Computing Partial Transposes and Related Entanglement Functions

Jonas Maziero¹,²

Abstract The partial transpose (PT) is an important function for entanglement testing and quantification and also for the study of geometrical aspects of the quantum state space. In this article, considering general bipartite and multipartite discrete systems, explicit formulas ready for the numerical implementation of the PT and of related entanglement functions are presented and the Fortran code produced for that purpose is described. What is more, we obtain an analytical expression for the Hilbert-Schmidt entanglement of two-qudit systems and for the associated closest separable state. In contrast to previous works on this matter, we only use the properties of the PT, not applying Lagrange multipliers.

Keywords Quantum information · Entanglement · Partial transpose · Hilbert-Schmidt

1 Introduction

The correlations among the constituent particles of physical systems are of central importance for science [1]. In quantum information science (QIS) [2–4], there are several types of correlations [5–10]. Entanglement is one kind of quantum correlation, one which is widely recognized as being the fuel for the more efficient realization of several information manipulation tasks [11–14].

Entanglement quantifiers (EQs) are functions which are null only for states that can be prepared using local quantum operations and classical communication (the separable states) and which do not increase under such kind of transformation [6]. Nowadays, there are several proposals of EQs in the literature [15, 16]. One common feature of these quantities is that they are very hard to compute analytically in the general case [17, 18]. This motivates the consideration of entanglement functions (EFs), which possess some, but not all, of the properties one may request for a good EQ. The partial transposition (PT) provides the most famous and tractable separability criterion and EFs [19–22] and is relevant for a myriad of investigations in QIS.

In this article, we present a detailed description of the partial transposition map and of related EFs. In addition to that, we obtain an analytical formula for the Hilbert-Schmidt entanglement (HSE) of two-qudit¹ systems and for the associated nearest separable state. We also describe the Fortran code² produced to compute all the functions regarded here.

The remainder of this article is structured as follows. In the next section, we start introducing the transposition map (Section 2.1). In the sequence, we use it to discuss the partial transposition operation in the contexts of bipartite (Section 2.2) and of multipartite discrete systems (Section 2.3). In Section 2.4, we recall Peres’ separability criterion and some related EFs. The analytical calculation of the HSE

¹A qudit is a d-level quantum system.
²The Fortran code used in this article is part of the Fortran Library for Quantum Information Science and can be accessed freely in: https://github.com/jonasmaziero/LibForQ. For the description of some related tools, see Refs. [23–27].
is addressed in Section 3. Some final remarks and open questions are included in Section 4.

2 Partial Transposes and Related Entanglement Functions

2.1 The Transposition Map

Before introducing the partial transposition map, let us discuss the transposition operation. Let \( \rho \) be a general linear operator defined on the Hilbert space \( \mathcal{H} \). Let \( \{|j\rangle\}_{j=1}^d \) be an orthonormal basis for \( \mathcal{H} \), with \( d = \dim \mathcal{H} \). Then, we can write the matrix representation: \( \rho = \sum_{j,k=1}^d \langle j | \rho | k \rangle | j \rangle \langle k | \).

In the sequence, \( |j\rangle \) is assumed to be the standard computational basis in \( \mathcal{H} \). By definition, the transposition map \( T \) is linear and acts on the computational basis as follows:

\[
T \left( \sum_{j,k} c_{jk} | j \rangle \langle k | \right) := \sum_{j,k} c_{jk} T(| j \rangle \langle k |) := \sum_{j,k} c_{jk} | k \rangle \langle j |,
\]

with \( c_{jk} \in \mathbb{C} \). Thus,

\[
T(\rho) = T \left( \sum_{j,k=1}^d \langle j | \rho | k \rangle | j \rangle \langle k | \right) = \sum_{j,k=1}^d \langle j | \rho | k \rangle T(| j \rangle \langle k |) = \sum_{j,k=1}^d \langle k | (T(\rho)) j \rangle \langle j | \langle k | \langle j | \langle k | \rangle .
\]

Hence, the familiar relation between the matrix elements of \( \rho \) and of \( T(\rho) \) is obtained, i.e., \( \langle k | (T(\rho)) j \rangle = \langle j | \rho | k \rangle \).

We remark that the definition in (1) is base dependent. So, for another basis \( \{|\beta_j\rangle\} := U|j\rangle \), with \( UU^\dagger = I \) (\( I \) is the identity operator in \( \mathcal{H} \)), the last simple relation would be valid only for the “rotated” versions of \( T(\rho) \) and of \( \rho \), i.e., \( \langle \beta_j | (U T(\rho) U^\dagger) | \beta_k \rangle = \langle \beta_j | U \rho U^\dagger | \beta_k \rangle \).

Let us end this subsection observing that once we have \( det(T(\rho - \lambda I)) = det(\rho - \lambda I) \) [28] and \( T(\rho - \lambda I) = T(\rho) - \lambda \mathbb{1} \), then the eigenvalues of \( T(\rho) \) are the same as those of \( \rho \).

An immediate consequence of this result is that their traces are also equal, i.e., \( \text{Tr}(T(\rho)) = \text{Tr}(\rho) \). Thus, if \( \rho \) is a density operator, i.e., it is positive semidefinite \( (\rho \geq 0) \) and has unit trace \( (\text{Tr}(\rho) = 1) \), then \( T(\rho) \) is also a valid density operator. This fact is key for Peres’ separability criterion, which shall be recalled in Section 2.4.

2.2 Partial Transposition for Bipartitions

In what follows, we shall introduce the partial transposition (PT) operation and obtain expressions which are useful for its numerical implementation. Let us start regarding a bipartition of \( \mathcal{H} \), \( \mathcal{H}_a \otimes \mathcal{H}_b \), with dimensions \( d_s := \dim \mathcal{H}_s \) for \( s = a, b \). Any computational base state in \( \mathcal{H} \) can be cast in terms of the local computational bases as follows:

\[
\langle j | = | j_a \rangle \otimes | j_b \rangle = | (j_a - 1) d_b + j_b \rangle, \quad \text{with } | j_s \rangle \text{ being the computational basis in } \mathcal{H}_s.
\]

Hereafter, we assume the matrix elements of \( \rho \) in the product-local computational basis \( | j_a j_b \rangle \) are known:

\[
\rho = \sum_{j_a,k_a=1}^{d_a} \sum_{j_b,k_b=1}^{d_b} | j_a j_b | \rho | k_a k_b \rangle \langle k_a | \otimes | j_b \rangle \langle k_b | .
\]

With this, we are ready to introduce the, also linear, partial transposition operator, which, when taken over subsystem \( a \), is defined by \( T_a \equiv T \otimes id \), with \( id \) being the identity map, i.e., \( id(X) = X \) for all linear operator \( X \) on \( \mathcal{H}_s \). So,

\[
T_a(\rho) = T \otimes id(\rho) = \sum_{j_a,k_a=1}^{d_a} \sum_{j_b,k_b=1}^{d_b} | j_a j_b | \rho | k_a k_b \rangle T(| j_a \rangle \langle k_a |) \otimes id(| j_b \rangle \langle k_b |)
\]

\[
= \sum_{j_a,k_a=1}^{d_a} \sum_{j_b,k_b=1}^{d_b} (| j_a j_b \rangle \rho | k_a k_b \rangle) | k_a \rangle \otimes | j_a \rangle \langle j_a \langle k_a | \langle k_a \langle j_a | \langle j_a \langle k_a |, \quad (4)
\]

In an analogous manner, when applied to subsystem \( b \) the partial transpose leads to

\[
T_b(\rho) = id(\rho) \otimes T(\rho) = \sum_{j_a,k_a=1}^{d_a} \sum_{j_b,k_b=1}^{d_b} | j_a j_b | \rho | k_a k_b \rangle T(| j_b \rangle \langle k_b |) \otimes | j_a \rangle \langle j_a \langle k_a | \langle k_a \langle j_a | \langle j_a \langle k_a |, \quad (5)
\]

In terms of matrix elements, we get

\[
| k_a k_b | T_a(\rho) | j_a j_b \rangle = | k_a j_b | T_a(\rho) | j_a k_b \rangle, \quad (6)
\]

\[
| k_a k_b | T_b(\rho) | j_a j_b \rangle = | j_a j_b | T_b(\rho) | k_a k_b \rangle. \quad (7)
\]

For numerical calculations, with the notation \( T^a \equiv T_a(\rho) \), we just set

\[
\rho^a T^a ((k_a - 1) d_b + j_b, (j_a - 1) d_b + k_a) = \rho(\alpha, \beta), \quad (8)
\]

\[
\rho^b T^b ((j_a - 1) d_b + k_b, (k_a - 1) d_b + j_a) = \rho(\alpha, \beta), \quad (9)
\]

with \( \alpha = (j_a - 1) d_b + j_b \) and \( \beta = (k_a - 1) d_b + k_b \) for all \( j_s, k_s = 1, \ldots , d_s \). The PT for multipartite systems is returned by the subroutines partial transpose_\_s(d_a, d_b, \rho, T_s(\rho)), with \( s = a, b \).

2.3 Partial Transposition for Multipartitions

Let us consider a density operator \( \rho \) in the Hilbert space \( \mathcal{H}_a \otimes \mathcal{H}_b \otimes \mathcal{H}_c \):

\[
\rho = \sum_{j_a,j_b,j_c} | j_a j_b j_c \rangle \rho | k_a k_b k_c \rangle \langle k_a k_b k_c |, \quad (10)
\]
with |j⟩ and |k⟩ being the computational base for \(\mathcal{H}_s\) (\(s = a, b, c\)) and the sum is made over all \(j\)'s and \(k\)'s, which run from 1 to \(d_s\). Analogously to the previous calculations, we apply the definition for the partial transposition over the inner subsystem,

\[
T_b(\rho) = \text{id} \otimes T \otimes \text{id}(\rho),
\]

(11)

to see that

\[
\langle j a k b j c | \tilde{\rho}^b | k a j b k c \rangle = \langle j a j b j c | \rho | k a j b k c \rangle.
\]

(12)

For numerical calculations, we use

\[
|x y z \rangle = (x - 1) d_b d_c + (y - 1) d_c + z
\]

(13)

to directly relate the matrix elements of \(\tilde{\rho}^b\) and of \(\rho\) in the global computational basis. The subroutine provided to compute the inner partial transposition map is \text{partial\_transpose\_3}\((d_a, d_b, d_c, \rho, T_b(\rho))\).

Now, given any multipartite state space \(\mathcal{H}_s \otimes \mathcal{H}_{s+1} \otimes \cdots \otimes \mathcal{H}_{s'-1} \otimes \mathcal{H}_{s'} \otimes \mathcal{H}_{s'+1} \otimes \cdots\), we notice that the partial transposition over the parties \(s\) and \(s'\) can be composed as follows:

\[
T_{ss'}(\rho) \equiv T_s \otimes T_{s'}(\rho).
\]

(14)

With this, the partial transposition over an arbitrary number of subsystems (with arbitrary finite dimensions) can be computed through the composition of the left (4), right (5), and inner (11) partial transpositions described above. We also provide a subroutine, \text{partial\_transpose}\((d, \rho, T_p(\rho), nss, \text{di}, \text{ssys})\), which returns the partial transposition in the general case. Regarding the arguments therein, \(nss\) is the number of subsystems, \(d\) is the total dimension, \(\text{di}\) is a vector containing the dimensions of the subsystems, and \(\text{ssys}\) is a vector with components equal to 0 or 1 for those subsystems over which the PT shall or shall not be applied, respectively. The dimension of \(\text{di}\) and \(\text{ssys}\) is equal to \(nss\).

### 2.4 Peres’ Criterion and Entanglement Negativity

In 1996, A. Peres [19] made the insightful observation that if a state is separable, i.e., if it can be cast as

\[
\sigma = \sum_j p_j \sigma^a_j \otimes \sigma^b_j
\]

(15)

with \(p_j\) being a probability distribution and \(\sigma^a_j\) being valid density operators for the subsystem \(s\), then its PT,

\[
\tilde{\sigma} = T_b(\sigma) = \sum_j p_j \sigma^a_j \otimes T(\sigma^b_j) = \sum_j p_j \sigma^a_j \otimes \tilde{\sigma}^b_j,
\]

(16)

is also a valid (and separable) state, because \(\tilde{\sigma}^b_j = T(\sigma^b_j)\) are valid density operators (see Section 2.1) and the convex combination of positive semidefinite matrices is also a positive semidefinite matrix [29]. So, \(\tilde{\sigma}\) is a positive semidefinite matrix. Therefore, if the PT of a generic density matrix \(\rho\) is negative, then this state has to be entangled. This fact indicates that the absolute value of the negative eigenvalues of the PT of a state would be a possible entanglement quantifier. Actually, the entanglement negativity [21],

\[
E_n(\rho) = 2^{-1}(||T_b(\rho)||_{tr} - 1),
\]

(17)

is an entanglement function [6]. In the last equation, \(||X||_{tr} := \text{Tr} \sqrt{X^\dagger X}\) is the trace norm. The Fortran function negativity\((d, T_p(\rho))\) returns \(E_n\) once provided the PT of \(\rho\) and its dimension. In order to obtain the logarithmic negativity [21, 22],

\[
E_{ln}(\rho) := \log_2(2E_n(\rho) + 1),
\]

(18)

just change the name of the function to \text{log\_negativity}.

It was shown later that the Peres’ condition is necessary and sufficient only for systems with dimension up to six [20]. For larger dimensions, there may exist entangled states with positive PT [30]. As a matter of fact, there is no known analytically computable entanglement measure for general states [6]. In the next section, we will consider another entanglement function which is not an entanglement quantifier, but which may be a useful analytical tool in several circumstances.

### 3 Analytical Formula for the Hilbert-Schmidt Entanglement

In this section, we shall obtain an analytical expression for the Hilbert-Schmidt entanglement (HSE) and for the associated closest separable state. Our approach is motivated by Ref. [31], but here we do not use the Lagrange multipliers. With this, our calculations gain in clarity and avoid possible drawbacks of that method [32].

As mentioned in Section 1, computing entanglement quantifiers (EQs) for general states is a very complex task. So, one of the motivations for studying entanglement functions, such as the HSE, is that the insights gained while doing that can shed some light on how we can effectively tackle the complicated optimizations problems involved in the calculation of EQs. On the other hand, the consideration of the HSE, in addition to the entanglement negativity (EN), is appealing because of the geometrical nature of the first. For instance, contrary to the EN, when computing the HSE we can get as a byproduct the closest separable state. And this kind of information can be useful, for example, for studying the geometrical aspects of the quantum state space and as an initial ansatz for the calculation of EQs induced by other, more faithful, distinguishability measures.

Let us recall that the Hilbert-Schmidt (HS) norm of matrix \(A\) is defined and given by

\[
||A||_s := \sqrt{\text{Tr}(A^\dagger A)} = \sqrt{\sum_{j,k} |\langle j|A|k\rangle|^2}.
\]

(19)
The HSE of state $\rho$ is then defined, using the HS distance, as
\[
E_{hs}(\rho) := \min_{\sigma} ||\rho - \sigma||_{hs},
\] (20)
with the minimization running over all separable states.

Since the HS norm is invariant under unitary transformations, i.e., it is base independent, we can use the computational basis to verify that the HS distance does not change under taking the PT of its arguments:
\[
||T_b(\rho - \sigma)||_{hs}^2 = \sum_{j_a, k_a=1}^{d_a} \sum_{j_b, k_b=1}^{d_b} |\langle j_a j_b \rho | k_a k_b \rangle|^2 - |\langle j_a j_b \sigma | k_a k_b \rangle|^2
\]
\[
= \sum_{j_a, k_a=1}^{d_a} \sum_{j_b, k_b=1}^{d_b} |\langle j_a j_b T_b(\rho)| k_a k_b \rangle|^2 - |\langle j_a j_b T_b(\sigma)| k_a k_b \rangle|^2
\]
\[
= \sum_{j_a, k_a=1}^{d_a} \sum_{j_b, k_b=1}^{d_b} |\langle j_a j_b | T_b(\rho)| k_a k_b \rangle|^2 - |\langle j_a j_b | T_b(\sigma)| k_a k_b \rangle|^2
\]
\[
= \sum_{j_a, k_a=1}^{d_a} \sum_{j_b, k_b=1}^{d_b} |\langle j_a j_b (\rho - \sigma)| k_a k_b \rangle|^2
\]
\[
= ||\rho - \sigma||_{hs}^2.
\] (21)
Thus, using this equivalence, we can write
\[
E_{hs}(\rho) = \min_{\sigma} ||T_b(\rho) - T_b(\sigma)||_{hs} =: \min_{\sigma} ||\rho - \sigma||_{hs}.
\] (22)

In the sequence, we use once more the invariance under unitaries of the HS norm to see that:
\[
E_{hs}(\rho) = \min_{\sigma} ||U(\rho T_b - \sigma) U^\dagger||_{hs} =: \min_{\sigma} ||D - \sigma||_{hs},
\] (23)
where, considering that $T_b(\rho)$ is an Hermitian operator:
\[
(T_b(\rho))^\dagger = \sum_{j_a, k_a=1}^{d_a} \sum_{j_b, k_b=1}^{d_b} \langle j_a j_b | \rho | k_a k_b \rangle^\dagger \langle j_a j_b \rangle \langle k_a k_b \rangle
\]
\[
= \sum_{j_a, k_a=1}^{d_a} \sum_{j_b, k_b=1}^{d_b} \langle j_a j_b | \rho | k_a k_b \rangle^\dagger \langle j_a j_b \rangle \langle k_a k_b \rangle
\]
\[
= \sum_{j_a, k_a=1}^{d_a} \sum_{j_b, k_b=1}^{d_b} \langle j_a j_b | \rho | k_a k_b \rangle \langle j_a j_b \rangle \langle k_a k_b \rangle = T_b(\rho),
\] (24)
we assumed that $U$ diagonalizes $\rho T_b$, i.e.,
\[
U \rho T_b U^\dagger = D := \sum_{j=1}^{d} |D_j \rangle \langle D_j |,
\] (25)
with $d = d_a d_b$. Besides we defined the, in principle general and possibly entangled, density operator:
\[
\hat{\zeta} = U \hat{\sigma} U^\dagger.
\] (26)
We remark at this point that once we find the optimal $\zeta$, let us call it $\zeta^\ast$, then, as
\[
T_b(\hat{\sigma}) = T_b(T_b(\sigma)) = \sigma,
\] (27)
we have found also the optimal separable state:
\[
\sigma^\ast = T_b(\hat{\sigma}^\ast) = T_b(U^\dagger \zeta^\ast U).
\] (28)
Following with the calculation of the HSE, we use (23), (25), and (26) to write
\[
E_{hs}(\rho) = \min_{\zeta} \sqrt{\text{Tr}(D - \zeta)^2}
\] (29)
\[
= \min_{\zeta} \sqrt{\sum_{j=1}^{d} (|D_j \rangle \langle D_j |)^2 - \sum_{j=1}^{d} |D_j \rangle \langle D_j |^2}
\]
\[
= \min_{\zeta} \left( \sum_{j,k} (|D_j \rangle \langle D_k | - \langle D_j | \langle D_k |) \right) (|D_k \rangle \langle D_j |)^{1/2}
\]
\[
= \min_{\zeta} \left( \sum_{j,k} (|D_j \rangle \langle D_k | - \langle D_j | \langle D_k |) \right)^{1/2}
\]
\[
= \min_{\zeta} \left( \sum_{j,k} (|D_j \rangle \langle D_k | - \langle D_j | \langle D_k |) \right)^2 + \sum_{j \neq k} \langle D_j | \langle D_k |)^2.
\] (30)
From this last expression, we see that $E_{hs}$ is minimized if $\zeta$ has no coherences in the eigenbasis of $D$, i.e., if
\[
\zeta = \sum_{j=1}^{d} |\zeta_j \rangle \langle D_j |angle |D_j |.
\] (30)
So,
\[
E_{hs}(\rho) = \min_{\{\zeta_j\}_{j=1}^{d}} \sqrt{\sum_{j=1}^{d} (|D_j \rangle \langle D_j | - \langle D_j | \langle D_j |)^2}.
\] (31)
In what follows, it will be useful noticing that, as $\zeta$ is a density operator, we have to have $\zeta_j \geq 0$ and $\text{Tr}(\zeta) = \sum_{j=1}^{d} \zeta_j = 1$. In addition to that, it will be important for our calculations seeing that $T_b(\rho)$ has unit trace:
\[
\text{Tr}(T_b(\rho)) = \sum_{j_a, k_a=1}^{d_a} \sum_{j_b, k_b=1}^{d_b} \langle j_a j_b | \rho | k_a k_b \rangle \text{Tr}(|j_a k_b \rangle \langle j_a k_b |)
\]
\[
= \sum_{j_a, k_a=1}^{d_a} \sum_{j_b, k_b=1}^{d_b} \langle j_a j_b | \rho | k_a k_b \rangle \delta_{j_a k_b} \delta_{j_a k_b}
\]
\[
= \sum_{j_a, k_a=1}^{d_a} \sum_{j_b, k_b=1}^{d_b} \langle j_a j_b | \rho | j_a j_b \rangle = \text{Tr}(\rho) = 1.
\] (32)
Now, let $D_+^j$, $D_-^j$, and $D_0^j$ denote the (real) positive, negative, and null eigenvalues of $D$ (and of $T_b(\rho)$). The dimension of the corresponding eigenspaces are denoted, respectively, by $d_+$, $d_-$, and $d_0$; thus, $d_+ + d_- + d_0 = d$. Hence, the unit trace of $T_b(\rho)$ leads to:
\[
\text{Tr}(T_b(\rho)) = 1 = \text{Tr}(U \rho T_b U^\dagger) = \text{Tr}(D) = \sum_{j=1}^{d} D_j
\]
\[
= \sum_{j=1}^{d} D_+^j + \sum_{j=1}^{d} D_-^j + \sum_{j=1}^{d} 0 = \sum_{j=1}^{d} D_+^j - \sum_{j=1}^{d} |D_j |.\] (33)
which is obtained only if $\sum_{j=1}^{d_+} D_+^j \geq 1$. Thus, the HSE in (31) can be written as
\[
E_{hs}(\rho) = \min_{\{\zeta_j\}_{j=1}^{d}} \left( \sum_{j=1}^{d} (\zeta_j^+ - \zeta_j^-)^2 \right.
\]
\[
\left. + \sum_{j=1}^{d_+} (\zeta_j^+ - \zeta_j^-)^2 + \sum_{j=1}^{d_0} (0 - \zeta_j^0)^2 \right)^{1/2}.
\] (34)
where \( \xi_j^+, \xi_j^-, \) and \( \xi_j^0 \) are the eigenvalues of \( \xi \) with eigenvectors in the positive, negative, and null eigenspaces of \( D \), respectively. Of course, we shall minimize \( E_{hs} \) if we set \( \xi_j^0 := 0 \) for \( j = 1, \ldots, d_0 \). We also minimize \( E_{hs} \) if we set \( \xi_j^- := 0 \) for \( j = 1, \ldots, d_- \) (because any \( \xi_j^- > 0 \) would make \( D_j^- - \xi_j^- \) more negative and hence lead to a greater value of \( (D_j^- - \xi_j^-)^2 \)). Next, let the positive eigenvalues \( D_j^+ \) be arranged in decreasing order and let \( d_+ \) be defined such that

\[
1 - \xi := \sum_{j=1}^{d_+} D_j^+ \leq 1 \quad \text{and} \quad \sum_{j=1}^{d_+} D_j^+ > 1. \tag{35}
\]

Then, considering that S. Rana showed in Ref. [33] that for two-qudit states the eigenvalues of the PT of \( \rho \) lie in interval \([-1/2, 1]\), we shall minimize \( E_{hs} \) if we set

\[
\xi_j^+ = D_j^+ \quad \text{for} \quad j = 1, \ldots, d_+ - 1,
\]

\[
\xi_d^+ = \xi,
\]

\[
\xi_j^- = 0 \quad \text{for} \quad j = d_+ + 1, \ldots, d_+.
\tag{36}
\]

With these choices for \( \xi_j \), we will have a valid density operator \( \rho \). Thus, substituting these values of \( \xi_j \) in (34), the minimum value for the Hilbert-Schmidt entanglement of an arbitrary bipartite density matrix shall be given by:

\[
E_{hs}^2(\rho) = (d_+^2 - \xi)^2 + \sum_{j=d_+ + 1}^{d_+} (D_j^+)^2 + \sum_{j=1}^{d_-} (D_j^-)^2
\]

\[
= \left( \sum_{j=1}^{d_+} D_j^+ - 1 \right)^2 + \sum_{j=d_+ + 1}^{d_+} (D_j^+)^2 + \sum_{j=1}^{d_-} (D_j^-)^2
\]

\[
= \left( \sum_{j=1}^{d_-} D_j^- \right)^2 - \sum_{j=d_+ + 1}^{d_+} (D_j^+)^2
\]

\[
+ \sum_{j=d_+ + 1}^{d_+} (D_j^+)^2 + \sum_{j=1}^{d_-} (D_j^-)^2. \tag{37}
\]

We observe that \( E_{hs} \) is written above in terms of (all) the negative eigenvalues of \( T_b(\rho) \) and in terms of its \( d_+ - d_+^* \) smaller positive eigenvalues. If the state under analysis is separable, then, in addition to the eigenvalues of \( T_b(\rho) \) being positive (i.e., \( d_- = 0 \)), we have \( d_+ = d_+^* - 1 \); and, therefore \( E_{hs}(\sigma) = 0 \), as expected. Besides, \( E_{hs}(\rho) > 0 \) whenever \( E_n(\rho) > 0 \).

To obtain the closest separable state (CSS), we start using the optimal \( \xi_j \)'s to write (30) as follows:

\[
\xi^* = \sum_{j=1}^{d_+} \xi_j^* |D_j^+ \rangle \langle D_j^+|
\]

\[
= \sum_{j=1}^{d_+} D_j^+ |D_j^+ \rangle \langle D_j^+| + \xi |D_{d_+}^* \rangle \langle D_{d_+}^*|
\]

\[
= \sum_{j=d_+ + 1}^{d_+} 0 |D_j^+ \rangle \langle D_j^+| + \sum_{j=1}^{d_-} 0 |D_j^- \rangle \langle D_j^-| + \sum_{j=1}^{d_+} 0 |D_j^0 \rangle \langle D_j^0|
\]

\[
= \sum_{j=1}^{d_+} D_j^+ |D_j^+ \rangle \langle D_j^+| + \xi |D_{d_+}^* \rangle \langle D_{d_+}^*|. \tag{38}
\]

Thus, using (28) and noticing from (25) that \( T_b(\rho) := \sum_{j=1}^{d_+} D_j |R_j \rangle \langle R_j| \) then \( |R_j \rangle = U^\dagger |D_j \rangle \), we get

\[
\sigma^* = T_b(\sum_{j=1}^{d_+} D_j^+ |R_j^+ \rangle \langle R_j^+| + \xi |R_{d_+}^- \rangle \langle R_{d_+}^-|) =: T_b(\Xi). \tag{39}
\]

So, as \( |R_j^+ \rangle \) is the eigenvector of \( T_b(\rho) \) corresponding to its \( j \)-th positive eigenvalue, we have written \( \sigma^* \) in terms of quantities directly related to the PT of \( \rho \). Actually, the closest separable state from \( \rho \) seems to be the PT of the mixture of the \( d_+ \) eigenvectors of \( T_b(\rho) \) corresponding to its \( d_+ \) greater eigenvalues; with the weights given by the eigenvalues themselves or by \( \xi \).

The HSE, (37), and the matrix \( \Xi \) in (39), whose PT gives the CSS, are returned by the subroutine

Fig. 1 Entanglement negativity and the Hilbert-Schmidt entanglement for the two- and three-qubit Werner states of (40). These states are fully separable for \( w \) less than \( 1/3 \) and \( 1/5 \), respectively [34]. In the two cases, we apply the partial transposition to one of the qubits, the other two are regarded as a ququart. For \( \rho_{w_1}^x \), the positive eigenvalues of its partial transpose are not used and the increasing rate of \( E_{hs} \) with \( w \) is constant. However, for \( \rho_{w_2}^x \), because of the changes of \( d_w \) with \( w \), the number of positive eigenvalues involved in the calculation of \( E_{hs} \) also changes, and this leads to the behavior shown in the plot.
entanglement hs (d, T_b(ρ), E_{hs}, css), with css being a character (1) variable. If css = ‘γ’ then, on exit, Ξ is returned in T_b(ρ). If css = ‘n’ and/or E_{hs}(ρ) = 0 then Ξ is not computed and T_b(ρ) is not modified. As an example, in Fig. 1, we show E_n and E_{hs} calculated for the two- and three-qubit Werner states:

\[ ρ_w^n = w|Φ_n⟩⟨Φ_n| + (1 - w)2^{-n}I_{2^n}, \quad (40) \]

where w \in [0, 1], |Φ_2⟩ = 2^{-1/2}(|00⟩ + |11⟩), |Φ_3⟩ = 2^{-1/2}(|000⟩ + |111⟩), and \( I_{2^n} \) is the 2^n x 2^n identity matrix.

4 Concluding Remarks

In this article, we presented a thorough description of the partial transposition (PT) map and of related entanglement functions. We produced and described free Fortran code to compute all of these functions. Besides, considering two-qudit systems, we obtained an analytical expression for the Hilbert-Schmidt entanglement (HSE) and for the associated properties of the PT of a state. So, in addition to its simplicity and clarity, our approach may be more suitable when compared to the application of Lagrange multipliers [32].

It is worthwhile remarking that the HS distance (HSD) is not generally contractive under quantum operations [35, 36]. This fact has motivated critiques regarding its use for quantum correlations quantification [37, 38]. Although the HSD can still be a formidable tool for several kinds of inquires [39–46], it would be interesting verifying if the procedure presented here to compute the HSE can be extended to other distance measures possessing more of the wanted “good” properties. In this direction, it is interesting observing that the \( l_1 \)-norm, which when computed using the basis \( B = \{|b⟩\} \), is given by \( ||A||_{l_1}^B = \sum_j |b⟩|A|b⟩ \), was shown to lead to a faithful quantum coherence quantifier (in contrast to \( ||A||_{hs} \)) [47]. In fact, if \( B \) is the computational basis: \( C = \{|j⟩_A|b⟩ \} \), we can show, in an analogous manner to the verification in Section 3, that

\[ ||ρ - σ||_{l_1}^C = ||T_b(ρ - σ)||_{l_1}^C. \quad (41) \]

However, the lack of unitary invariance of the \( l_1 \)-norm [48] seems to complicate its application in this scenario; so we leave the verification of this possibility as an open problem. As an alternative, it would be interesting considering also the \( r_1 \)-norm, introduced in Ref. [49], and its quantum extension for application in this context. It remains though to be investigated if the induced distance measure retains the properties of unitary-invariance, computability, PT-invariance, and contractivity under quantum operations.

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References

1. N.D. Mermin, What is quantum mechanics trying to tell us? Am. J. Phys. 66, 753 (1998)
2. M.A. Nielsen, I.L. Chuang, Quantum Computation and Quantum Information (Cambridge University Press) (2000)
3. J. Preskill, Quantum Information and Computation, http://theory.caltech.edu/people/preskill/ph229
4. M.M. Wilde, Quantum Information Theory (Cambridge University Press) (2013)
5. B. Groisman, S. Popescu, A. Winter, On the quantum, classical and total amount of correlations in a quantum state. Phys. Rev. A 72, 032317 (2005)
6. R. Horodecki, P. Horodecki, M. Horodecki, K. Horodecki, Quantum entanglement. Rev. Mod. Phys. 81, 865 (2009)
7. L.C. Céleri, J. Maziero, R.M. Serra, Quantum entanglement and correlated states. Int. J. Quantum Inf. 9, 1837 (2011)
8. O.D. Soares-Pinto, R. Aucaisse, J. Maziero, A. Gavini-Viana, R.M. Serra, L.C. Céleri, On the quinnerness of correlations in magnetic resonance. Phil. Trans. R. Soc. A 370, 4821 (2012)
9. N. Brunner, D. Cavalcanti, S. Pironio, V. Scarani, S. Wehner, Bell nonlocality. Rev. Mod. Phys. 86, 419 (2014)
10. D. Cavalcanti, P. Skrzypczyk, Quantum steering: A short review with focus on semidefinite programming. arXiv:1604.00501
11. M.D. Reid, P.D. Drummond, W.P. Bowen, E.G. Cavalcanti, P.K. Lam, H.A. Bachor, U.L. Andersen, G. Leuchs. Rev. Mod. Phys. 81, 1727 (2009)
12. C.S. Castro, O.S. Duarte, D.P. Pires, D.O. Soares-Pinto, M.S. Reis, Thermal entanglement and teleportation in a dipolar interacting system. Phys. Lett. A 380, 1571 (2016)
13. N. Gisin, R. Ribordy, W. Tittel, H. Zbinden, Quantum cryptography. Rev. Mod. Phys. 74, 145 (2002)
14. L. Maccone, Quantum metrology: why entanglement?. Phys. Rev. A 88, 042109 (2013)
15. M.B. Plenio, S. Virmani. An introduction to entanglement measures. Quant. Inf. Comput. 7, 1 (2007)
16. L. Aolita, F. de Melo, L. Davidovich, Open-system dynamics of entanglement. Rep. Prog. Phys. 78, 042001 (2015)
17. S. Gharibian, Strong NP-hardness of the quantum separability problem. Quant. Inf. Comp. 10, 343 (2010)
18. Y. Huang, Computing quantum discord is NP-complete. New J. Phys. 16, 033027 (2014)
19. A. Peres, Separability criterion for density matrices. Phys. Rev. Lett. 77, 1413 (1996)
20. M. Horodecki, P. Horodecki, R. Horodecki, Separability of mixed states: necessary and sufficient conditions. Phys. Lett. A 223, 1 (1996)
21. G. Vidal, R.F. Werner, A computable measure of entanglement. Phys. Rev. A 65, 032314 (2002)
22. M.B. Plenio, The logarithmic negativity: a full entanglement monotone that is not convex. Phys. Rev. Lett. 95, 090503 (2005)
23. J. Maziero, Generating pseudo-random discrete probability distributions: about the iid, normalization, and trigonometric methods. Braz. J. Phys. 45, 377 (2015)
24. J. Maziero, Random sampling of quantum states: a survey of methods. Braz. J. Phys. 45, 575 (2015)
25. J. Maziero, Fortran code for generating random probability vectors, unitaries, and quantum states. Front. ICT 3, 4 (2016)
26. J. Maziero, Computing coherence vectors and correlation matrices, with application to quantum discord quantification. Adv. Math. Phys. 2016, 6892178 (2016)
27. J. Maziero, Computing partial traces and reduced density matrices. Int. J. Mod. Phys. C 28, 1750005 (2017)
28. K. Kuttler, Elementary Linear Algebra (Textbook Equity Edition) (2014)
29. R.A. Horn, C.R. Johnson, Matrix Analysis (Cambridge University Press) (2013)
30. M. Horodecki, P. Horodecki, R. Horodecki, Mixed-state entanglement and distillation: is there a “bound” entanglement in nature. Phys. Rev. Lett. 80, 5239 (1998)
31. F. Verstraete, J. Dehaene, B. De Moor, On the geometry of entangled states. J. Mod. Opt. 49, 1277 (2002)
32. N. Jing, B. Yu, Quantum discord of X-states as optimization of one variable function. J. Phys. A: Math. Theor. 49, 385302 (2016)
33. S. Rana, Negative eigenvalues of partial transposition of arbitrary bipartite states. Phys. Rev. A 87, 054301 (2013)
34. A.O. Pittenger, M.H. Rubin, Note on separability of the Werner states in arbitrary dimensions. Opt. Comm. 179, 447 (2000)
35. D. Pérez-García, M.M. Wolf, D. Petz, M.B. Ruskai, Contractivity of positive and trace-preserving maps under $L_p$ norms. J. Math. Phys. 47, 083506 (2006)
36. X. Wang, S.G. Schirmer, Contractivity of the Hilbert-Schmidt distance under open-system dynamics. Phys. Rev. A 79, 052326 (2009)
37. M. Ozawa, Entanglement measures and the Hilbert-Schmidt distance. Phys. Lett. A 268, 158 (2000)
38. M. Piani, The problem with the geometric discord. Phys. Rev. A 86, 034101 (2012)
39. B. Dakic, Y.O. Lipp, X. Ma, M. Ringbauer, S. Kropatschek, S. Barz, T. Paterek, V. Vedral, A. Zeilinger, C. Brukner, P. Walther, Quantum discord as resource for remote state preparation. Nat. Phys. 8, 666 (2012)
40. R.A. Bertlmann, H. Narnhofer, W. Thirring, A geometric picture of entanglement and Bell inequalities. Phys. Rev. A 66, 032319 (2002)
41. R.A. Bertlmann, K. Durstberger, B.C. Hiesmayr, P. Krammer, Optimal entanglement witnesses for qubits and qudits. Phys. Rev. A 72, 052331 (2005)
42. J. Lee, M.S. Kim, C. Brukner, Operationally invariant measure of the distance between quantum states by complementary measurements. Phys. Rev. Lett. 91, 087902 (2003)
43. B. Tamir, E. Cohen, A Holevo-type bound for a Hilbert Schmidt distance measure. J. Quant. Inf. Science 05, 127 (2015)
44. V.V. Dodonov, O.V. Man’ko, V.I. Man’ko, A. Wünsche, Hilbert-Schmidt distance and non-classicality of states in quantum optics. J. Mod. Opt. 47, 633 (2000)
45. K. Zyczkowski, H.-J. Sommers, Hilbert-Schmidt volume of the set of mixed quantum states. J. Phys. A: Math. Gen. 36, 10115 (2003)
46. S. Popescu, A.J. Short, A. Winter, Entanglement and the foundations of statistical mechanics. Nat. Phys. 2, 754 (2006)
47. T. Baumgratz, M. Cramer, M.B. Plenio, Quantifying coherence. Phys. Rev. Lett. 113, 140401 (2014)
48. T. Nakano, M. Piani, G. Adesso, Negativity of quantumness and its interpretations. Phys. Rev. A 88, 012117 (2013)
49. C. Ding, D. Zhou, X. He, H. Zha, R1-PCA: Rotational invariant L1-norm principal component analysis for robust subspace factorization. In Proceedings of the 23rd international conference on Machine Learning 281–288 ACM (2006)