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Bipartite quantum systems: on the realignment criterion and beyond

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Abstract

Inspired by the 'computable cross norm' or 'realignment' criterion, we propose a new point of view about the characterization of the states of bipartite quantum systems. We consider a Schmidt decomposition of a bipartite density operator. The corresponding Schmidt coefficients, or the associated symmetric polynomials, are regarded as quantities that can be used to characterize bipartite quantum states. In particular, starting from the realignment criterion, a family of necessary conditions for the separability of bipartite quantum states are derived. We conjecture that these conditions, which are weaker than the parent criterion, can be strengthened in such a way to obtain a new family of criteria that are independent of the original one. This conjecture is supported by numerical examples for the low dimensional cases. These ideas can be applied to the study of quantum channels, leading to a relation between the rate of contraction of a map and its ability to preserve entanglement.

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(Some figures in this article are in colour only in the electronic version)

1. Introduction

The relation between the state of a composite quantum system as a whole and the configuration of its parts is a very peculiar feature of quantum theory. As recognized since the early stages of development of the theory [1–3], this is a consequence of the tensor product structure

of the state space of a composite quantum system. This feature of quantum mechanics has its most evident manifestation in the fact that it allows the presence of non-classical correlations, i.e. of *entanglement*, between the subsystems of a composite system. Nowadays, we may say that quantum entanglement is not only regarded as a key for the interpretation of quantum mechanics or as a mere scientific curiosity, but also as a fundamental resource for quantum information, communication and computation tasks [4, 5]. However, despite the great efforts made by the scientific community in the past few decades, there are still several open issues regarding the mathematical characterization of composite quantum states, even in the ‘elementary case’ of a bipartite system with a finite number of levels.

A major challenge is to characterize those states of a bipartite system that are entangled. According to the definition of Werner [6], *entangled* (mixed) states differ from *separable* states since they cannot be prepared, not even in principle, from product states by means of local operations and classical communication only. In mathematical terms, a (mixed) state $\hat{\rho}$ —a positive (trace class) operator of unit trace—in a composite Hilbert space $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$ is called *separable* if it can be represented as a convex sum of product states:

$$\hat{\rho} = \sum_i p_i \hat{\rho}_i^A \otimes \hat{\rho}_i^B, \quad (1)$$

with $p_i \geq 0$ and $\sum_i p_i = 1$; otherwise, $\hat{\rho}$ is said to be *entangled*. We remark that, if $\hat{\rho}$ is separable, decomposition (1) is in general not unique, and the smallest number of terms in the sum (usually called *cardinality*), due to Caratheodory’s theorem, is not larger than the squared dimension of the *total* Hilbert space of the system \mathcal{H} (see [7]).

Since quantum entanglement is a very important subject, also in view of its several potential applications, separability criteria are regarded as extremely precious tools. Among a plethora of proposed separability criteria—i.e. suitable conditions satisfied by all separable states whose violation allows us to detect entanglement (see, for instance, [8–11])—the present contribution is mainly inspired by the criterion that was proposed in [12] with the name of a ‘realignment criterion’ (RC) and in [13] with the name of a ‘computable cross norm’ criterion. As we will try to argue, the RC brings attention to the role played by the *Schmidt coefficients* [18] of a bipartite quantum state in the characterization of entanglement. Trying to shed light on this role will be the main goal of our contribution.

The paper develops along the following lines. In section 2, we introduce a ‘Schmidt equivalence relation’ in the set of states of a bipartite quantum system, and we show the link between this notion and the RC. Section 3 is devoted to the characterization of the Schmidt equivalence classes. We follow two different approaches: the characterization of some groups acting on the Schmidt equivalence classes and the analysis of the local geometry of these equivalence classes regarded as manifolds. A family of separability criteria are presented in section 4, which are extensions of the RC. These criteria are based on the ‘symmetric polynomials’ in the Schmidt coefficients, and are weaker than the parent criterion. In section 5, the well-known correspondence between quantum states and quantum maps (see, e.g., [14–16]), i.e. completely positive trace-preserving (CPT) maps, is considered, and a straightforward application of the derived family of separability criteria to the study of CPT maps is discussed. Through this correspondence, separable states are associated with entanglement breaking (EB) channels [17]. The proposed family of criteria, applied to this context, leads to a purely geometrical characterization of EB maps. In section 6, we formulate the conjecture that the proposed criteria can be strengthened in order to obtain new necessary conditions for separability which are independent of the parent RC. Numerical examples in support of this thesis are provided in section 7 for low dimensional bipartite systems.

2. Schmidt equivalence classes of states of a bipartite quantum system

Let us consider a bipartite, finite-dimensional, complex Hilbert space $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$ — $\mathcal{H}_A \cong \mathbb{C}^{N_A}$, $\mathcal{H}_B \cong \mathbb{C}^{N_B}$, $N_A, N_B \geq 2$ —and the corresponding real vector spaces of Hermitian operators $\mathcal{L}_{\mathbb{R}}(\mathcal{H})$, $\mathcal{L}_{\mathbb{R}}(\mathcal{H}_A)$ and $\mathcal{L}_{\mathbb{R}}(\mathcal{H}_B)$ (the spaces of observables) in \mathcal{H} , \mathcal{H}_A and \mathcal{H}_B , respectively, that are naturally endowed with a scalar product, namely the *bilinear* Hilbert–Schmidt (HS) product:

$$\langle \hat{A}, \hat{B} \rangle_{\text{HS}} = \text{tr}(\hat{A}\hat{B}), \quad (\hat{A}, \hat{B} \text{ Hermitian}). \quad (2)$$

In particular, the *density operators*—i.e. the positive operators of unit trace—in \mathcal{H} (\mathcal{H}_A and \mathcal{H}_B , respectively) can be regarded as elements of the real vector space $\mathcal{L}_{\mathbb{R}}(\mathcal{H})$ ($\mathcal{L}_{\mathbb{R}}(\mathcal{H}_A)$ and $\mathcal{L}_{\mathbb{R}}(\mathcal{H}_B)$, respectively), in which they form a convex body that will be denoted by $\mathcal{D}(\mathcal{H})$. Observe that $\mathcal{L}_{\mathbb{R}}(\mathcal{H}) = \mathcal{L}_{\mathbb{R}}(\mathcal{H}_A) \otimes \mathcal{L}_{\mathbb{R}}(\mathcal{H}_B)$, with $\mathcal{L}_{\mathbb{R}}(\mathcal{H}_A) \cong \mathbb{R}^{N_A^2}$ and $\mathcal{L}_{\mathbb{R}}(\mathcal{H}_B) \cong \mathbb{R}^{N_B^2}$. The HS product allows us to write a (nonunique) *Schmidt decomposition* [18] of a density operator $\hat{\rho} \in \mathcal{D}(\mathcal{H})$, i.e.⁷

$$\hat{\rho} = \sum_{k=1}^d \lambda_k \hat{F}_k^A \otimes \hat{F}_k^B, \quad \lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_d \geq 0, \quad (3)$$

where

$$\text{tr}(\hat{F}_h^A \hat{F}_k^A) = \delta_{hk} = \text{tr}(\hat{F}_h^B \hat{F}_k^B), \quad h, k \in \{1, \dots, d\}, \quad (4)$$

and the real positive numbers $\{\lambda_k\}_{k=1}^d$ are the (uniquely determined) *Schmidt coefficients* (in short, SCs). Note that the number of terms in the sum equals $d = \min\{N_A^2, N_B^2\}$ (we will also set $D = \max\{N_A^2, N_B^2\}$). The definition of the SCs of a bipartite density operator is the natural generalization of the standard definition for pure states (see, for instance, [19]). It is worth stressing that, since the operators forming the orthonormal systems $\{\hat{F}_k^A\}_{k=1}^d$ and $\{\hat{F}_k^B\}_{k=1}^d$ (in $\mathcal{L}_{\mathbb{R}}(\mathcal{H}_A)$ and $\mathcal{L}_{\mathbb{R}}(\mathcal{H}_B)$, respectively) are Hermitian, the operators $\{\hat{F}_k^A \otimes \hat{F}_k^B\}_{k=1}^d$ are *observables*. Hence—at least in principle—the SCs are *physically measurable quantities*:

$$\lambda_k = \text{tr}(\hat{\rho} \hat{F}_k^A \otimes \hat{F}_k^B). \quad (5)$$

The set of ‘local’ operators $\{\hat{F}_k^A \otimes \hat{F}_k^B\}_{k=1}^d$ is also referred to as *local orthogonal observables* [20]. Decomposition (3) has been recently considered—see [21]—in connection with the formulation of new separability criteria.

We observe that the convex body $\mathcal{D}(\mathcal{H})$ can also be regarded as immersed in the *complex* vector space $\mathcal{L}(\mathcal{H})$ of linear operators in \mathcal{H} , vector space that can be endowed with the *sesquilinear* HS product (denoted, again, as $\langle \cdot, \cdot \rangle_{\text{HS}}$). Then, one can consider a Schmidt decomposition of a density operator $\hat{\rho}$ in \mathcal{H} with respect to the complex Hilbert space $\mathcal{L}(\mathcal{H})$. It is clear that such a decomposition will contain the same SCs as decomposition (3), but this time will involve an orthonormal system of, in general, non-Hermitian operators.

Given a bipartite density operator, one can uniquely determine its SCs. On the other hand, it is clear that the SCs do not identify a unique quantum state. It is then natural to formulate the following definition.

Definition 1 (Schmidt equivalence relation). *We say that two bipartite density operators are Schmidt equivalent if they share the same set of Schmidt coefficients.*

Then the convex set of density operators in the Hilbert space \mathcal{H} —which will be denoted by $\mathcal{D}(\mathcal{H})$ —is partitioned into Schmidt equivalence classes.

⁷ We remark that actually any operator in $\mathcal{L}_{\mathbb{R}}(\mathcal{H})$ admits a Schmidt decomposition.

It is known that a bipartite *pure* state is completely characterized, with respect to entanglement, by the corresponding SCs [22]. Although the same characterization cannot be extended to a generic state, it is reasonable to suppose that there exists some relation between the SCs of a bipartite density operator and the entanglement properties of this state, and to address the following questions: ‘What relevant properties are encoded by the SCs of a bipartite density operator, and how can one characterize the Schmidt equivalence classes?’ In the following, we will try to analyze these questions and provide some reasonable answers.

A first observation is that the SCs determine the *purity* of a state. Let us recall that the purity is defined as the trace of the square of the density operator:

$$\mathcal{P}(\hat{\rho}) := \text{tr}(\hat{\rho}^2); \tag{6}$$

hence, $\mathcal{P}(\hat{\rho}) \in]0, 1], \forall \hat{\rho} \in \mathcal{D}(\mathcal{H})$. It follows from the definition of Schmidt decomposition that the purity equals the sum of the squares of the SCs:

$$\frac{1}{N_A N_B} \leq \mathcal{P}(\hat{\rho}) = \langle \hat{\rho}, \hat{\rho} \rangle_{\text{HS}} = \sum_{k=1}^d \lambda_k^2 \leq 1. \tag{7}$$

Thus, the purity is the simplest property which is (completely) described by the SCs of a density operator. Another relevant fact is the existence of a link between the separability of a density operator and its SCs.

Indeed, the ‘realignment criterion’ (in short, RC, see [12, 13]; also see [19], where a generalization of the RC is obtained) establishes a necessary condition for the separability of a quantum state (or a sufficient condition for the nonseparability). It can be formulated in various equivalent ways. From our point of view, it can be regarded as a condition on the SCs of a separable density operator $\hat{\rho}$. Precisely, it imposes an upper bound for the sum of its SCs.

Theorem 1 (the ‘realignment criterion’). *If a bipartite density operator $\hat{\rho}$ is separable, then its Schmidt coefficients $\{\lambda_k\}_{k=1}^d$ satisfy the following inequality:*

$$\sum_{k=1}^d \lambda_k \leq 1. \tag{8}$$

The RC is easily implementable. In particular, in [12], the notion of a *realigned matrix* ρ^R was introduced which is associated with the bipartite density operator $\hat{\rho}$ in order to compute the lhs of inequality (8). Fixed orthonormal bases $\{|n\rangle\}_{n=1, \dots, N_A}$ and $\{|v\rangle\}_{v=1, \dots, N_B}$ in the local Hilbert spaces \mathcal{H}_A and \mathcal{H}_B , respectively, and assuming that $\rho_{(m\mu)(nv)}$ is the representative matrix of the density operator $\hat{\rho}$ with respect to the product basis $\{|n\rangle \otimes |v\rangle\}_{n=1, \dots, N_A}^{v=1, \dots, N_B}$ —where $(m\mu)$ and (nv) are double indices—the corresponding realigned matrix (with respect to the given basis) is defined as

$$\rho_{(mn)(\mu\nu)}^R := \rho_{(m\mu)(nv)}. \tag{9}$$

It turns out that the SCs of $\hat{\rho}$ are the *singular values* of the realigned matrix ρ^R , see [19]. Precisely, consider a *singular value decomposition* of the realigned matrix, i.e.

$$\rho^R = \mathcal{U} \Delta \mathcal{V}, \tag{10}$$

where \mathcal{U} and \mathcal{V} are unitary matrices, belonging respectively to the unitary groups $U(N_A^2)$ and $U(N_B^2)$, and Δ is a rectangular matrix such that its nonvanishing entries are positive and placed along the principal diagonal only. Then, the diagonal entries of Δ are the singular values of ρ^R , hence the SCs of $\hat{\rho}$. At this point, observing that the singular values of the realigned

matrix ρ^R coincide with the eigenvalues of the positive matrix $|\rho^R| = \sqrt{\rho^{R\dagger}\rho^R}$, one concludes that inequality (8) can also be written as

$$\|\rho^R\|_{\text{tr}} = \text{tr}(|\rho^R|) \leq 1. \tag{11}$$

Given a density operator $\hat{\rho} \in \mathcal{D}(\mathcal{H})$, we will denote by $\mathfrak{S}_{\hat{\rho}}$ the Schmidt equivalence class containing $\hat{\rho}$. Beside the Schmidt equivalence class $\mathfrak{S}_{\hat{\rho}}$, we will consider the *extended Schmidt equivalence class* containing $\hat{\rho}$, namely the set $\mathfrak{S}_{\hat{\rho}}^{\text{ext}}$ of all the Hermitian operators in \mathcal{H} that share with $\hat{\rho}$ the same set of Schmidt coefficients. Thus, we have that $\mathfrak{S}_{\hat{\rho}} = \mathfrak{S}_{\hat{\rho}}^{\text{ext}} \cap \mathcal{D}(\mathcal{H})$.

3. Characterization of the Schmidt equivalence classes

The aim of the present section is to give a basic characterization of the Schmidt equivalence classes of states; see definition 1. In this regard, one can adopt two different approaches. On one hand, one can try to characterize some ‘natural’ groups for which an action on the Schmidt equivalence classes is defined; see subsection 3.1. On the other hand, one can regard the Schmidt equivalence classes as manifolds and study their local geometry considering the action of the local orthogonal groups; see subsection 3.2. Although the results that we obtain are still somewhat ‘preliminary’, we think that it is worthwhile to report them since a description of Schmidt equivalence classes seems to be completely missing in the literature.

3.1. Groups acting on the Schmidt equivalence classes

Note that, since $\mathcal{L}_{\mathbb{R}}(\mathcal{H}), \mathcal{L}_{\mathbb{R}}(\mathcal{H}_A)$ and $\mathcal{L}_{\mathbb{R}}(\mathcal{H}_B)$ are *real* Hilbert spaces, the unitary (super)operators in these spaces belong to orthogonal groups. For instance, a unitary operator in $\mathcal{L}_{\mathbb{R}}(\mathcal{H})$ belongs to the orthogonal group $O(N_A^2 N_B^2)$. The class of unitary operators in $\mathcal{L}_{\mathbb{R}}(\mathcal{H})$ that are decomposable as the tensor product of two unitary operators in $\mathcal{L}_{\mathbb{R}}(\mathcal{H}_A)$ and $\mathcal{L}_{\mathbb{R}}(\mathcal{H}_B)$, respectively—i.e. of the form $\hat{T}_A \otimes \hat{T}_B$, with \hat{T}_A in $O(N_A^2)$ and \hat{T}_B in $O(N_B^2)$ —will be denoted by $O \otimes O(\mathcal{H})$. It is clear that the maps in $O \otimes O(\mathcal{H})$ preserve the SCs of every element of $\mathcal{L}_{\mathbb{R}}(\mathcal{H})$, but, in general, $\hat{T}_A \otimes \hat{T}_B(\mathcal{D}(\mathcal{H})) \not\subset \mathcal{D}(\mathcal{H})$. Note, moreover, that the set $O \otimes O(\mathcal{H})$ is a group (isomorphic to the direct product $O(N_A^2) \times O(N_B^2)$) with respect to the usual composition of maps. The orbit in $\mathcal{L}_{\mathbb{R}}(\mathcal{H})$, under the action of this group, passing through $\hat{\rho} \in \mathcal{D}(\mathcal{H})$, will be denoted by $\tilde{\mathfrak{S}}_{\hat{\rho}}$; i.e.

$$\tilde{\mathfrak{S}}_{\hat{\rho}} := \{\hat{T}(\hat{\rho}) \in \mathcal{L}_{\mathbb{R}}(\mathcal{H}) : \hat{T} = \hat{T}_A \otimes \hat{T}_B \in O \otimes O(\mathcal{H})\}. \tag{12}$$

Proposition 1. *The orbit $\tilde{\mathfrak{S}}_{\hat{\rho}}$ of the group $O \otimes O(\mathcal{H})$ through $\hat{\rho} \in \mathcal{D}(\mathcal{H})$ coincides with the extended Schmidt equivalence class containing $\hat{\rho}$:*

$$\tilde{\mathfrak{S}}_{\hat{\rho}} = \mathfrak{S}_{\hat{\rho}}^{\text{ext}}. \tag{13}$$

It follows that

$$\mathfrak{S}_{\hat{\rho}} = \tilde{\mathfrak{S}}_{\hat{\rho}} \cap \mathcal{D}(\mathcal{H}). \tag{14}$$

Therefore, two states $\hat{\rho}$ and $\hat{\sigma}$ in $\mathcal{D}(\mathcal{H})$ are Schmidt equivalent if and only if

$$\hat{\rho} = \hat{T}_A \otimes \hat{T}_B(\hat{\sigma}), \tag{15}$$

for some unitary operators \hat{T}_A and \hat{T}_B in $\mathcal{L}_{\mathbb{R}}(\mathcal{H}_A)$ and $\mathcal{L}_{\mathbb{R}}(\mathcal{H}_B)$, respectively.

Proof. As already observed, given $\hat{\rho} \in \mathcal{D}(\mathcal{H})$, for every \hat{T} in the group $O \otimes O(\mathcal{H})$, $\hat{T}(\hat{\rho})$ belongs to $\mathfrak{S}_{\hat{\rho}}^{\text{ext}}$; hence, $\tilde{\mathfrak{S}}_{\hat{\rho}} \subset \mathfrak{S}_{\hat{\rho}}^{\text{ext}}$. On the other hand, let $\hat{\rho} = \sum_{k=1}^d \lambda_k \hat{F}_k^A \otimes \hat{F}_k^B$ be a Schmidt decomposition of $\hat{\rho}$ and $\hat{C} = \sum_{k=1}^d \lambda_k \hat{G}_k^A \otimes \hat{G}_k^B$ a Schmidt decomposition of an arbitrary

element \hat{C} of $\mathfrak{S}_\rho^{\text{ext}}$. Then, for every couple of unitary operators \hat{T}_A and \hat{T}_B in $\mathcal{L}_\mathbb{R}(\mathcal{H}_A)$ and $\mathcal{L}_\mathbb{R}(\mathcal{H}_B)$, respectively, such that $\hat{T}_A(\hat{F}_k^A) = \hat{G}_k^A$ and $\hat{T}_B(\hat{F}_k^B) = \hat{G}_k^B$, $k = 1, \dots, d$, we have $\hat{T}_A \otimes \hat{T}_B(\hat{\rho}) = \hat{C}$. Hence, $\tilde{\mathfrak{S}}_\rho \supset \mathfrak{S}_\rho^{\text{ext}}$. \square

The set of all the maps of the form $\hat{T}_A \otimes \hat{T}_B$ —with \hat{T}_A and \hat{T}_B unitary operators in $\mathcal{L}_\mathbb{R}(\mathcal{H}_A)$ and $\mathcal{L}_\mathbb{R}(\mathcal{H}_B)$, respectively—such that \mathfrak{S}_ρ is *stable* under the action of $\hat{T}_A \otimes \hat{T}_B$, i.e. such that

$$\hat{T}_A \otimes \hat{T}_B(\mathfrak{S}_\rho) \subset \mathfrak{S}_\rho, \quad (16)$$

is a semigroup (with respect to composition) with identity, contained in the group $\mathcal{O} \otimes \mathcal{O}(\mathcal{H})$, which will be denoted by $\mathcal{O} \otimes \mathcal{O}_{\text{st}}(\hat{\rho})$. The subset $\mathcal{O} \otimes \mathcal{O}_{\text{inv}}(\hat{\rho})$ of $\mathcal{O} \otimes \mathcal{O}_{\text{st}}(\hat{\rho})$ defined by

$$\mathcal{O} \otimes \mathcal{O}_{\text{inv}}(\hat{\rho}) := \{\hat{T}_A \otimes \hat{T}_B \in \mathcal{O} \otimes \mathcal{O}_{\text{st}}(\hat{\rho}) : (\hat{T}_A \otimes \hat{T}_B)^\dagger \in \mathcal{O} \otimes \mathcal{O}_{\text{st}}(\hat{\rho})\} \quad (17)$$

is a group. It is easy to check that $\mathcal{O} \otimes \mathcal{O}_{\text{inv}}(\hat{\rho})$ coincides with the subset of $\mathcal{O} \otimes \mathcal{O}_{\text{st}}(\hat{\rho})$ containing those maps that leave \mathfrak{S}_ρ *invariant*, i.e.

$$\mathcal{O} \otimes \mathcal{O}_{\text{inv}}(\hat{\rho}) = \{\hat{T}_A \otimes \hat{T}_B \in \mathcal{O} \otimes \mathcal{O}_{\text{st}}(\hat{\rho}) : \hat{T}_A \otimes \hat{T}_B(\mathfrak{S}_\rho) = \mathfrak{S}_\rho\}. \quad (18)$$

As an example of an operator belonging to $\mathcal{O} \otimes \mathcal{O}_{\text{inv}}(\hat{\rho})$, for all $\hat{\rho} \in \mathcal{D}(\mathcal{H})$, consider the linear map $\hat{J}_A \otimes \hat{J}_B : \mathcal{L}_\mathbb{R}(\mathcal{H}) \rightarrow \mathcal{L}_\mathbb{R}(\mathcal{H})$, with \hat{J}_A and \hat{J}_B unitary operators defined by

$$\hat{J}_A : \mathcal{L}_\mathbb{R}(\mathcal{H}_A) \ni \hat{A} \mapsto \hat{J}_A \hat{A} \hat{J}_A \in \mathcal{L}_\mathbb{R}(\mathcal{H}_A), \quad \hat{J}_B : \mathcal{L}_\mathbb{R}(\mathcal{H}_B) \ni \hat{B} \mapsto \hat{J}_B \hat{B} \hat{J}_B \in \mathcal{L}_\mathbb{R}(\mathcal{H}_B), \quad (19)$$

where \hat{J}_A and \hat{J}_B are ‘local’ *complex conjugations* (i.e. self-adjoint anti-unitary operators) in \mathcal{H}_A and \mathcal{H}_B , respectively. The maps \hat{J}_A and \hat{J}_B are partial transpositions, so that the map $\hat{J}_A \otimes \hat{J}_B$ is the transposition associated with a tensor product basis in $\mathcal{H}_A \otimes \mathcal{H}_B$ (recall that transposition, as complex conjugation, is a basis-dependent notion). As is well known, a transposition is a *positive trace-preserving* map (in short, PT map), and it is self-adjoint with respect to the HS scalar product. Therefore, the self-adjoint unitary operator $\hat{J}_A \otimes \hat{J}_B$ is contained in the group $\mathcal{O} \otimes \mathcal{O}_{\text{inv}}(\hat{\rho})$, for all $\hat{\rho} \in \mathcal{D}(\mathcal{H})$.

It is natural to wonder how states belonging to the same Schmidt equivalence class can be connected by physically realizable transformations. We will then consider the semigroup with identity of PT maps in $\mathcal{L}_\mathbb{R}(\mathcal{H})$, which will be denoted by $\text{PT}(\mathcal{H})$. It is worth defining the following subset of $\text{PT}(\mathcal{H})$:

$$\text{PT}_\mathfrak{S}(\mathcal{H}) := \{\hat{\mathcal{E}} \in \text{PT}(\mathcal{H}) : \hat{\mathcal{E}} \text{ bijective, } \hat{\mathcal{E}}^{-1} \in \text{PT}(\mathcal{H}), \hat{\mathcal{E}}(\mathfrak{S}_\rho) = \mathfrak{S}_\rho, \forall \hat{\rho} \in \mathcal{D}(\mathcal{H})\}. \quad (20)$$

It is clear that the set $\text{PT}_\mathfrak{S}(\mathcal{H})$ is a group.

As already observed, unitary maps in $\mathcal{L}_\mathbb{R}(\mathcal{H})$ of the form $\hat{T}_A \otimes \hat{T}_B$ —with \hat{T}_A and \hat{T}_B unitary operators in $\mathcal{L}_\mathbb{R}(\mathcal{H}_A)$ and $\mathcal{L}_\mathbb{R}(\mathcal{H}_B)$, respectively—preserve the SCs of every element of $\mathcal{L}_\mathbb{R}(\mathcal{H})$, but, in general, $\hat{T}_A \otimes \hat{T}_B(\mathcal{D}(\mathcal{H})) \not\subset \mathcal{D}(\mathcal{H})$. It is therefore natural to consider the class of linear maps in $\mathcal{L}_\mathbb{R}(\mathcal{H})$ belonging to the set $\mathcal{O} \otimes \mathcal{O}(\mathcal{H}) \cap \text{PT}(\mathcal{H})$. It is clear that this set is a semigroup (with respect to composition of maps) with identity contained in $\mathcal{O} \otimes \mathcal{O}_{\text{st}}(\hat{\rho})$. We will now show that it is actually a group which is a subgroup of $\mathcal{O} \otimes \mathcal{O}_{\text{inv}}(\hat{\rho})$. We need two preliminary results; the proof of the first one is trivial.

Lemma 1. *The inverse of a bijective trace-preserving map from $\mathcal{L}_\mathbb{R}(\mathcal{H})$ onto $\mathcal{L}_\mathbb{R}(\mathcal{H})$ is trace-preserving.*

Lemma 2. *A positive linear map $\hat{T} : \mathcal{L}_\mathbb{R}(\mathcal{H}) \rightarrow \mathcal{L}_\mathbb{R}(\mathcal{H})$ which is unitary transforms the convex cone of positive operators in \mathcal{H} onto itself; therefore, \hat{T}^\dagger is a positive map. Hence, in particular, if a linear map belonging to $\mathcal{O} \otimes \mathcal{O}(\mathcal{H})$ is a positive map, then its inverse is a positive map too.*

Proof. We will prove the statement by contradiction. Suppose that $\hat{B} = \hat{T}(\hat{A})$ is positive and assume that \hat{A} is not a positive operator. Then, for some $\psi \in \mathcal{H}$, we should have

that $\langle \psi, \hat{A}\psi \rangle < 0$; hence, $\text{tr}(\hat{T}(|\psi\rangle\langle\psi|)\hat{T}(\hat{A})) = \text{tr}(|\psi\rangle\langle\psi|\hat{A}) = \langle \psi, \hat{A}\psi \rangle < 0$, where we have used the unitarity of \hat{T} . On the other hand, since \hat{T} is a positive injective linear map, $\hat{\Psi} \equiv \hat{T}(|\psi\rangle\langle\psi|)$ is a nonzero positive operator, so that it admits a decomposition of the form $\hat{\Psi} = \sum_{k=1}^K \epsilon_k |\phi_k\rangle\langle\phi_k|$, where $\{\phi_k\}_{k=1}^K$ is an orthonormal system and $\{\epsilon_k\}_{k=1}^K$ is a set of strictly positive numbers. Therefore, since \hat{B} is positive, we have

$$\text{tr}(\hat{\Psi}\hat{B}) = \sum_{k=1}^K \epsilon_k \text{tr}(|\phi_k\rangle\langle\phi_k|\hat{B}) = \sum_{k=1}^K \epsilon_k \langle \phi_k, \hat{B}\phi_k \rangle > 0. \tag{21}$$

But this is in contrast with the inequality $\text{tr}(\hat{\Psi}\hat{B}) < 0$ previously found. □

From lemmas 1 and 2, one immediately obtains the following result.

Proposition 2. *The inverse of a linear map belonging to the set $\text{O} \otimes \text{O}(\mathcal{H}) \cap \text{PT}(\mathcal{H})$ belongs to this set too. Hence, $\text{O} \otimes \text{O}(\mathcal{H}) \cap \text{PT}(\mathcal{H})$ is a subgroup of $\text{O} \otimes \text{O}_{\text{inv}}(\hat{\rho})$.*

We now consider the set $\text{PTO} \otimes \text{PTO}(\mathcal{H})$ consisting of those linear maps in $\mathcal{L}_{\mathbb{R}}(\mathcal{H})$ of the form $\hat{E}_A \otimes \hat{E}_B$, where \hat{E}_A and \hat{E}_B are linear maps in $\mathcal{L}_{\mathbb{R}}(\mathcal{H}_A)$ and $\mathcal{L}_{\mathbb{R}}(\mathcal{H}_B)$, respectively, that are positive, trace-preserving and unitary. An analogous definition holds for the set $\text{CPTO} \otimes \text{CPTO}(\mathcal{H})$, with the ‘local maps’ \hat{E}_A and \hat{E}_B assumed to be *completely positive* rather than simply positive. It is clear that the sets $\text{PTO} \otimes \text{PTO}(\mathcal{H})$ and $\text{CPTO} \otimes \text{CPTO}(\mathcal{H})$ are semigroups with identity. We will see that they are actually groups. Also consider the group of *local unitary transformations*:

$$\begin{aligned} \underline{\text{O}} \otimes \underline{\text{O}}(\mathcal{H}) := \{ \hat{T} \in \text{O} \otimes \text{O}(\mathcal{H}) : \hat{T}(\hat{A}) &= (\hat{U} \otimes \hat{V})\hat{A}(\hat{U}^\dagger \otimes \hat{V}^\dagger), \forall \hat{A} \in \mathcal{L}_{\mathbb{R}}(\mathcal{H}), \\ &\text{for some unitary operators } \hat{U}, \hat{V} \text{ in } \mathcal{L}_{\mathbb{R}}(\mathcal{H}_A), \mathcal{L}_{\mathbb{R}}(\mathcal{H}_B) \text{ respectively}, \end{aligned} \tag{22}$$

which is obviously a subgroup of both $\text{PTO} \otimes \text{PTO}(\mathcal{H})$ and $\text{CPTO} \otimes \text{CPTO}(\mathcal{H})$. In a similar way, one defines the group of *local unitary–anti-unitary transformations* $\overline{\text{O}} \otimes \overline{\text{O}}(\mathcal{H})$ (include local anti-unitary operators \hat{U}, \hat{V} on the rhs of (22)). An example of a map that belongs to $\overline{\text{O}} \otimes \overline{\text{O}}(\mathcal{H})$, but not to $\underline{\text{O}} \otimes \underline{\text{O}}(\mathcal{H})$, is the tensor product $\hat{J}_A \otimes \hat{J}_B$ of two partial transpositions \hat{J}_A and \hat{J}_B .

Proposition 3. *The set $\text{PTO} \otimes \text{PTO}(\mathcal{H})$ is a group (with respect to composition of maps); hence, it is a subgroup of the group $\text{O} \otimes \text{O}(\mathcal{H}) \cap \text{PT}(\mathcal{H})$.*

Proof. Given a map $\hat{E}_A \otimes \hat{E}_B$ in $\text{PTO} \otimes \text{PTO}(\mathcal{H})$ —where \hat{E}_A, \hat{E}_B are linear maps in $\mathcal{L}_{\mathbb{R}}(\mathcal{H}_A), \mathcal{L}_{\mathbb{R}}(\mathcal{H}_B)$, respectively, that are positive, trace-preserving and unitary—the inverse map $\hat{E}_A^{-1} \otimes \hat{E}_B^{-1}$ is positive; to show this, apply lemmas 1 and 2 identifying the (generic) Hilbert space \mathcal{H} with the local Hilbert spaces \mathcal{H}_A and \mathcal{H}_B . □

A *Kadison automorphism* is a bijective map from $\mathcal{D}(\mathcal{K})$ —the convex set of density operators in a Hilbert space \mathcal{K} —onto itself that is convex linear. We now state as a lemma a property of this kind of automorphisms that can be obtained ‘by duality’ from a well-known result due to Kadison [23] (concerning C^* -algebras).

Lemma 3 (Kadison). *Every Kadison automorphism $\hat{\mathcal{E}}: \mathcal{D}(\mathcal{K}) \rightarrow \mathcal{D}(\mathcal{K})$ is of the form*

$$\hat{\mathcal{E}}(\hat{\rho}) = \hat{T}\hat{\rho}\hat{T}^\dagger, \quad \forall \hat{\rho} \in \mathcal{D}(\mathcal{K}), \tag{23}$$

where \hat{T} is a unitary or anti-unitary operator.

Assume that the Hilbert space \mathcal{K} is finite-dimensional. Then, since any operator $\hat{C} \in \mathcal{L}_{\mathbb{R}}(\mathcal{K})$ can be written as $\hat{C} = c_1\hat{\rho}_1 - c_2\hat{\rho}_2$, for some $\hat{\rho}_1, \hat{\rho}_2 \in \mathcal{D}(\mathcal{K})$ and some non-negative numbers

c_1, c_2 , it is clear that every Kadison automorphism $\hat{\mathcal{E}}: \mathcal{D}(\mathcal{K}) \rightarrow \mathcal{D}(\mathcal{K})$ extends (uniquely) in a natural way to a linear map in $\mathcal{L}_{\mathbb{R}}(\mathcal{K})$; conversely, a linear map in $\mathcal{L}_{\mathbb{R}}(\mathcal{K})$ which is bijective on $\mathcal{D}(\mathcal{K})$ can be regarded as a Kadison automorphism.

Let us denote by $\overline{\mathcal{O}}(\mathcal{H})$ the group of unitary–anti-unitary transformations in $\mathcal{L}_{\mathbb{R}}(\mathcal{H})$. We are now able to prove the following result.

Theorem 2. *The group $\mathcal{O} \otimes \mathcal{O}(\mathcal{H}) \cap \text{PT}(\mathcal{H})$ coincides with the group $\mathcal{O} \otimes \mathcal{O}(\mathcal{H}) \cap \overline{\mathcal{O}}(\mathcal{H})$. The group $\text{PTO} \otimes \text{PTO}(\mathcal{H})$ coincides with the group $\overline{\mathcal{O}} \otimes \overline{\mathcal{O}}(\mathcal{H})$. The set $\text{CPTO} \otimes \text{CPTO}(\mathcal{H})$ is a group which coincides with the group of local unitary transformations $\underline{\mathcal{O}} \otimes \underline{\mathcal{O}}(\mathcal{H})$. All the mentioned groups are subgroups of $\text{PT}_{\mathfrak{S}}(\mathcal{H})$, and $\text{PT}_{\mathfrak{S}}(\mathcal{H})$ is a subgroup of $\overline{\mathcal{O}}(\mathcal{H})$.*

Proof. It is clear that the group $\mathcal{O} \otimes \mathcal{O}(\mathcal{H}) \cap \overline{\mathcal{O}}(\mathcal{H})$ is a subgroup of $\mathcal{O} \otimes \mathcal{O}(\mathcal{H}) \cap \text{PT}(\mathcal{H})$. On the other hand, by lemmas 1 and 2, a map in the group $\mathcal{O} \otimes \mathcal{O}(\mathcal{H}) \cap \text{PT}(\mathcal{H})$ is a Kadison automorphism; hence, by lemma 3, it is contained in $\mathcal{O} \otimes \mathcal{O}(\mathcal{H}) \cap \overline{\mathcal{O}}(\mathcal{H})$. This proves the first assertion of the theorem. Next, given a map $\hat{\mathcal{E}}_A \otimes \hat{\mathcal{E}}_B$ in $\text{PTO} \otimes \text{PTO}(\mathcal{H})$ —where $\hat{\mathcal{E}}_A, \hat{\mathcal{E}}_B$ are linear maps in $\mathcal{L}_{\mathbb{R}}(\mathcal{H}_A), \mathcal{L}_{\mathbb{R}}(\mathcal{H}_B)$, respectively, that are positive, trace-preserving and unitary—the maps $\hat{\mathcal{E}}_A$ and $\hat{\mathcal{E}}_B$ are Kadison automorphisms. Hence, by lemma 3,

$$\hat{\mathcal{E}}_A(\hat{A}) = \hat{U} \hat{A} \hat{U}^\dagger, \quad \forall \hat{A} \in \mathcal{L}_{\mathbb{R}}(\mathcal{H}_A), \quad \hat{\mathcal{E}}_A(\hat{B}) = \hat{V} \hat{B} \hat{V}^\dagger, \quad \forall \hat{B} \in \mathcal{L}_{\mathbb{R}}(\mathcal{H}_B), \quad (24)$$

for some unitary or anti-unitary operators \hat{U}, \hat{V} in $\mathcal{L}_{\mathbb{R}}(\mathcal{H}_A), \mathcal{L}_{\mathbb{R}}(\mathcal{H}_B)$, respectively. Therefore, the group $\text{PTO} \otimes \text{PTO}(\mathcal{H})$ coincides with the group $\overline{\mathcal{O}} \otimes \overline{\mathcal{O}}(\mathcal{H})$. Note that, since an anti-unitary operator is the composition of a unitary operator with a complex conjugation, if in (24) we let the operators \hat{U}, \hat{V} be anti-unitary, we have that the maps $\hat{\mathcal{E}}_A, \hat{\mathcal{E}}_B$ are the composition of unitary transformations with transpositions. Transpositions are positive but not completely positive maps; hence, the set $\text{CPTO} \otimes \text{CPTO}(\mathcal{H})$ coincides with the group of local unitary transformations $\underline{\mathcal{O}} \otimes \underline{\mathcal{O}}(\mathcal{H})$. Finally, observe that the maps in the group $\text{PT}_{\mathfrak{S}}(\mathcal{H})$ are Kadison automorphisms. Thus, by lemma 3, the last assertion of the theorem follows. □

3.2. Local analysis

In [24], the authors considered the Schmidt decomposition of *pure* states, and, in that setting, analyzed the geometry of the sets of Schmidt-equivalent pure states (that turn out to be differentiable manifolds). Since two pure states are Schmidt equivalent if and only if they are mutually convertible via local unitary transformations, they called such manifolds ‘the manifolds of *interconvertible* states’. The aim of the present section is to apply the same line of reasoning to study the structure of the manifolds of Schmidt-equivalent (mixed) states. Here we assume for simplicity that $N_A = N_B = N$; hence $d = N^2$. This is not necessary for our purposes but it allows a convenient simplification of our formulae.

As is discussed below, there is a major limitation to the straightforward extension of the aforementioned results from pure to mixed states. The definition of SCs is based on the fact that density operators are elements of a vector space. On the other hand, they are constrained to be positive operators (of unit trace) because of their physical interpretation. This leads to the main difference between the results in [24] and our forthcoming discussion: while in [24] the geometry of the manifolds of interconvertible states can be characterized globally, here we are limited to a ‘local’ analysis (i.e. we are forced to consider transformations in a neighborhood of the identity).

As stated in proposition 1, the transformations of the form $\hat{\rho} \mapsto \hat{T}(\hat{\rho})$, where \hat{T} belongs to $\mathcal{O} \otimes \mathcal{O}(\mathcal{H})$, preserve the SCs. The converse is also true: if two operators have the same SCs then they are connected by a map in the group $\mathcal{O} \otimes \mathcal{O}(\mathcal{H})$. Therefore, we can build the different

equivalence classes acting locally on ‘fiducial states’ with the group $O \otimes O(\mathcal{H})$. Actually, we need to consider the component connected to the identity of this group, which is isomorphic to (and will be identified with) the Lie group $SO(d) \times SO(d)$. We then need to impose two conditions on the local (i.e. close to the identity) transformations: (a) the positivity of a fiducial state $\hat{\rho}$ must be preserved and (b) the trace of $\hat{\rho}$ has to be preserved as well. The first is a *global constraint* that does not ‘reduce the number of dimensions’, although characterizing a neighborhood of the identity in $SO(d) \times SO(d)$ preserving the positivity of a given fiducial state is a challenging open problem. The second constraint, normalization, is a *local constraint* that reduces the dimension of the manifold by 1: the condition that $\text{tr}(\hat{\rho}) = 1$ amounts to fixing the projection of the vector $\hat{\rho}$ along the direction $\hat{\mathbb{1}}$. Let us consider an orthonormal basis in the real Hilbert space of the form $\{\hat{\mathbb{1}}^A \otimes \hat{\mathbb{1}}^B, \hat{F}_i^A \otimes \hat{\mathbb{1}}^B, \hat{\mathbb{1}}^A \otimes \hat{F}_j^B, \hat{F}_i^A \otimes \hat{F}_j^B\}_{1 \leq i, j \leq d-1}$; clearly, $\text{tr}(\hat{F}_i^A) = 0 = \text{tr}(\hat{F}_j^B)$, because of the orthogonality condition with $\hat{\mathbb{1}} = \hat{\mathbb{1}}^A \otimes \hat{\mathbb{1}}^B$. Given a state $\hat{\rho} \in \mathcal{D}(\mathcal{H})$, we have

$$\hat{\rho} = \frac{\hat{\mathbb{1}}^A \otimes \hat{\mathbb{1}}^B}{d} + \sum_{i=1}^{d-1} \alpha_i^A \hat{F}_i^A \otimes \hat{\mathbb{1}}^B + \sum_{i=1}^{d-1} \alpha_i^B \hat{\mathbb{1}}^A \otimes \hat{F}_i^B + \sum_{i, j=1}^{d-1} \beta_{ij} \hat{F}_i^A \otimes \hat{F}_j^B. \quad (25)$$

The infinitesimal action of the Lie group $SO(d) \times SO(d)$ on the basis elements is of the form

$$\hat{F}_i^{A,B} \mapsto (\delta_{ij} + \phi_{ij}^{A,B}) \hat{F}_j^{A,B} + \epsilon_i^{A,B} \hat{\mathbb{1}}^{A,B}, \quad (26)$$

$$\hat{\mathbb{1}}^{A,B} \mapsto \hat{\mathbb{1}}^{A,B} - \epsilon_i^{A,B} \hat{F}_i^{A,B}, \quad (27)$$

where contraction of repeated indices is understood. Here ϕ^A and ϕ^B are real, $(d-1) \times (d-1)$ antisymmetric matrices and ϵ^A and ϵ^B are real $(d-1)$ -dimensional vectors.

Hence, by applying an infinitesimal transformation to $SO(d) \times SO(d)$ with generators $(\phi^A, \epsilon^A; \phi^B, \epsilon^B)$ it is not difficult to see that the coefficient of $\hat{\mathbb{1}} = \hat{\mathbb{1}}^A \otimes \hat{\mathbb{1}}^B$ —and hence $\text{tr}(\hat{\rho})$ —undergoes the following change:

$$\delta \text{tr}(\hat{\rho}) = \alpha_i^A \epsilon_i^A + \alpha_i^B \epsilon_i^B + \beta_{ij} \epsilon_i^A \epsilon_j^B. \quad (28)$$

In this equation we have kept the leading non-trivial infinitesimal changes, discarding those of the type $(\epsilon^A)^2$ and $(\epsilon^B)^2$. This is the correct expansion in the space of jets of regular functions of two vectors with nonvanishing gradients. Equation (28) defines a surface similar to an hyperboloid. In order to visualize it, one can simply take $\epsilon_i^{A,B} = \delta_{1i} \epsilon^{A,B}$. For a simple choice of α, β , the result is plotted in figure 1. Clearly, connection to the identity implies that only the branch containing the origin has to be considered.

Therefore, the vectors $\epsilon^{A,B}$ are constrained while the matrices $\phi^{A,B}$ are unconstrained⁸. Assuming that *the SCs are all different* (i.e. that $\hat{\rho}$ is a ‘typical state’), one finds out that the Schmidt equivalence class $\mathfrak{S}_{\hat{\rho}}$ is locally diffeomorphic to

$$\frac{SO(d) \times SO(d)}{SO(2)}, \quad (29)$$

where the subgroup $SO(2)$ is generated by the linear combination of the coefficients $\{\epsilon_i^A, \epsilon_i^B\}_{i=1}^{d-1}$ derived above. Then, the dimension of the manifold $\mathfrak{S}_{\hat{\rho}}$ is

$$d_{\hat{\rho}} = 2 \frac{d(d-1)}{2} - 1 = d^2 - d - 1. \quad (30)$$

⁸ We neglect here the case $\alpha_i^{A,B} = 0, \beta_{ij} \neq 0$. In this atypical case, we need to keep terms of $\mathcal{O}(\epsilon^2)$ in the transformation law of $\hat{\mathbb{1}}^{A,B}$. Once this is done, one checks that the codimension is still 1. The really degenerate case $\alpha = \beta = 0$, instead, corresponds to the class of equivalence of a single point $\hat{\rho} = \hat{\mathbb{1}}^A \otimes \hat{\mathbb{1}}^B / d$, with dimension 0. This point has to be considered as the ‘tip’, the extremal point of the space of states.

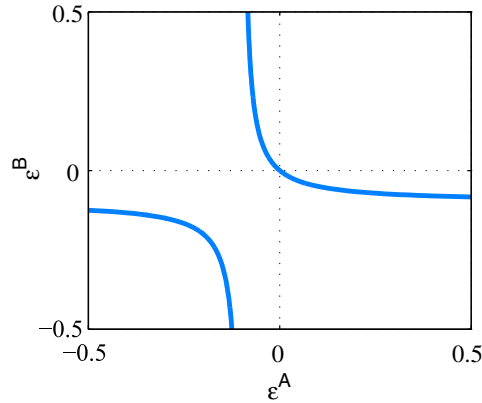


Figure 1. An example of the parameter space of allowed orthogonal transformations. Only the branch of the hyperboloid which contains the origin must be considered.

It is easy to see how this counting is consistent with the intuition that changing one of the SCs $\lambda_1, \dots, \lambda_d$ of $\hat{\rho}$ brings this operator out of the equivalence class $\mathfrak{S}_{\hat{\rho}}$. Indeed, subtracting the number of the SCs from the number of dimensions— $(d^2 - 1) - d = d^2 - d - 1$ —we obtain the dimensionality of a typical orbit. For example, take the case of 2-qubits: $N_A = N_B = 2$. We have $d = 4$ and $d^2 - 1 = 15$; hence, the manifold $\mathfrak{S}_{\hat{\rho}}$, for a typical bipartite state $\hat{\rho} \in \mathcal{D}(\mathcal{H})$, is $(15 - 4 = 11)$ -dimensional.

If $\hat{\rho} \in \mathcal{D}(\mathcal{H})$ is a non-typical state, the dimension of the manifold $\mathfrak{S}_{\hat{\rho}}$ is smaller than $d^2 - d - 1$. In fact, in the case where the d SCs of $\hat{\rho}$ cluster into subsets of m_1, \dots, m_h identical values—by means of an argument analogous to that adopted in [24]—one can check that there is a ‘local stabilizer subgroup’ isomorphic to $SO(m_1) \times \dots \times SO(m_h)$; therefore, in this case, $\mathfrak{S}_{\hat{\rho}}$ is locally diffeomorphic to

$$\frac{SO(d) \times SO(d)/SO(2)}{SO(m_1) \times \dots \times SO(m_h)}. \tag{31}$$

Then, the dimension $d_{\hat{\rho}}$ of $\mathfrak{S}_{\hat{\rho}}$ is given, in general, by

$$d_{\hat{\rho}} = d(d - 1) - 1 - \sum_{k=1}^h \frac{m_k(m_k - 1)}{2}. \tag{32}$$

In order to make the above argument *rigorous*, one should actually *prove* that the Schmidt equivalence classes are actually differentiable manifolds. In that case, our previous argument would provide the correct dimension of such manifolds. As we learn from mathematicians [25], a standard tool for characterizing a subset of a differentiable manifold (like the manifold of Hermitian operators in \mathcal{H}) as a submanifold is the study of the (possible) Lie groups acting transitively on the given subset and of the associated stabilizer subgroups. Therefore, suitably improving the analysis of subsection 3.1 may allow us to achieve such a remarkable result.

4. Entanglement and symmetric polynomials in the Schmidt coefficients

We will now consider the role played by Schmidt coefficients in the characterization of entanglement. Our starting point will be the realignment criterion (RC). It is natural to wonder if the *whole set* of the SCs of a bipartite state may allow a stronger characterization of entanglement with respect to the RC.

As we have seen, the RC, like other separability criteria, is based on the evaluation of a single functional in terms of which a necessary condition for separability can be stated. In the case of the RC, this functional coincides with the sum of the Schmidt coefficients. On the other hand, the evaluation of a single functional might not be sufficient to completely determine the presence of entanglement [22] (from a more general point of view, we may say, to characterize classical and quantum correlations). In particular, as the RC is only a necessary condition for separability, one is led to consider additional functionals in order to gain information about the presence of entanglement.

Here we propose to consider the *symmetric polynomials* in the Schmidt coefficients, namely

$$\begin{aligned}
 M^{[1]} &= \sum_{k=1}^d \lambda_k \\
 M^{[2]} &= \sum_{h \neq k=1}^d \lambda_h \lambda_k \\
 &\dots \\
 M^{[l]} &= \sum_{\{i_1, i_2, \dots, i_l\}} \lambda_{i_1} \lambda_{i_2} \dots \lambda_{i_l} \\
 &\dots \\
 M^{[d]} &= \prod_{k=1}^d \lambda_k.
 \end{aligned}
 \tag{33}$$

Note that the RC involves the symmetric polynomial of degree 1.

A naive argument says that if the sum of the Schmidt coefficients is equal to S , their product is upper bounded by $(S/d)^d$. Hence, we have the following condition for a separable density matrix ρ :

$$\hat{\rho} \text{ separable} \Rightarrow M^{[d]} \leq \left(\frac{1}{d}\right)^d,
 \tag{34}$$

which obviously defines a weaker separability criterion. Analogously, one can consider the symmetric polynomial of degree l and obtain the following necessary conditions for separability:

$$\hat{\rho} \text{ separable} \Rightarrow M^{[l]} \leq y_l(d) = \binom{d}{l} \left(\frac{1}{d}\right)^l.
 \tag{35}$$

In particular, if $\hat{\rho}$ has Schmidt rank R , we can write the conditions

$$M^{[l]} \leq \binom{R}{l} \left(\frac{1}{R}\right)^l
 \tag{36}$$

for $l \leq R$, while $M^{[l]} = 0$ for $l > R$.

It is worth noting that the symmetric polynomials $\{M^{[l]}\}$ are in one-to-one correspondence with the Schmidt coefficients $\{\lambda_k\}$. Inequalities (35) are consequences of the RC. Hence, as separability criteria, they are weaker than the parent one. Section 6 will be devoted to the study of possible stronger generalization.

Finally, we note that in the approach followed in [12], which makes use of the associated realigned matrix ρ^R , the symmetric polynomials are the coefficients of the characteristic polynomial:

$$\chi_{\rho^R}(x) = \det(|\rho^R| - x\mathbb{I}) = \sum_{l=1}^d M^{[l]}(|\rho^R|)(-x)^{d-l}, \quad (37)$$

where, with abuse of notation, we indicated with $M^{[l]}(A)$ the principal minor of order l of the matrix A .

5. Quantum states and quantum maps

This section is devoted to the application of the ideas presented in section 4 to the study of quantum channels, i.e. CPT maps. In order to do that, we exploit the well-known correspondence between quantum channels and quantum states (see [14–16]).

Here we consider quantum systems with Hilbert spaces \mathcal{H}_A and \mathcal{H}_B , the set of states in the composite system $\mathcal{D}(\mathcal{H}_A \otimes \mathcal{H}_B)$ and the set of CPT maps from system B to system A, which is denoted by $\text{CPT}(\mathcal{H}_B, \mathcal{H}_A)$.

Given a CPT map $\hat{\mathcal{E}} \in \text{CPT}(\mathcal{H}_B, \mathcal{H}_A)$, one can associate a state $\hat{\rho} \in \mathcal{D}(\mathcal{H}_A \otimes \mathcal{H}_B)$ in the following *canonical* way:

$$\hat{\mathcal{E}} \longrightarrow \hat{\rho} = (\hat{\mathcal{E}} \otimes \hat{\mathcal{I}})(\hat{\beta}), \quad (38)$$

where $\hat{\beta} = |\phi\rangle\langle\phi| \in \mathcal{D}(\mathcal{H}_B \otimes \mathcal{H}_B)$ denotes a maximally entangled state, for instance $|\phi\rangle = \frac{1}{\sqrt{N_B}} \sum_{\alpha=1}^{N_B} |\alpha\rangle|\alpha\rangle$, and $\hat{\mathcal{I}}$ is the identical map in the system B.

A CPT map $\hat{\mathcal{E}}$ is said to be entanglement breaking (EB) if $\hat{\mathcal{E}} \otimes \hat{\mathcal{I}}$ maps any state into a separable one [26]. One can show that a CPT is EB if and only if the map $\hat{\mathcal{E}} \otimes \hat{\mathcal{I}}$ transforms a maximally entangled state into a separable one. It follows that the CPT map is EB if and only if the canonically associated state is separable.

One can select a local orthogonal basis $\hat{F}_{(mn)}^A = |m\rangle\langle n|$ and $\hat{F}_{(\mu\nu)}^B = |\mu\rangle\langle\nu|$ and write the matrix elements of the CPT map in that basis as follows:

$$\mathcal{E}_{(mn)(\mu\nu)} = \text{tr}(\hat{F}_{(mn)}^A \hat{\mathcal{E}}(\hat{F}_{(\mu\nu)}^B)). \quad (39)$$

It is easy to check that, with the canonical association (38), the matrix representation of the state $\hat{\rho}$ and the map $\hat{\mathcal{E}}$ are related in the following way:

$$\rho_{(i\alpha)(j\beta)} = \frac{1}{N_B} \mathcal{E}_{(ij)(\alpha\beta)}. \quad (40)$$

Following the definition in [12], it is immediate to recognize that, apart from the normalization factor $1/N_B$, the matrix expression of $\hat{\mathcal{E}}$ is identical to the realigned matrix ρ^R (see equation (9)). Identifying the CPT map with the realigned matrix of the corresponding density matrix, one can consider the characteristic polynomial

$$P_{\mathcal{E}}(x) = \det(|\mathcal{E}| - x\mathbb{I}), \quad (41)$$

where $|\mathcal{E}| = \sqrt{\mathcal{E}^\dagger \mathcal{E}}$ and $\mathcal{E} \equiv \mathcal{E}_{(ij)(\alpha\beta)}$. To fix the ideas, let us consider the case in which \mathcal{E} has full rank. One obtains from (34) the following necessary condition for $\hat{\mathcal{E}}$ to be entanglement breaking:

$$\det(|\mathcal{E}|) \leq \left(\frac{N_B}{d}\right)^d. \quad (42)$$

The determinant of quantum channels was also considered in [27], in which some of its properties were presented and discussed in the context of factorization of CPT maps. The

present result relates a geometric property of the map, such as the rate of contraction of volume (which is equal to $\det(|\mathcal{E}|)$), to the property of being entanglement breaking. Analogously, from (36), if the matrix $\mathcal{E}_{(ij)(\alpha\beta)}$ has rank R , we can write the following necessary conditions for $\hat{\mathcal{E}}$ to be entanglement breaking:

$$M^{[l]}(|\mathcal{E}|) \leq \binom{R}{l} \left(\frac{N_B}{R}\right)^l \quad (43)$$

for $l = 1, \dots, R$.

6. Beyond the realignment criterion

In section 4, we introduced a family of separability conditions which are weaker than (or equivalent to) the RC. In this section, we argue about the possibility of extending the family of separability criteria defined in (35) in order to write criteria which are independent of the RC. As a first step in this direction, we may ask whether it is possible to find strict upper bounds $x_l(d, D)$ such that

$$\hat{\rho} \text{ separable} \Rightarrow M^{[l]} \leq x_l(d, D) < \binom{d}{l} \left(\frac{1}{d}\right)^l. \quad (44)$$

However, in the following we consider a weaker statement⁹, namely

$$M^{[1]} \leq 1 \Rightarrow M^{[l]} \leq \tilde{x}_l(d, D) < \binom{d}{l} \left(\frac{1}{d}\right)^l, \quad (45)$$

which establishes a strict upper bound for the functionals $M^{[l]}$ over the set of states satisfying the RC.

The following proposition holds true.

Proposition 4. *The upper bounds $\tilde{x}_l(d, D)$ in equation (45) exist for $D < d^3$.*

Proof. The proposition is proven by contradiction. Let us suppose the existence of a density matrix ρ_0 such that $M^{[1]} \leq 1$ and the inequalities in (35) are saturated. This implies that the density matrix has the maximum rank, $R = d$, and all its SCs are equal to d^{-1} . Hence, referring to the singular value decomposition in equation (10), we can write the Schmidt decomposition of the density matrix in the following way:

$$\rho_{0(\alpha i)(\beta j)} = \frac{1}{d} \sum_{k,l=1}^d u_{(\alpha\beta)(kl)} v^*_{(kl)(ij)}, \quad (46)$$

where $v_{(ij)(i'j')}$ and $u_{(\alpha\beta)(\alpha'\beta')}$ are respectively the entries of the unitary matrices \mathcal{V} and \mathcal{U} (see equation (10)), with dimensions N_A^2 and N_B^2 . We introduce the following notation:

$$u_{(\alpha\beta)(kl)} v^*_{(kl)(ij)} = \langle \hat{v}_{ij}, \hat{u}_{\alpha\beta} \rangle, \quad (47)$$

where $\hat{u}_{\alpha\beta}$ and \hat{v}_{ij} indicate the vectors respectively defined as the rows and the columns of the matrices \mathcal{U} and \mathcal{V} . We have

$$\text{tr}(\rho_0) = \frac{1}{d^2} \sum_{i,\alpha} \langle \hat{v}_{ii}, \hat{u}_{\alpha\alpha} \rangle = \frac{1}{d^2} \left\langle \sum_{i=1}^{N_A} \hat{v}_{ii}, \sum_{\alpha=1}^{N_B} \hat{u}_{\alpha\alpha} \right\rangle, \quad (48)$$

⁹ Note that (45) is weaker as a separability criterion, while it is stronger in the sense that (45) implies (44). In particular, $x_l(d, D) \leq \tilde{x}_l(d, D)$

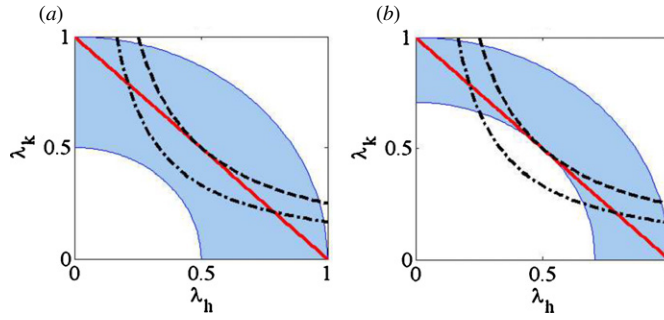


Figure 2. A pictorial representation of the set of the equivalence classes, for the generic case $d \neq D$ (a) and for the degenerate one $d = D$ (b). The Schmidt coefficients are represented along the axes. States are contained in the colored region, which fulfills the constraints on the purity (7). The region on the bottom left of the solid line fulfill the RC (hence separable states are contained in this region). The region on the bottom left of the dashed line contains the states that fulfill one of the *naive* inequalities (35) for some $l > 1$. Finally, the region on the bottom left of the dot-dashed line contains the states that fulfill the proposed criterion *RCl*. Note that the RC (or RC1) bounds separable states with a hyperplane, while the higher order *RCl*, for $l > 1$, bounds the set of separable states with nonlinear hypersurfaces. Note that the *RCs* can in principle allow a finer characterization of entangled states.

and we obtain

$$\text{tr}(\rho_0) = |\text{tr}(\rho_0)| = \frac{|\langle \sum_i \hat{v}_{ii}, \sum_\alpha \hat{u}_{\alpha\alpha} \rangle|}{d^2} \leq \frac{|\sum_i \hat{v}_{ii}| |\sum_\alpha \hat{u}_{\alpha\alpha}|}{d^2} = \frac{\sqrt{N_A N_B}}{d^2} \quad (49)$$

(the last equality holds true since $\hat{u}_{\alpha\alpha}$ and \hat{v}_{ii} are two systems of orthonormal vectors) which, for $D < d^2$, is in contradiction with the hypothesis that ρ_0 has unit trace. Since the set of states satisfying the RC is compact and the symmetric polynomials $M^{[l]}$ are continuous functionals, the lower upper bounds $\tilde{x}_l(d, D)$ do exist. \square

In the following, we indicate with *RCl* the suggested criterion

$$\hat{\rho} \text{ separable} \Rightarrow M^{[l]} \leq x_l(d, D). \quad (50)$$

Figure 2 shows a pictorial representation of the relation between the parent RC, the weaker criteria (35) and the proposed extensions *RCl*. As the figure suggests, the *RCl* can in principle be used, with respect to the information given by the RC, as refinements of the knowledge about the region of separable states.

It is worth noting, however, that there are still two main open problems:

- (i) the actual values of the upper bounds $x_l(d, D)$ (as well as $\tilde{x}_l(d, D)$) are still undetermined,
- (ii) it is not clear whether the criteria *RCl* are independent of the RC, i.e. if there are entangled states such that RC is not violated while *RCl* is for some $l > 1$. That is equivalent to the strict inequality $x_l(d, D) < \tilde{x}_l(d, D)$.

In the following section, we face these problems with a numerical approach. We are going to restrict our discussion to the case of lower dimensional systems, namely $\mathcal{H}_A \otimes \mathcal{H}_B = \mathbb{C}^2 \otimes \mathbb{C}^2, \mathbb{C}^2 \otimes \mathbb{C}^3$. For these cases, one can exploit the fact that the PPT (positive partial transpose) criterion [8] is necessary and sufficient for separability.

7. Examples for low dimensional systems

In analogy with what can be done for the RC (see, for instance, [19]), one could determine the value of the strict upper bounds $x_l(d, D)$ by convex linearity starting from the properties

Table 1. For a qubit–qubit system, the table shows the upper bounds on the sums of the symmetric polynomials $M^{[l]}$. $y_l(4)$ denotes the naive bounds (35). $\tilde{x}_l(4, 4)$ denotes the numerically estimated strict bounds over the states satisfying the RC (45). Finally, $x_l(4, 4)$ indicates the numerically estimated strict bounds over the set of separable states (44). Note that in this case, we found $x_l(d, D) = \tilde{x}_l(d, D)$ suggesting that the criteria RC1 *cannot be* independent of the RC.

	$l = 1$	$l = 2$	$l = 3$	$l = 4$
$y_l(4)$	1	0.3750	0.06250	0.003906
$\tilde{x}_l(4, 4)$	1	0.3333	0.04630	0.00231
$x_l(4, 4)$	1	0.3333	0.04630	0.00231

Table 2. For a qubit–qutrit system, the table shows the upper bounds on the sums of the symmetric polynomials $M^{[l]}$. $y_l(4)$ denotes the naive bounds (35). $\tilde{x}_l(4, 9)$ denotes the numerically estimated strict bounds over the states satisfying the RC (45). Finally, $x_l(4, 9)$ indicates the numerically estimated strict bounds over the set of separable states (44). Note that in this case, we found $x_l(d, D) < \tilde{x}_l(d, D)$ suggesting that the criteria RC1 *can be* in principle independent of the RC.

	$l = 1$	$l = 2$	$l = 3$	$l = 4$
$y_l(4)$	1	0.3750	0.06250	0.003906
$\tilde{x}_l(4, 9)$	1	0.3583	0.05533	0.003133
$x_l(4, 9)$	1	0.3469	0.05249	0.00291

of pure separable states. Nevertheless, it is worth noting that this can be a rather difficult task since the symmetric polynomials $M^{[l]}$ are not easy to manipulate with respect to the convex structure of the set of separable states. For this reason, in the following we present a numerical analysis which allows us to present some interesting results.

For a preliminary analysis of the potentialities of the proposed family of criteria, they have been numerically tested in the case of a bipartite qubit–qubit and qubit–qutrit system. A numerical search of the upper bounds can be done by exploiting the PPT criterion [8]. The constraints $\rho \geq 0$ and $\rho^{T_A} \geq 0$, where T_A indicates the partial transposition, are known to be necessary and sufficient to characterize separable states in the low dimensional cases. Hence, the determination of the lower upper bounds $x_l(d, D)$ reduces to a problem of constrained maximization.

We have numerically estimated the maxima of the functions $M^{[l]}$ over separable states (hence determining estimates for $x_l(d, D)$) and over the set of states satisfying the RC (hence estimating the upper bounds $\tilde{x}_l(d, D)$). For a qubit–qubit system ($d = D = 4$), the results are shown in table 1 together with *naive* bounds in (35). The analogous quantities are shown in table 2 for the case of a qubit–qutrit system ($d = 4, D = 9$). In the latter case, we found $x_l(d, D) < \tilde{x}_l(d, D)$ suggesting that the criteria RC1 *can be in principle* stronger than the RC. Figures 3 and 4 show the maxima of the functionals $M^{[l]}$ for $l = 2, 3, 4$, computed for fixed values of $M^{[1]}$, respectively for qubit–qubit and qubit–qutrit systems, as functions of the value of $M^{[1]}$. The maxima are computed over generic states and over separable states. In the case of a qubit–qutrit system, the plots show the region in which the criteria RC1 can in principle be stronger than—or independent to—the RC.

To conclude this section, we consider the case of 2-qubit (generalized) Werner states of the form

$$\hat{\rho}_p = p|\phi\rangle\langle\phi| + (1 - p)\mathbb{1}/4, \tag{51}$$

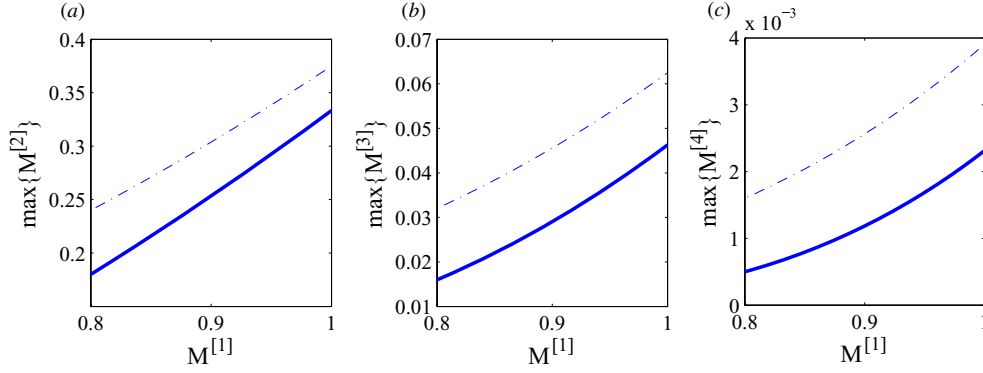


Figure 3. Numerically estimated upper bounds of the symmetric polynomials $M^{[2]}$ (a), $M^{[3]}$ (b) and $M^{[4]}$ (c), as functions of the value of $M^{[1]}$ for a qubit-qubit system: naive upper bounds (dash-dotted line) and numerically estimated upper bounds over the set of separable states (solid line) which coincide with upper bounds over the set of all states (separable and entangled).

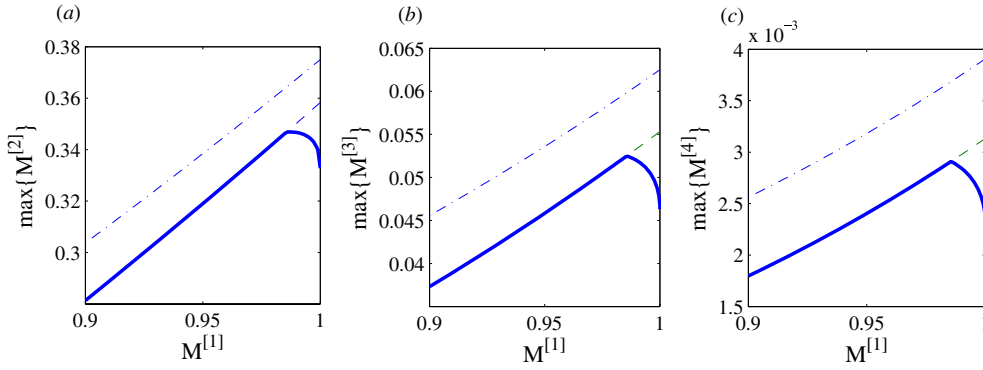


Figure 4. Numerically estimated upper bounds of the symmetric polynomials $M^{[2]}$ (a), $M^{[3]}$ (b) and $M^{[4]}$ (c), as functions of the value of $M^{[1]}$ for a qubit-qutrit system: naive upper bounds (dash-dotted line) and numerically estimated upper bounds over the set of separable states (solid line) and over the set of all states (dashed line). Note the presence of a region in which the functionals have a lower upper bound over the set of separable states.

for $p \in [0, 1]$, where $|\phi\rangle$ indicates a maximally entangled pure state. The Schmidt coefficients of the state (51) are easily calculated to be $\{1/2, p/2, p/2, p/2\}$, yielding

$$\begin{aligned}
 M^{[1]} &= (1 + 3p)/2 \\
 M^{[2]} &= 3(p + p^2)/4 \\
 M^{[3]} &= (3p^2 + p^3)/8 \\
 M^{[4]} &= p^3/16.
 \end{aligned}
 \tag{52}$$

Note that the symmetric polynomials are monotonically increasing functions of the state parameter p . It was shown in [28] that the realignment criterion is necessary and sufficient for this family of states (indeed it is so for all the two-qubit states with *maximally disordered subsystems*). The state in (51) is known to be separable for $p \in [0, 1/3]$ and entangled otherwise. We can compute the maximal value of the symmetric polynomials $M^{[l]}$ over the

separable states in that family. These maxima are reached in correspondence of the value $p = 1/3$, hence yielding

$$\hat{\rho}_p \text{ separable} \Rightarrow \begin{aligned} M^{[1]} &\leq 1 \\ M^{[2]} &\leq 1/3 \\ M^{[3]} &\leq 5/108 \simeq 0.04630 \\ M^{[4]} &\leq 1/432 \simeq 0.00231. \end{aligned} \quad (53)$$

Note that the values in (53) computed for 2-qubit generalized Werner states saturates the numerical estimated upper bounds reported in table 1.

8. Conclusions

The main goal of the present paper is to bring attention to the Schmidt coefficients of a bipartite density operator and to their role for entanglement detection. The notion of Schmidt equivalence classes has been introduced and a preliminary characterization of such classes has been provided.

We have presented a family of separability criteria, written in terms of the Schmidt coefficients, which are derived from the realignment criterion. These separability criteria are a consequence of the fact that the symmetric polynomials in the Schmidt coefficients are upper bounded on the set of separable states.

The application of that family of criteria to the study of quantum channels determines a relation between a physical feature, such as the preservation of entanglement under the action of the channel, and a geometrical quantity, such as the determinant—or the sum of principal minors of order l —of a corresponding matrix.

We conjecture—also with support of numerical examples—that a strengthened version of these criteria, independent of the realignment criterion, exists. In particular, we have given numerical examples for the case of the qubit–qutrit system. These numerical results are of course not sufficient for achieving independent separability criteria. However, they can open the way to an analytical determination of stricter upper bounds on the symmetric polynomials, and this may eventually lead to new separability criteria.

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