposed. (Also, analyses in the real and quaternionic (cf. [14, 37]) domains might be conducted.)

Let us now perform a third qubit-qutrit analysis, after those in secs. [11] and [IVA] in which we found evidence for the invariance of separability probabilities over both the generalized (qutrit) Bloch radius \( R = \sqrt{c_3^2} \) and the cubic Casimir invariant \( c_3 \). Those analyses were conducted using Hilbert-Schmidt measure, implicitly the symmetric instance, with an ancillary Hilbert space of dimension six, that is, \( N = K = 6 \), of more generally random induced measure [16]. We, thus, modify the analyses by employing an ancillary space of, we choose, dimension nine, \( K = 9 \).

1,097 million \( 6 \times 6 \) density matrices were generated with respect to the corresponding measure (following the prescription in [23]). 285,823,317 of these were separable, yielding a separability probability estimate of 0.260549969917958. (The associated 95% confidence interval was \( \{0.260524, 0.260570\} \).) For each density ma-

![FIG. 11. Qubit-qutrit separability probabilities as a function of the cubic Casimir invariant \( c_3 \)](image)

![FIG. 12. Two-qubit (clearly, now non-uniform) separability probabilities as a function of the second-degree separability polynomial invariant \( C^{(002)} \) given in eq. (5).](image)
In the case of $8 \times 8$ (qubit-qudit) density matrices, there are three independent Casimir invariants for the qudit subsystem [35, eqs. (46)-(48)] [35, eqs. (28)-(30)], with the PPT-probabilities conjecturally holding constant over each of the three invariants. (We already have acquired evidence [Fig. 10] as to apparent invariance over $R_{\text{qudit}} = \sqrt{c_2}$.)

Let us note the existence of but only a limited body of formally rigorous results (theorems, lemmas, . . . ) pertaining to properties of Hilbert-Schmidt (finite-dimensional) separability probabilities [5, 69] (cf. [40]).

Proofs are certainly still lacking for the interesting generalized Bloch radii/Casimir invariants conjectures made above, as well as those in a number of other recent reports [11–14, 20, 22, 36], and the infinite summation formula given above ((1)-(3)).

On the other hand, clear evidence has been provided [22, Fig. 31] that the apparent $r$-invariance phenomenon revealed by the work of Milz and Strunz [19] and supported above and in [22] does not continue to hold if one employs, rather than Hilbert-Schmidt measure, its Bures (minimal monotone) counterpart.

Let us also indicate the interesting paper of Altafini, entitled ”Tensor of coherences parametrization of multiqubit density operators for entanglement characterization” [42]. In it, he applies the term ”partial quadratic Casimir invariant” in relation to reduced density matrices. He notes that a quadratic Casimir invariant can be regarded as the specific form ($q = 2$) of Tsallis entropy. Further, he remarks that ”partial transposition is a linear norm preserving operation: $\text{tr}(\rho^2) = \text{tr}((\rho^T_1)^2) = \text{tr}((\rho^T_2)^2)$. Hence entanglement violating PPT does not modify the quadratic Casimir invariants of the density and the necessary [separability] conditions $[\text{tr}(\rho^n_A) \geq \text{tr}(\rho^2), \text{tr}(\rho^n_B) \geq \text{tr}(\rho^2)]$ are insensible to it”.

The space of two-qubit density matrices has been explicitly defined in terms of polynomial inequalities in the Casimir operators of the enveloping algebra of the $SU(4)$ group [38]. Additionally, the Peres-Horodecki separability conditions have been given in the form of polynomial inequalities in three $SU(4)$ Casimir invariants and two $SU(2) \otimes SU(2)$ scalars; namely determinants of the so-called correlation and Schlienz-Mahler entanglement matrices.
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