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ON THE GEOMETRIC PROBABILITY OF ENTANGLED MIXED STATES

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The state space of a composite quantum system, the set of density matrices $\mathfrak{P}_+$, is decomposable into the space of separable states $\mathfrak{S}_+$ and its complement, the space of entangled states. An explicit construction of such a decomposition constitutes the so-called separability problem. If the space $\mathfrak{P}_+$ is endowed with a certain Riemannian metric, then the separability problem admits a measure-theoretic formulation. In particular, one can define the "geometric probability of separability" as the relative volume of the space of separable states $\mathfrak{S}_+$ with respect to the volume of all states. In the present note, using the Peres–Horodecki positive partial transposition criterion, we discuss the measure-theoretic aspects of the separability problem for bipartite systems composed either of two qubits or of a qubit-qutrit pair. Necessary and sufficient conditions for the separability of a two-qubit state are formulated in terms of local $\mathrm{SU}(2)\otimes\mathrm{SU}(2)$ *invariant polynomials, the determinant of the correlation matrix, and the determinant of the Schlienz–Mahler matrix. Using the projective method of generating random density matrices distributed according to the Hilbert–Schmidt or Bures measure, we calculate the probability of separability (including that of absolute separability) of a two-qubit and qubit-qutrit pair. Bibliograhpy: 47 titles.*

1. Introduction

The word "*entanglement*," "*verschränkung*" in the original Austrian phrasing, was introduced into the glossary of quantum mechanics by Ervin Schrödinger in the 1930s. The name is due to a strange type of correlations in composite systems predicted by the newly created quantum theory [1]. The existence of "entangled" states in quantum theory seemed very problematic and mysterious since its inception, but at present it is experimentally verified and, moreover, used in practice in a variety of quantum engineering applications. Undoubtedly, nowadays entanglement has found its place among the fundamental notions of quantum physics and gains popularity similar to that the words "energy" and "force" had in the 19th century.

Being highly counterintuitive and strange, entanglement has a transparent mathematical formulation. Mathematics certainly dispels the aura of mystery, reducing the understanding of correlations between parts of a composite system to the analysis of a set of correctly stated algebraic problems. One problem of primary importance, the so-called "separability problem," is formulated as follows. Consider a system composed of two d_A- and d_B-dimensional subsystems with Hilbert spaces $\mathcal{H}^{d_A}$ and $\mathcal{H}^{d_B}$, respectively. According to the axioms of quantum mechanics, any state of the composite system is given by a density matrix $\varrho \in \mathfrak{P}_+$, which acts on a Hilbert space of tensor product form:

$$\mathcal{H}^{d_A\, d_B} = \mathcal{H}^{d_A} \otimes \mathcal{H}^{d_B}.$$

For a given factorization $\mathcal{H}^{d_A} \otimes \mathcal{H}^{d_B}$, an element $\varrho_{\mathrm{sep}} \in \mathfrak{P}_+$ belongs to the subset $\mathfrak{S}_+$ of *separable* states if and only if ϱ_{sep} admits a convex decomposition into r tensor product states

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with some probability distribution ω_k [2]:

$$\varrho_{\text{sep}} = \sum_{k=1}^{r} \omega_k \, \varrho_k^A \otimes \varrho_k^B . \tag{1}$$

The operators ϱ_k^A and ϱ_k^B in (1) are the density operators of the subsystems A and B, respectively. The states complementary to the separable ones are called *entangled*.[1]

The definition (1) is implicit, and hence the question of whether a given state is separable or entangled is worth further attention. Even at first glance it becomes clear that the "separability" question is highly intricate. Moreover, as shown by Gurvits (cf. [4, 5]), even for a bipartite system the separability problem is categorized computationally as NP-hard.

The complexity of the problem brings into play alternative approaches. In particular, by considering the state space of a quantum mechanical system as an object with measure (cf. [6, 7]), the "separability problem" can be reshaped into a probability issue [8, 9].

Below, adopting the above approach, we consider in detail bipartite systems consisting of two- and three-level subsystems. Equipping the state space with a certain measure, we compute the relative volume of the entangled states with respect to all possible states:

$$\mathcal{P}_{\text{E}} = \frac{\text{Vol(Space of entangled states)}}{\text{Vol(Space of all states)}} . \tag{2}$$

This number determines the geometric probability of entanglement, which can be treated as a certain measure of "capacity of quantumness" of the system.

The paper is organized as follows. In Secs. 2 and 3, the basic elements from the mathematical description of finite-dimensional quantum systems are given. Then, using this background, we introduce the notion of the separability probability of states. Using the Peres–Horodecki positive partial transposition criterion, we formulate necessary and sufficient conditions for the separability of a state of the two-qubit system in terms of local SU(2)⊗SU(2) scalars, the determinants of the correlation matrix and the Schlienz–Mahler matrix [10]. In Sec. 3, adopting the projective method of generating random density matrices, we study the probabilistic aspects of separability characteristics of two-qubit and qubit-qutrit pairs, including the computation of the separability and absolute separability probability, as well as a numerical evaluation of distributions of separable matrices with respect to the determinants of the correlation and Schlienz–Mahler matrices.

2. Settings

Below, the relevant definitions and notions, including the basic algebraic and geometric characteristics of composite quantum systems, are given in a form suitable for introducting a probability of quantum states. Note that we consider only finite-dimensional quantum systems.

2.1. The state space. At the beginning of the "Golden Age" of quantum mechanics, John von Neumann and Lev Landau became aware of limitations on the applicability of Schrödinger's Ψ-function and introduced the notion of a *"mixed quantum state"* [11, 12]. A mixed state is characterized by a self-adjoint, positive semidefinite *"density operator"* acting on the Hilbert space of a quantum system. For a nonrelativistic n-dimensional system, the Hilbert space $\mathcal{H}$ is $\mathbb{C}^n$ and the density operator can be identified with an $n \times n$ Hermitian, unit trace, positive

[1] Note that the representation (1) is not unique, and even if one knows that a state is separable, to find its decomposition is not an easy task. Furthermore, speaking about separability, one must always keep in mind that a fixed factorization $\mathcal{H}^{d_A} \otimes \mathcal{H}^{d_B}$ has been picked out. Using a global unitary transformation U acting on the total space, one can switch to another factorization $U\left(\mathcal{H}^{d_A} \otimes \mathcal{H}^{d_B}\right) U^+$. As a result, a separable state can become entangled and vice versa (cf. the discussion in [3]).

semidefinite matrix ϱ. This matrix, termed the *density matrix*, completely specifies a state of an n-level quantum system. All possible density matrices form the set $\mathfrak{P}_+$, the *state space* of the n-dimensional quantum system.

2.1.1. *The state space as a semialgebraic variety.* The space of Hermitian matrices is topologically isomorphic to $\mathbb{R}^{n^2}$. Due to the positive semidefiniteness, any density matrix ϱ represents a point of the semialgebraic variety $\mathfrak{P}_+(\mathbb{R}^{n^2-1})$ in the affine subspace determined by the unit trace equation $\mathrm{Tr}\varrho = 1$. In spite of the long story of studies of finite-dimensional systems, very little is known about $\mathfrak{P}_+(\mathbb{R}^{n^2-1})$ for arbitrary n. It turns out that even for small n the structure of $\mathfrak{P}_+(\mathbb{R}^{n^2-1})$ is quite cumbersome.[2]

• **Density matrices and the universal enveloping algebra** $\mathfrak{U}(\mathfrak{su}(n))$**.** The state space has a useful algebraic description in terms of the universal enveloping algebra $\mathfrak{U}(\mathfrak{su}(n))$ of the Lie algebra $\mathfrak{su}(n)$. Let $e_1, e_2, \dots, e_{n^2-1}$ form a basis for $\mathfrak{su}(n)$:

$$\mathfrak{su}(n) = \sum_{i=1}^{n^2-1} \xi_i \, e_i. \tag{3}$$

Consider elements from $\mathfrak{U}(\mathfrak{su}(n))$ of the following form:

$$\varrho = \frac{1}{n}\left(\mathbb{I}_{n\times n} + \imath\sqrt{\frac{n(n-1)}{2}} \sum_{i=1}^{n^2-1} \xi_i \, e_i \right), \tag{4}$$

with a real (n^2-1)-dimensional vector $\boldsymbol{\xi} = (\xi_1, \xi_2, \dots, \xi_{n^2-1})$. As mentioned above, expression (4) represents an element of the state space $\mathfrak{P}_+$ if the vector $\boldsymbol{\xi}$ satisfies a finite set of polynomial inequalities:

$$f_\alpha(\boldsymbol{\xi}) \geq 0. \tag{5}$$

Moreover, it turns out that the semialgebraic set described by (5) admits a representation with polynomial functions f_α that are invariant under the adjoint action of the unitary group $\mathrm{SU}(n)$ on $\mathfrak{P}_+(\mathbb{R}^{n^2-1})$. More precisely, consider the ring $\mathbb{R}[\mathfrak{P}_+]^{\mathrm{SU}(n)}$ of $\mathrm{SU}(n)$-invariant polynomials and a set of homogeneous polynomials $\mathcal{P} = (t_1, t_2, \dots, t_n)$ that form an integrity basis of this ring:

$$\mathbb{R}[\xi_1, \xi_2, \dots, \xi_{n^2-1}]^{\mathrm{SU}(n)} = \mathbb{R}[t_1, t_2, \dots, t_n]. \tag{6}$$

Then the state space $\mathfrak{P}_+(\mathbb{R}^{n^2-1})$ for every n is a semialgebraic subset given by inequalities of the following type:

$$p_i(t_1, t_2, \dots, t_n) \geq 0\,, \quad i = 1, 2, \dots, s, \tag{7}$$

where $p_i \in \mathbb{R}[\mathfrak{P}_+]^{\mathrm{SU}(n)}$. Below, analyzing the Hermiticity and semipositivity requirements for density matrices, we will give an explicit form of inequalities (7). With this aim, a brief digression is in order on constructing an integrity basis $\mathcal{P} = (t_1, t_2, \dots, t_n)$ from elements of the center $\mathcal{Z}(\mathfrak{su}(n))$ of the universal algebra.

DIGRESSION 1

• **The** $\mathrm{SU}(n)$**-invariance.** Constructing adjoint $\mathrm{SU}(n)$-invariants from elements of $\mathcal{Z}(\mathfrak{su}(n))$ is a well-known procedure. Referring the reader to the literature on this subject (see, e.g., [14]),

[2] A neighborhood of a generic point of $\mathfrak{P}_+(\mathbb{R}^{n^2-1})$ is locally isometric to $\left(\mathrm{SU}(n)/\mathrm{U}(1)^{n-1}\right) \times D^{n-1}$, where D^{n-1} is the $(n-1)$-dimensional disc (cf. [13]).

we briefly state the results and discuss constraints on these invariants due to the Hermiticity and positive semidefiniteness of density matrices. We are looking for polynomials

$$\phi(\boldsymbol{\xi}) = \sum c_{i_1\cdots i_r}\, \xi_{i_1}\xi_{i_2}\dots\xi_{i_r} \tag{8}$$

in variables $\xi_1, \xi_2, \dots, \xi_{n^2-1}$ that are invariant under the adjoint action

$$\phi(\boldsymbol{\xi}) = \phi((\mathrm{Ad}g)^T\boldsymbol{\xi})\,, \tag{9}$$

where $(\mathrm{Ad}g)^T$ is the transpose of the adjoint operator calculated in the basis $e_{i_1}, e_{i_2}, \dots, e_{n^2-1}$:

$$g\, e_i\, g^{-1} = (\mathrm{Ad}g\,)_{ij} e_j\,, \qquad g \in \mathrm{SU}(n)\,. \tag{10}$$

These polynomials are in a one-to-one correspondence with the elements of the center $\mathcal{Z}(\mathfrak{su}(n))$:

$$\mathfrak{C}_r = \sum \frac{1}{r!} c_{i_1\cdots i_r} \sum_{\sigma\in S_r} e_{i_{\sigma(1)}} e_{i_{\sigma(2)}} \dots\, e_{i_{\sigma(r)}}, \tag{11}$$

where S_r is the group of permutations of $1, 2, \dots, r$.

Furthermore, the $n-1$ independent Casimir operators $\mathfrak{C}_r$ in (11) serve as a source for an integrity basis of the polynomial ring $\mathbb{R}[\mathfrak{P}_+]^{\mathrm{SU}(n)}$. The scalars arising from the above isomorphism are commonly referred to as Casimir invariants. The first Casimir invariants up to the sixth order in $\boldsymbol{\xi}$ are

$$\mathfrak{C}_2 = (n-1)\, \boldsymbol{\xi}\cdot\boldsymbol{\xi}, \tag{12}$$

$$\mathfrak{C}_3 = (n-1)\, (\boldsymbol{\xi}\vee\boldsymbol{\xi}\,)\cdot\boldsymbol{\xi}, \tag{13}$$

$$\mathfrak{C}_4 = (n-1)\, (\boldsymbol{\xi}\vee\boldsymbol{\xi}\,)\cdot(\boldsymbol{\xi}\vee\boldsymbol{\xi}\,), \tag{14}$$

$$\mathfrak{C}_5 = (n-1)\Big((\boldsymbol{\xi}\vee\boldsymbol{\xi}\,), \vee(\boldsymbol{\xi}\vee\boldsymbol{\xi}\,)\Big)\cdot\boldsymbol{\xi}, \tag{15}$$

$$\mathfrak{C}_6 = (n-1)\, (\boldsymbol{\xi}\vee\boldsymbol{\xi}\vee\boldsymbol{\xi}\,)^2, \tag{16}$$

$$\dots\dots,$$

where

$$(\boldsymbol{U}\vee\boldsymbol{V}\,)_a := \kappa\, d_{abc} U_a V_b\,,$$

d_{abc} are symmetric structure constants for $\mathfrak{su}(n)$, and $\kappa = \sqrt{n(n-1)/2}$ is a normalization constant. Another equivalent set of invariants, useful from a computational point of view, is given by the so-called trace invariants, power series in the eigenvalues $\{\lambda\} = \lambda_1, \lambda_2, \dots, \lambda_n$ of the density matrix:

$$t_k := \mathrm{tr}(\varrho^k) = \lambda_1^k + \lambda_2^k + \dots + \lambda_n^k\,, \qquad k = 1, 2, \dots, n. \tag{17}$$

Below we formulate the Hermiticity and semipositivity requirements for density matrices directly in terms of (17).

• **The Hermiticity of ϱ in terms of $\mathrm{SU}(n)$-invariants.** Since ϱ is a Hermitian matrix, all solutions (eigenvalues $\{\lambda\}$) of the characteristic equation

$$\det\|\lambda - \varrho\| = \lambda^n - S_1\lambda^{n-1} + S_2\lambda^{n-2} - \dots + (-1)^n S_n = 0 \tag{18}$$

are real numbers. According to a classical result, certain information on the properties of the roots can be extracted from the so-called *Bézoutian*, the matrix $\mathrm{B} = \Delta^T\Delta$ constructed from the Vandermonde matrix

$$\Delta = \begin{pmatrix} 1 & \lambda_1 & \lambda_1^2 & \dots & \lambda_1^{n-1} \\ 1 & \lambda_2 & \lambda_2^2 & \dots & \lambda_2^{n-1} \\ 1 & \lambda_3 & \lambda_3^2 & \dots & \lambda_3^{n-1} \\ \vdots & \vdots & \vdots & \vdots\vdots\vdots & \\ 1 & \lambda_n & \lambda_n^2 & \dots & \lambda_n^{n-1} \end{pmatrix} . \tag{19}$$

The entries of the Bézoutian are simply the trace invariants:

$$\mathrm{B}_{ij} = t_{i+j-2} \,. \tag{20}$$

The Bézoutian accummulates information on the number of distinct roots (via its rank), the number of real roots (via its signature), as well as the Hermiticity condition. A real characteristic polynomial has all its roots *real and distinct* if and only if the Bézoutian is positive definite. Here we are interested only in generic density matrices (the space of degenerate matrices with coinciding roots is a set of zero measure). For this case, the positivity of the Bézoutian reduces to the requirement

$$\det \|\mathrm{B}\| > 0 \,. \tag{21}$$

Since $\det \|\mathrm{B}\| = (\det \|\Delta\|)^2$, the determinant of the Bézoutian is nothing else but the *discriminant* of the characteristic equation (18),

$$\mathrm{Disc} = \prod_{i>j} (\lambda_i - \lambda_j)^2 \,, \tag{22}$$

rewritten in terms of the trace polynomials:

$$\mathrm{Disc}(t_1, t_2, \dots, t_n) := \det \|\mathrm{B}\|. \tag{23}$$

The dependence of the discriminant on the trace invariants only up to order n emphasized in the left-hand side of (23) implicates that all higher trace invariants t_k with $k > n$ in (20) are expressed via polynomials in $t_1, t_2, \dots, t_n$ (the Cayley–Hamilton theorem).

• **The semipositivity of ϱ in terms of SU(n)-invariants.** The positive semidefiniteness implies the nonnegativity of the roots of (18):

$$\lambda_k \geq 0 \,, \qquad k = 1, 2, \dots, n. \tag{24}$$

Inequalities (24) are not computationally efficient, the eigenvalues $\{\lambda\}$ are nonpolynomial SU(n)-invariants. Fortunately, it is known (see, e.g., [15, 16] and references therein) that instead of (24) an equivalent set of inequalities can be formulated in terms of the first n symmetric polynomials in the eigenvalues of ϱ:

$$S_k \geq 0 \,, \qquad k = 1, 2, \dots, n. \tag{25}$$

In contrast to the eigenvalues, the coefficients S_k are SU(n)-invariant polynomial functions of density matrix elements and thus are expressible in terms of trace invariants. An elegant expression for S_k is given by the following determinant:

$$S_k = \frac{1}{k!} \det \begin{pmatrix} t_1 & 1 & 0 & \cdots & 0 \\ t_2 & t_1 & 2 & \cdots & 1 \\ t_3 & t_2 & t_1 & \cdots & \\ \vdots & \vdots & \vdots & \vdots\vdots\vdots & k-1 \\ t_k & t_{k-1} & t_{k-2} & \cdots & t_1 \end{pmatrix} . \tag{26}$$

Summarizing, the algebraic set of inequalities in SU(n)-invariants describing the state space $\mathfrak{P}_+(\mathbb{R}^{n^2-1})$ as a semialgebraic variety in the affine subspace $\mathrm{Tr}\varrho = 1$, reads

$$\mathrm{Disc} \geq 0 \qquad \text{(Hermiticity)}\,, \tag{27}$$

$$S_k \geq 0 \qquad \text{(semipositivity)}. \tag{28}$$

Now we are in a position to pose the following question: *Is the space of separable states* $\mathfrak{S}_+$ *also a semialgebraic set*? In spite of many efforts in the last decades, a complete answer for the generic case is yet unknown. But for a simplest bipartite system $2 \otimes 2$, composed of a pair of two-dimensional subsystems (qubits), the space of separable states $\mathfrak{S}^{2\otimes 2}$ admits a nice description as a basic semialgebraic variety. The next section is devoted to a detailed demonstration of this particular result.

2.1.2. *Decomposing the state space: separable vs. entangled.* As mentioned in the introduction, due to the quantum superposition principle, an arbitrary state of a composite system is described by an element of the tensor product of the density operators of its subsystems. For a given factorization of the system into parts, the state space $\mathfrak{P}_+(\mathbb{R}^{n^2-1})$ decomposes into the separable component $\mathfrak{S}_+$ and the entangled component. Furthermore, since the separability property is independent of the choice of a basis in each subsystem, it was conjectured (see the discussion in [17]) that $\mathfrak{S}_+$ is a so-called basic closed semialgebraic set, which is determined by polynomial inequalities in variables that are invariant under the independent action of unitary transformations of each subsystem. Below, starting with the necessary definitions, we will give a description of $\mathfrak{S}_+$ for a pair of qubits.

A generic 15-parameter density matrix for the composite $2 \otimes 2$ system consisting of two qubits reads as

$$\varrho = \frac{1}{4}\left[\mathbb{I}_4 + \boldsymbol{a}\cdot\boldsymbol{\sigma}\otimes\mathbb{I}_2 + \mathbb{I}_2\otimes\boldsymbol{\sigma}\cdot\boldsymbol{b} + c_{ij}\,\boldsymbol{\sigma}_i\otimes\boldsymbol{\sigma}_j\,\right]. \tag{29}$$

The representation (29) is often called the Fano [18] decomposition of a two-qubit state with parameters $\boldsymbol{a}$ and $\boldsymbol{b}$ assigned to the Bloch vectors of the reduced density matrices ϱ_A and ϱ_B extracted from ϱ by taking the partial traces over the second and first qubit, respectively:

$$\varrho_A = \mathrm{Tr}_B\,\varrho, \qquad \varrho_B = \mathrm{Tr}_A\,\varrho. \tag{30}$$

Nine real coefficients c_{ij} are usually collected in the *"correlation matrix"* $\|\mathrm{C}\|_{ij} = c_{ij}$. As follows from its name, the C-matrix contains information on interactions between the parts of a composite system.

• **The separability criterion.** Perhaps the most useful tool for evaluating separability is the famous Peres–Horodecki criterion [19–21], which is based on the idea of partial transposition. The partial transpose ϱ^{T_B} of a two-qubit density matrix is defined as

$$\varrho^{T_B} = I\otimes T\varrho, \tag{31}$$

where T is the standard transposition. Under this transposition, the Pauli matrices change as $T(\sigma_1, \sigma_2, \sigma_3) \to (\sigma_1, -\sigma_2, \sigma_3)\,.$

States for which the partial transposition preserves positivity are called positive partial transpose (PPT) states. It is easy to verify that any separable state is PPT. The converse is not true, even for low-dimensional bipartite systems. Counterexamples for the 3×3 case show that there are entangled states with positive partial transpose. However, for composite binary systems of type 2×2 and 2×3, the Peres–Horodecki criterion asserts that a state ϱ is separable if and only if its partial transpose ϱ^{T_B} is positive too.[3]

[3]More generally, consider a family of so-called bipartite $k\times l$ states ϱ, i.e., states whose partial traces are matrices with $\mathrm{rank}\varrho_A = k$ and $\mathrm{rank}\varrho_A = l$, respectively. For such $k\times l$ states, it was proved that ϱ is separable if it is PPT and $(k-1)(l-1)\leq 2$ [19,20].

Intuitively, it is clear that entanglement in composite systems is a function of the "relative orientation" of its subsystems only, any "local characteristics" of subsystems are irrelevant for the separability problem. To give a precise sense to this view, the second digression on the so-called local invariance of composite systems is in order.

DIGRESSION 2

• **The local unitary invariance.** The characterization of entanglement for two qubits, as well as for more general multipartite systems, admits a formulation in terms of invariants of the so-called local groups [22]. To introduce this notion, consider a generic multipartite system composed of r subsystems with $d_1, d_2, \ldots, d_r$ levels, respectively. The special subgroup

$$\mathrm{SU}(d_1) \otimes \mathrm{SU}(d_2) \otimes \cdots \otimes \mathrm{SU}(d_r) \tag{32}$$

of the unitary group $\mathrm{SU}(n)$ with $n = d_1 \times d_2 \times \cdots \times d_r$ acting on the state space is called the group of *local unitary transformations* (LUT). This action introduces equivalence relations on $\mathfrak{P}_+(\mathbb{R}^{n^2-1})$ and determines its orbit decomposition. Two states of a composite system connected by LUT (32) have the same nonlocal properties. Any characteristic of entanglement is a function of LUT invariants. In particular, the separability criterion can be given in terms of the corresponding polynomial LUT invariants. Before presenting an algebraic formulation of the separability criterion, we turn to a basic description of LUT invariants (see, e.g., [22–26]).

• **SU(2)⊗ SU(2) invariants.** LUT invariants of the mixed two-qubit system are polynomials in the elements of the density matrix ϱ that are constant under the adjoint action of the group SU(2)⊗ SU(2). These invariants and the corresponding ring $\mathcal{R}^{\mathrm{SU(2)}\otimes\mathrm{SU(2)}}$ have been the subject of intensive studies. In this general setting, $\mathcal{R}^{\mathrm{SU(2)}\otimes\mathrm{SU(2)}}$ necessarily has the Cohen–Macaulay property, i.e., there exists a homogeneous system of parameters $K_1, K_2, \ldots, K_n$, for some n, such that $\mathcal{R}^{\mathrm{SU(2)}\otimes\mathrm{SU(2)}}$ is finitely generated as a free module over $\mathbb{C}[K_1, K_2, \ldots, K_n]$. It is known that the polynomial ring of $\mathrm{SU}(2) \otimes \mathrm{SU}(2)$ invariants admits the Hironaka decomposition, namely ([24]),

$$\mathcal{R}^{\mathrm{SU(2)}\otimes\mathrm{SU(2)}} = \bigoplus_{k=0}^{15} J_k\, \mathbb{C}[K_1, K_2, \ldots, K_{10}], \tag{33}$$

where ten primary algebraically independent polynomials K_r have degrees

$$\mathrm{deg}K = (1, 2, 2, 2, 3, 3, 4, 4, 4, 6);$$

and fifteen secondary linearly independent invariants J_k, $k = 0, 1, 2, \ldots, 15$, are polynomials of degrees $\mathrm{deg}J = (4, 5, 6, 6, 6, 7, 7, 8, 8, 9, 9, 9, 10, 11, 15)$ with $J_0 = 1$.

An integrity basis of SU(2)⊗ SU(2) invariants in the enveloping algebra $\mathfrak{U}(\mathfrak{su}(n))$ is known [24, 27]. Following Quesne's notation, below we list the invariants (up to the fourth order) necessary for our analysis (all repeated indices should be summed from 1 to 3):

3 invariants of the second degree

$$C^{(200)} = a_i a_i\,, \quad C^{(020)} = b_i b_i\,, \quad C^{(002)} = c_{ij} c_{ij}; \tag{34}$$

2 invariants of the third degree

$$C^{(003)} = \frac{1}{3!}\epsilon_{ijk}\epsilon_{\alpha\beta\gamma} c_{i\alpha} c_{j\beta} c_{k\gamma}, \quad C^{(111)} = a_i c_{ij} b_j; \tag{35}$$

4 invariants of the fourth degree

$$C^{(004)} = c_{i\alpha}c_{i\beta}c_{j\alpha}c_{j\beta}, \quad (36)$$

$$C^{(202)} = a_i a_j c_{i\alpha}c_{j\alpha}\,, \quad (37)$$

$$C^{(022)} = b_\alpha b_\beta c_{i\alpha}c_{i\beta}, \quad (38)$$

$$C^{(112)} = \epsilon_{ijk}\epsilon_{\alpha\beta\gamma}a_i b_\alpha c_{j\beta}c_{k\gamma}. \quad (39)$$

Now we will show that two LUT invariants, namely, $C^{(003)}$ and $C^{(112)}$, play a special role in the algebraic form of the Peres–Horodecki separability criterion.

• **Separability in terms of local invariants.** As follows from the Peres–Horodecki criterion, a density matrix ϱ for the two-qubit system is separable if the coefficients $S_k^{T_B}$ of the characteristic equation for the corresponding partially transposed matrix ϱ^{T_B} are nonnegative:

$$S_k^{T_B} \geq 0\,, \qquad k = 2, 3, 4. \quad (40)$$

As calculations show, the second coefficient of the characteristic equation is invariant under the partial transposition (31):

$$S_2^{T_B} = S_2, \quad (41)$$

while the higher coefficients change as follows:

$$S_3^{T_B} = S_3 + \det \|\mathrm{C}\|, \quad (42)$$

$$S_4^{T_B} = S_4 + \det \|\mathrm{M}\|, \quad (43)$$

where M stands for the Schlienz–Mahler matrix [10]:

$$\mathrm{M}_{ij} := c_{ij} - a_i b_j. \quad (44)$$

Comparing with (35), one can easily verify that both determinants $\det\|\mathrm{C}\|$ and $\det\|\mathrm{M}\|$ are invariant under the local group $\mathrm{SU}(2) \otimes \mathrm{SU}(2)$:

$$\det\|\mathrm{C}\| = C^{003}, \quad \det\|\mathrm{M}\| = C^{003} - \frac{1}{2}C^{112}. \quad (45)$$

It is interesting that Eqs. (42) and (43) allow one to formulate sufficient conditions for entanglement of two qubits.

• **Sufficient conditions for entanglement of two qubits.** Consider a pair of qubits in a generic mixed state (29). Then from (41)–(43) it follows that *any density matrix ρ obeying the inequalities*

$$\det{}^2\|\mathrm{M}\| > 1, \qquad \det{}^2\|\mathrm{C}\| > 1 \quad (46)$$

is necessarily an entangled matrix. Density matrices from the complementary domain

$$-1 \leq \det\|\mathrm{M}\| \leq 1, \quad -1 \leq \det\|\mathrm{C}\| \leq 1 \quad (47)$$

are separable as well as entangled.

The separability vs. entanglement conditions described above are invariant under the LUT group, but can change under generic unitary transformations. However, observing that the maximally mixed state $\varrho_0 \sim \mathbb{I}_{n\times n}$ remains separable under arbitrary $\mathrm{U}(n)$ transformations, one can expect the existence of states in its neighborhood that possess separability properties independent of the chosen basis. Below, a short review of the characterization of such states is given.

• **Absolute separability.** The separability vs. entanglement property is sensitive to how the system is decomposed into parts. In general, it depends on a fixed factorization, but there are exceptions. M. Kuś and K. Zyczkowski in [28] drew attention to the states of an n-dimensional quantum system that are *absolutely separable*, i.e., to the $\mathrm{U}(n)$-invariant subspace $\mathcal{A}\mathfrak{S}_+ \subset \mathfrak{S}_+$:

$$\mathcal{A}\mathfrak{S}_+ = \{\varrho \in \mathfrak{S}_+ \mid \mathrm{U}\varrho\,\mathrm{U}^+ \in \mathfrak{S}_+, \quad \text{for every} \quad \mathrm{U} \in \mathrm{U}(n)\}. \tag{48}$$

What is the condition for a state to be absolutely separable? The answer to this question for a two-qubit system was found by Verstraete et al. [29], who showed that a necessary and sufficient condition is given by a quadratic inequality on the eigenvalues of the density matrix. Later, for the case of a bipartite system composed of qudits, a similar system of inequalities in the eigenvalues of the density matrix was derived by R. Hildebrand [30]. In particular, for the $2 \otimes 2$ and $2 \otimes 3$ cases, the inequalities read

$$\lambda_1 - \lambda_3 \leq 2\sqrt{\lambda_2 \lambda_4}, \tag{49}$$

$$\lambda_1 - \lambda_5 \leq 2\sqrt{\lambda_4 \lambda_6}. \tag{50}$$

The algebraic description of the state space and, in particular, of the separable states presented here is well adapted for the extraction of quantitative characteristics of entanglement. Now a few applications exemplifying this thesis will be given.

3. A probabilistic view on entanglement

Here probabilistic aspects of entanglement are discussed within the semialgebraic description given in the previous sections. Adopting the probability approach [8, 9, 31–33], we present probabilistic characteristics of the two-qubit and qubit-qutrit systems. Since standard methods of probability theory require the existence of a measure, below we start with the introduction of Riemannian structures on $\mathfrak{P}_+(\mathbb{R}^{n^2-1})$.

3.1. The Riemannian geometry of states. There is no way to single out a unique measure in the state space. Various physical and mathematical argumentations have been used to introduce different metrics on $\mathfrak{P}_+(\mathbb{R}^{n^2-1})$. Several popular distances between two density matrices ϱ_1 and ϱ_2 commonly used in the literature are as follows:

- the *trace distance*

$$D_{\mathrm{tr}}(\varrho_1, \varrho_2) = \mathrm{tr}\left(\sqrt{(\varrho_1 - \varrho_2)^2}\right), \tag{51}$$

- the *Hilbert–Schmidt distance*

$$D_{\mathrm{HS}}(\varrho_1, \varrho_2) = \sqrt{\mathrm{tr}\left[(\varrho_1 - \varrho_2)^2\right]}, \tag{52}$$

- the *Bures distance*

$$D_{\mathrm{B}}(\varrho_1, \varrho_2) = \sqrt{2\left(1 - \mathrm{tr}\left[(\varrho_1^{1/2}\varrho_2\varrho_1^{1/2})^{1/2}\right]\right)}. \tag{53}$$

These distances naturally appear in different approaches, e.g., the Bures distance [34] originates from the statistical distance between quantum states [35] and quantum fidelity [36]. Each of them possesses certain advantages as well as drawbacks, and often the obtained results strongly depend on the choice made. Below, in order to analyze this type of dependence, we use the measures on $\mathfrak{P}_+(\mathbb{R}^{n^2-1})$ corresponding to two of them, (52) and (53). They can be derived as follows.

- **The Hilbert–Schmidt measure.** Considering the distance (52) between two infinitesimally close points ϱ and $\varrho + \mathrm{d}\varrho$, we get the flat metric

$$\mathrm{g}_{\mathrm{HS}} = \mathrm{tr}\left(\mathrm{d}\varrho \otimes \mathrm{d}\varrho\right), \tag{54}$$

which in the Bloch coordinates (4) for the two-qubit system takes (up to a scale factor) the standard Euclidean form in $\mathbb{R}^{15}$:

$$g_{\text{HS}} = d\xi_1 \otimes d\xi_1 + d\xi_2 \otimes d\xi_2 + \cdots + d\xi_{15} \otimes d\xi_{15}. \tag{55}$$

The measure corresponding to (55),

$$d\mu_{\text{HS}} := d\xi_1 \wedge d\xi_2 \wedge \cdots \wedge d\xi_{15}\,, \tag{56}$$

admits the following decomposition:

$$d\mu_{\text{HS}} = d\mu_{{}^\star\Delta_4} \times d\nu_{U(4)/U(1)^4}\,, \tag{57}$$

where $d\mu_{{}^\star\Delta_4}$ is a certain measure on the ordered 3-dimensional simplex[4] in $\mathbb{R}^4$ and $d\nu_{\mathrm{U}(4)/\mathrm{U}(1)^4}$ is the measure on the coset $\mathrm{U}(4)/\mathrm{U}(1)^4$ induced from the standard Haar measure on the unitary group $\mathrm{U}(4)$. Note that the decomposition (57) follows from the principal axis transformation applied to density matrices. Since density matrices are Hermitian, for every ϱ there exists a unitary matrix $U \in \mathrm{U}(4)$ such that

$$\varrho = U \Lambda U^\dagger. \tag{58}$$

Since the adjoint action on a diagonal matrix Λ has stability group H_Λ, the matrix U is not unique, it belongs to a coset homeomorphic to $\mathrm{U}(4)/H_\Lambda$. To make the representation (58) one-to-one, we constraint the diagonal elements of the matrix

$$\Lambda = \begin{pmatrix} \lambda_1 & 0 & 0 & 0 \\ 0 & \lambda_2 & 0 & 0 \\ 0 & 0 & \lambda_3 & 0 \\ 0 & 0 & 0 & \lambda_4 \end{pmatrix} \tag{59}$$

to the ordered simplex ${}^\star\Delta_4$ by fixing the descending order

$$1 \geq \lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \lambda_4 \geq 0.$$

The stability group H_Λ depends on the matrix Λ, and all possible types of H_Λ are listed in Table 1.

Eigenvalues	Stability group H_Λ	$\dim(\frac{U(4)}{H_\Lambda})$	$\dim(\Lambda)$
$\lambda_1 > \lambda_2 > \lambda_3 > \lambda_4 > 0$	$\mathrm{U}(1)^4$	12	3
$\lambda_1 = \lambda_2 > \lambda_3 > \lambda_4 > 0$	$\mathrm{U}(2) \otimes \mathrm{U}(1)^2$	10	2
$\lambda_1 > \lambda_2 = \lambda_3 > \lambda_4 > 0$	$\mathrm{U}(1) \otimes \mathrm{U}(2) \otimes \mathrm{U}(1)$	10	2
$\lambda_1 > \lambda_2 > \lambda_3 = \lambda_4 > 0$	$\mathrm{U}(1)^2 \otimes \mathrm{U}(2)$	10	2
$\lambda_1 > \lambda_2 = \lambda_3 = \lambda_4 > 0$	$\mathrm{U}(1) \otimes \mathrm{U}(3)$	6	1
$\lambda_1 = \lambda_2 > \lambda_3 = \lambda_4 > 0$	$\mathrm{U}(2) \otimes \mathrm{U}(2)$	8	1
$\lambda_1 = \lambda_2 = \lambda_3 > \lambda_4 > 0$	$\mathrm{U}(3) \otimes \mathrm{U}(1)$	6	1
$\lambda_1 = \lambda_2 = \lambda_3 = \lambda_4 \geq 0$	$\mathrm{U}(4)$	0	0

Table 1. The stability groups and dimensions of $\mathrm{U}(4)/H_\Lambda$ cosets.

From Table 1 one can conclude that the measure is determined by the case with the minimal isotropy group $\mathrm{U}(1)^4$. Thus, passing to new coordinates via the transformation (58), we bring

[4] The ordered simplex ${}^\star\Delta_4$ is the standard simplex Δ_4 factored by the action of the permutation group S_4.

the measure (57) to the form

$$\mathrm{d}\mu_{\star_{\Delta_4}} = \prod_{i>j} (\lambda_i - \lambda_j)^2 \, \mathrm{d}\lambda_1 \wedge \cdots \wedge \mathrm{d}\lambda_4, \tag{60}$$

with the discriminant of the characteristic equation for ϱ as the Jacobian and the measure on the coset $SU(4)/U(1)^4$ depending on $4^2 - 4$ angles:

$$\mathrm{d}\mu_{SU(4)/U(1)^4} = \omega_1 \wedge \omega_2 \wedge \cdots \wedge \omega_{12}, \tag{61}$$

where $\omega_1, \ldots, \omega_{12}$ are the left-invariant 1-forms on U(4) projected to the coset $SU(4)/U(1)^4$. As a result, the Hilbert–Schmidt measure (56) induces the following joint distribution function on the simplex of eigenvalues of density matrices:

$$P_{HS}(\boldsymbol{\lambda}) = C_n^{HS} \, \delta\left(1 - \sum_{i=1}^{n} \lambda_i\right) \prod_{i=1}^{n} \Theta(\lambda_i) \prod_{i>j} (\lambda_i - \lambda_j)^2 \,, \tag{62}$$

where the normalization constant C_n is

$$C_n^{HS} := \frac{\Gamma(n^2)}{\prod\limits_{j=0}^{n-1} \Gamma(n-j)\Gamma(n-j+1)} .$$

It is important to note that the distribution (62) may be regarded as a special case of the family of measures induced by the partial tracing [31–33]. Below, we will use this observation for the numerical analysis of the geometric probability.

• **The Bures measure.** The infinitesimal form of the Bures distance (53) leads to the metric

$$\mathrm{g}_{\mathrm{Bures}} = \frac{1}{2} \operatorname{Tr}\left(G \mathrm{d}\varrho\right), \tag{63}$$

where G is defined from the equation $\mathrm{d}\varrho = G\varrho + \varrho G$, see [37, 38].

It is known (see, e.g., [36, 39]) that the Bures probability distribution on the simplex of eigenvalues reads

$$P_{\mathrm{Bures}}(\boldsymbol{\lambda}) = C_n^{\mathrm{Bures}} \delta\left(1 - \sum_{i=1}^{n} \lambda_i\right) \prod \Theta(\lambda_i) \frac{\mathrm{d}\lambda_i}{\sqrt{\lambda_i}} \prod_{i<j} \frac{(\lambda_i - \lambda_j)^2}{\lambda_i + \lambda_j}, \tag{64}$$

where

$$C_n^{\mathrm{Bures}} = 2^{n^2-n} \frac{\Gamma(n^2/2)}{\pi^{n/2} \prod_{j=1}^{n} \Gamma(j+1)}$$

is a normalization constant.

3.2. The probability of separability. Now, having introduced a measure on the space of states, we are in a position to define probabilistic characteristics of entanglement. The simplest one is the probability of finding separable states among all possible states distributed according to the introduced measure on the state space.

• **The geometric probability of separability.** Consider a bipartite system consisting of a pair of qubits or of a qubit and a qutrit. Taking into account the semialgebraic structure of the state space, one can define the probability of separability as

$$\mathcal{P}_{\mathrm{sep}} = \frac{\int_{\mathfrak{P}_+ \cap\, \widetilde{\mathfrak{P}}_+} \mathrm{d}\mu}{\int_{\mathfrak{P}_+} \mathrm{d}\mu} . \tag{65}$$

The denominator in (65) represents the volume of the total state space $\mathfrak{P}_+$, while the numerator is the volume of the separable states; the integral is over the intersection $\mathfrak{P}_+ \cap \widetilde{\mathfrak{P}}_+$ of $\mathfrak{P}_+$

and its image $\widetilde{\mathfrak{P}}_+$ under the partial transposition map. The set $\mathfrak{P}_+ \cap \widetilde{\mathfrak{P}}_+$ is the subset of $\mathfrak{P}_+$ invariant under the partial transposition map:

$$\mathfrak{P}_+ \cap \widetilde{\mathfrak{P}}_+ = \{\rho \in \mathfrak{P}_+ \,|\, \mathrm{I} \otimes \mathrm{T}\rho \in \mathfrak{P}_+\}\,.$$

In our computations below, the measure $\mathrm{d}\mu$ in the integrals (65) is assumed to be either the Hilbert–Schmidt one or the Bures one. Since the volume of the state space is known for both metrics, the Hilbert–Schmidt metric [40] and the Bures metric [36], the problem of computing the probability of separability reduces to the evaluation of the integral over the set $\mathfrak{P}_+ \cap \widetilde{\mathfrak{P}}_+$.

Leaving for future studies generic properties of (65), we will discuss how to evaluate the probability of separability for pairs of qubits and qubit-qutrit pairs. A direct numerical calculation of the multidimensional integral over the set $\mathfrak{P}_+ \cap \widetilde{\mathfrak{P}}_+$ is a hard computational problem. To avoid very cumbersome calculations, one can use a reliable remedy, the Monte-Carlo method.

3.3. Generation of ensembles of density matrices. The basic ingredient of the Monte-Carlo approach is the generation of a specific random variable. To generate random density matrices from the Hilbert–Schmidt and Bures ensembles, the ideology of the method of induced measures (cf. [31–33] and [41–43]) can be used. To proceed, let us first start with the generation of the so-called *Ginibre ensemble* [44], i.e., the set of complex matrices whose entries have real and imaginary parts distributed as independent normal random variables.

• **The Ginibre ensemble.** Let $\mathrm{M}(\mathbb{C}, n)$ be the space of $n \times n$ matrices whose entries are complex numbers. Assume that the entries of $Z \in \mathrm{M}(\mathbb{C}, n)$ are independent identically distributed standard normal complex random variables:

$$p(z_{ij}) = \frac{1}{\pi}\exp(-|z_{ij}|), \quad i, j = 1, 2, \ldots, n.$$

The joint probability distribution

$$P(Z) = \prod_{i,j=1}^{n} p(z_{ij}) = \frac{1}{\pi^{n^2}} \exp\left(-\mathrm{Tr}\left(Z^\dagger Z\right)\right) \tag{66}$$

and the linear measure on $\mathrm{M}(\mathbb{C}, n)$ determine the Ginibre probability distribution:

$$\mathrm{d}\mu_{\mathrm{G}}(Z) = P(z)\mathrm{Tr}\left(\mathrm{d}Z^\dagger \mathrm{d}Z\right). \tag{67}$$

Having random Ginibre matrices, one can use a simple prescription to generate elements from both Hilbert–Schmidt and Bures ensembles.

• **The Hilbert–Schmidt ensemble**. In order to generate Hilbert–Schmidt states

$$P(\varrho)_{\mathrm{HS}} \approx \Theta(\varrho)\delta(1 - \varrho), \tag{68}$$

consider a square $n \times n$ complex random matrix Z from the Ginibre ensemble. Then it is easy to check that the matrix

$$\varrho_{\mathrm{HS}} = \frac{Z^\dagger Z}{\mathrm{Tr}\,(Z^\dagger Z)} \tag{69}$$

is, by construction, Hermitian, semipositive, unit norm matrix that belongs to the Hilbert–Schmidt ensemble (68).

• **The Bures ensemble.** The density matrix distributed according to the Bures measure can also be generated using the Ginibre ensemble. Following [42], consider the random matrix

$$\varrho_{\mathrm{B}} = \frac{(\mathbb{I} + U)ZZ^+(\mathbb{I} + U^+)}{\mathrm{Tr}\,[(\mathbb{I} + U)ZZ^+(\mathbb{I} + U^+)]}, \tag{70}$$

where Z is a complex matrix belonging to the Ginibre ensemble, while U is a unitary matrix distributed according to the Haar measure on the unitary group $U(N)$. By a straightforward calculation one can verify that the matrices ϱ_{B} are distributed according to the Bures measure.

3.4. Numerical results

• **The distribution of separable matrices.** Now, having an algorithm for generating Hilbert–Schmidt and Bures matrices, one can analyze the character of the distribution of separable matrices in both ensembles. As concerns the two-qubit system, the distributions of separable density matrices with given entanglement characteristics, the determinants of the correlation and Schlienz–Mahler matrices, $\det \|\mathrm{C}\|$ and $\det \|\mathrm{M}\|$, have been found. The results of our calculations are presented in Figs. 1 and 2.

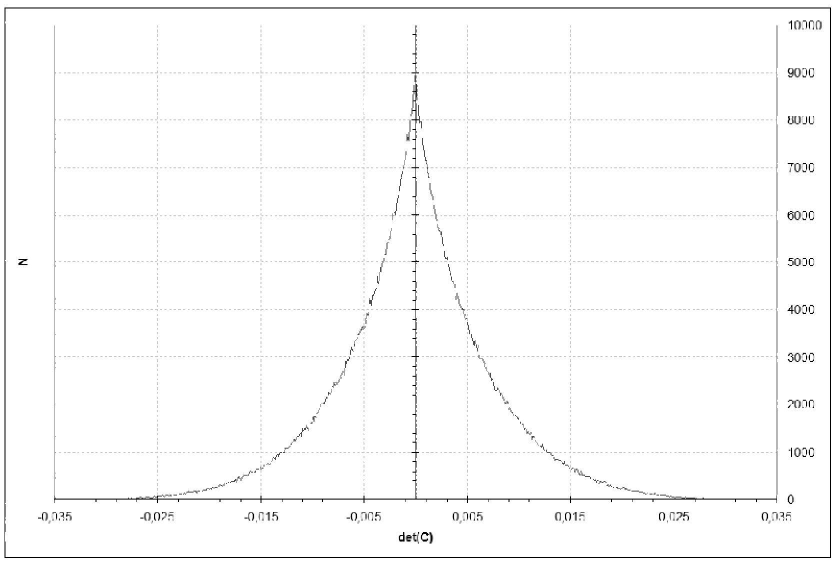

Fig. 1. The distribution of separable states with respect to the correlation measure $\det \|\mathrm{C}\|$ for 10^6 matrices from the Hilbert–Schmidt ensemble.

• **Probabilities and conjectures.** Finally, we give the values of probabilities for the two-qubit and qubit-qutrit composite systems whose density matrices are distributed according to the Hilbert–Schmidt and Bures measures.

Generating random density matrices as described above and then counting the number of matrices satisfying the PPT conditions

$$S_k^{T_B} \geq 0, \quad k = 1, 2, \ldots, 6,$$

we have found the probability of separability for the two measures. The results are as follows. For the Hilbert–Schmidt measure, the probabilities of separability are

$$\mathcal{P}_{\mathrm{H-S}}^{2\otimes 2} = 0.2424, \tag{71}$$

$$\mathcal{P}_{\mathrm{H-S}}^{2\otimes 3} = 0.0373, \tag{72}$$

while for the Bures measure they are

$$\mathcal{P}_{\mathrm{B}}^{2\otimes 2} = 0.073, \tag{73}$$

$$\mathcal{P}_{\mathrm{B}}^{2\otimes 3} = 0.001. \tag{74}$$

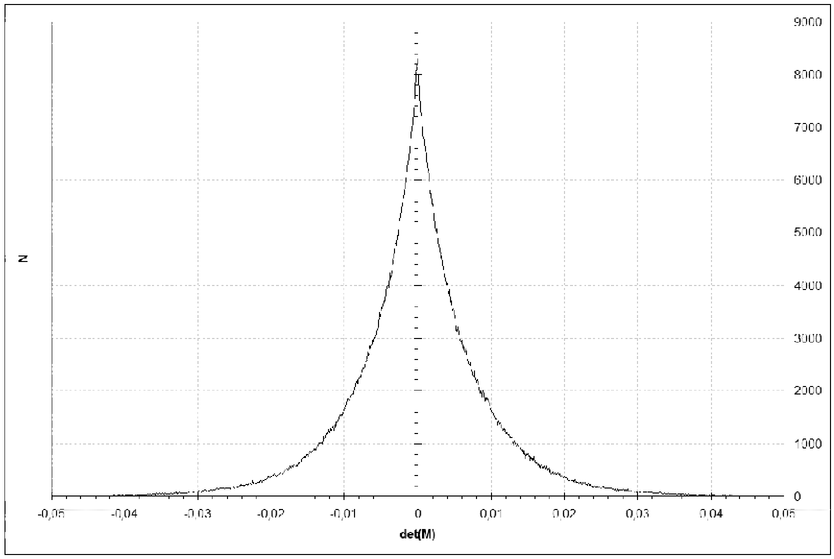

Fig. 2. The distribution of separable states with respect to the Schlienz–Mahler entanglement measure $\det \|\mathrm{M}\|$ for 10^6 random Hilbert–Schmidt matrices.

Besides, the probabilities of absolutely separable states for the two-qubit and qubit-qutrit systems have been determined. In this case, the problem reduces to the calculation of integrals over the domain in the ordered simplex given by inequalities (49) and (50):

$$\mathcal{P}^{2\otimes 2}_{\text{Measure}} = \int P_{\text{Measure}}(\boldsymbol{\lambda})\Theta(2\sqrt{\lambda_2\lambda_4} - \lambda_1 + \lambda_3), \tag{75}$$

$$\mathcal{P}^{2\otimes 3}_{\text{Measure}} = \int P_{\text{Measure}}(\boldsymbol{\lambda})\Theta(2\sqrt{\lambda_4\lambda_6} - \lambda_1 + \lambda_5). \tag{76}$$

These integrals have been evaluated using the `MATHEMATICA` package for the Hilbert–Schmidt (62) and Bures (64) distributions. Summarizing, all results, including the percentage of absolutely separable states, are collected in Table 2.

System	Separable		Abs. Sep.
H-S metric			
$2\otimes 2$	24.24 %	23,874174 %	0.365826 %
$2\otimes 3$	3.73 %	2,753321 %	0.976679 %
Bures metric			
$2\otimes 2$	7.3 %	7,2838208 %	0.0161792 %
$2\otimes 3$	0.1 %	0,1 %	-

Table 2. Probabilities for the two-qubit and qubit-qutrit systems.

4. Concluding remarks

In the present note, an algebraic description of low-dimensional binary composite systems, pairs of qubits and qubit-qutrit pairs, has been given in a form well adapted to computational purposes. Using this formulation, we have discussed a few probabilistic aspects of entanglement. Here a short comment on the results of our numerical experiments with probability of separability is in order. In particular, as concerns the probability of separability for the case of the Hilbert–Schmidt measure, one can observe the existence of intriguing simple rational approximations:

$$\mathcal{P}^{2\otimes 2}_{\mathrm{H-S}} = 0.2424 \approx \frac{8}{33} = \frac{2^3}{3*11}\,, \tag{77}$$

$$\mathcal{P}^{2\otimes 3}_{\mathrm{H-S}} = 0.0373 \approx \frac{16}{429} = \frac{2^4}{3*11*13}\,, \tag{78}$$

in agreement with the results conjectured by P. B. Slater a few years ago [45, 46]. It is interesting whether this observation has some deep background or is an accidental fact only.

Another interesting unclear issue discovered is the large value of the probability of absolute separability for the $2\otimes 3$ system with the Hilbert–Schmidt measure compared with the two-qubit system. Finally, we would also like to emphasize the strong dependence of entanglement characteristics on the choice of the measure (cf. [47]).

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