

Schmidt-number witnesses and bound entanglement

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The Schmidt number of a mixed state characterizes the minimum Schmidt rank of the pure states needed to construct it. We investigate the Schmidt number of an arbitrary mixed state by studying Schmidt-number witnesses that detect it. We present a canonical form of such witnesses and provide constructive methods for their optimization. Finally, we present strong evidence that all bound entangled states with positive partial transpose in $\mathcal{C}^3 \otimes \mathcal{C}^3$ have Schmidt number 2.

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Characterization of entanglement is one of the key features related to quantum information theory [1]. The resources needed to implement a particular protocol of quantum information processing (e.g., [2]) are closely linked to the entanglement properties of the states used in the protocol. Although recently a great effort has been devoted to detecting the presence of entanglement in a given state (see, for instance, [3,4]) and also to characterize multipartite entangled systems [5], many questions concerning bipartite mixed systems remain unanswered.

A bipartite pure state $|\psi\rangle$ can always be described by its Schmidt decomposition; i.e., the representation of $|\psi\rangle$ in an orthogonal product basis with minimal number of terms. The Schmidt rank is the number of nonvanishing terms in such an expansion. This decomposition gives a clear insight into the number of degrees of freedom that are entangled between both parties, and its coefficients provide a measure of entanglement.

The characterization of mixed states is a much harder task, and despite the fact that many entanglement measures have been introduced [6], there is not a “canonical” way of quantifying the entanglement. Nevertheless, in the context of mixed bipartite states it is legitimate and meaningful to ask: what is the minimum number of degrees of freedom that are entangled between both parties? Terhal and Horodecki [7] have recently addressed this question by introducing the concept of the *Schmidt number* of a density matrix. This number characterizes the minimum Schmidt rank of the pure states that are needed to construct such a density matrix. Furthermore, they proved that the Schmidt number is nonincreasing under local operations and classical communication, i.e., it provides a legitimate entanglement measure, or more precisely a monotone [8]. Finally, they introduced also the concept of k -positive maps that witness the Schmidt number, in the same way that positive maps witness entanglement. Recently, the concept of Schmidt rank and mean Schmidt number has been extended to pure [9] and mixed states [10] of multipartite systems.

Let us recall that a map is called positive (PM) if it maps positive operators into positive operators. A necessary and sufficient criterion for separability of a density matrix ρ was introduced by the Horodeckis [11] in terms of PM’s. Their criterion asserts that a state ρ acting on a composite Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$ is separable iff the tensor product of any positive map acting on A and the identity acting on B (or vice

versa) maps ρ onto a positive operator. This criterion, however, involves the characterization of the set of all PM’s, which is *per se* a formidable task. Similarly, the characterization of the set of k -positive maps [7] is a completely open problem. A complementary approach to study entanglement, introduced by Terhal [12], is based on the so-called entanglement witnesses (EW’s). An entanglement witness W is an observable that reveals the entanglement of some entangled state ρ , i.e., W is such that $\text{Tr}(W\sigma) \geq 0$ for all separable σ , but $\text{Tr}(W\rho) < 0$. The Hahn-Banach theorem implies that a state ρ is entangled iff there exists a witness that detects it [11]. There is an isomorphism between positive maps and entanglement witnesses [13].

A well-known example of a positive map is the transposition T : its tensor extension is the partial transposition (PT) $I \otimes T$ (see [14]). This map is positive on all separable states [15], and obviously detects all the entangled states that have nonpositive partial transposition (termed NPPT). However, given a PPT entangled state (PPTES), i.e. a state with bound entanglement [16(a)], it is in general very difficult to find an EW that detects it. A major step in the characterization of both, EW’s and the minimal set of them that are needed to detect all entangled states, has been presented in [17].

In this paper we extend the notion of entanglement witnesses (EW’s) to Schmidt-number k witnesses (k -SW’s), where $k \geq 2$. To this aim we define an observable which is non-negative (negative) for all (at least one) ρ of Schmidt number $k-1$ (k). Following [17], we express such operators in their canonical form, and show how to optimize them. Using this approach we obtain insight into the structure of the set of PPT-bound entangled states, determining the minimum number of degrees of freedom that must be entangled in order to prepare them. We present strong evidence that all PPTES’s in 3×3 systems have Schmidt number 2. In $N \times M$ systems ($N \geq M$) we expect PPTES states to have a Schmidt number $k < M$ in contrast with non-PPT entangled states that can have any Schmidt number $2 \leq k \leq M$. Before going into the details of the paper we recall the definitions of the Schmidt rank of a pure state $|\psi\rangle$, and the Schmidt number of a density matrix ρ :

Definition 1. A bipartite pure state $|\psi\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$, where $\dim \mathcal{H}_A = M$ and $\dim \mathcal{H}_B = N \geq M$, has Schmidt rank r if its Schmidt decomposition reads $|\psi\rangle = \sum_{i=1}^r a_i |e_i\rangle |f_i\rangle$, where $r \leq M$, $\sum_{i=1}^r a_i^2 = 1$, and $a_i > 0$.

Definition 2. Given the density matrix ρ of a bipartite system and all its possible decompositions in terms of pure states, namely $\rho = \sum_i p_i |\psi_i^r\rangle\langle\psi_i^r|$, where r_i denotes the Schmidt rank of $|\psi_i^r\rangle$, the Schmidt number of ρ , k , is defined as $k = \min\{r_{\max}\}$, where r_{\max} is the maximum Schmidt rank within a decomposition, and the minimum is taken over all decompositions [7].

Let us denote the whole space of density matrices in $N \times M$ by S_M , and the set of density matrices that have Schmidt number k or less by S_k . S_k is a convex compact subset of S_M [7]; a state from S_k will be called a state of (Schmidt) class k . Sets of increasing Schmidt number are embedded into each other, i.e., $S_1 \subset S_2 \subset \dots \subset S_k \subset \dots \subset S_M$. In particular, S_1 is the set of separable states (i.e., those that can be written as a convex combination of product states); S_2 contains S_1 plus the set of entangled states of Schmidt number 2, i.e., those with only two degrees of freedom between the two parties being entangled, etc. To determine which is the Schmidt number of a density matrix ρ , notice that due to the fact that the sets S_k are convex and compact, any arbitrary density matrix of class k can be decomposed as a convex combination of a density matrix of class $k-1$ and a remainder δ [20]:

Proposition 1. Any state of class k , ρ_k , can be written as a convex combination of a density matrix of class $k-1$ and a so-called k -edge state δ :

$$\rho_k = (1-p)\rho_{k-1} + p\delta, \quad 1 \geq p > 0, \quad (1)$$

where the edge state δ has Schmidt number $\geq k$.

The decomposition (1) is obtained by subtracting projectors onto pure states of Schmidt rank inferior to k , $P = |\psi^{<k}\rangle\langle\psi^{<k}|$, such that $\rho_k - \lambda P \geq 0$. Here $|\psi^{<k}\rangle$ stands for pure states of Schmidt rank $r < k$. Denoting by $K(\rho)$, $R(\rho)$, and $r(\rho)$ the kernel, range, and rank of ρ , respectively, we observe that $\rho' \propto \rho - \lambda |\psi^{<k}\rangle\langle\psi^{<k}|$ is non-negative iff $|\psi^{<k}\rangle \in R(\rho)$ and $\lambda \leq \langle\psi^{<k}|\rho^{-1}|\psi^{<k}\rangle^{-1}$ (see [20]). The idea behind this decomposition is that the edge state δ that has generically lower rank contains all the information concerning the Schmidt number k of the density matrix ρ_k .

There exists an optimal decomposition of the form (1) with p minimal. Also restricting ourselves to decompositions $\rho_k = \sum_i p_i |\psi_i^r\rangle\langle\psi_i^r|$ with all $r_i \leq k$, we can always find a decomposition of the form (1) with $\delta \in S_k$. We define below precisely what an edge state is.

Definition 3. A k -edge state δ is a state such that $\delta - \epsilon |\psi^{<k}\rangle\langle\psi^{<k}|$ is not positive, for any $\epsilon > 0$ and $|\psi^{<k}\rangle$.

Criterion 1. A mixed state δ is a k -edge state iff there exists no $|\psi^{<k}\rangle$ such that $|\psi^{<k}\rangle \in R(\delta)$.

Let us now define a Schmidt number k witness (k -SW):

Definition 4. A Hermitian operator W is a Schmidt witness of class k iff $\text{Tr}(W\sigma) \geq 0$ for all $\sigma \in S_{k-1}$, and there exists at least one $\rho \in S_k$ such that $\text{Tr}(W\rho) < 0$.

Notice that detecting inseparability is, thus, equivalent to searching for witnesses of Schmidt class 2. Also, the problem of distillability [4,16,18,19] can be recast in the language of witnesses of Schmidt number 2 and 3, i.e., if ρ^{TB} is a 2-SW (3-SW) then ρ is a distillable (one-copy nondistill-

able) state. It is straightforward to see that every SW that detects ρ given by Eq. (1) also detects the edge state δ , since if $\text{Tr}(W\rho) < 0$ then necessarily $\text{Tr}(W\delta) < 0$, too. Thus, the knowledge of all SW's of k -edge states fully characterizes all $\rho \in S_k$. Below, we show how to construct for any edge state a SW that detects it. Most of the technical proofs used to construct and optimize Schmidt witnesses are very similar to those presented in Ref. [17] for entanglement witnesses.

Let δ be a k -edge state, C an arbitrary positive operator such that $\text{Tr}(\delta C) > 0$, and P a positive operator whose range fulfills $R(P) = K(\delta)$. We define $\epsilon \equiv \inf_{|\psi^{<k}\rangle} \langle\psi^{<k}|P|\psi^{<k}\rangle$ and $c \equiv \sup \langle\psi|C|\psi\rangle$. Note that $c > 0$ by construction and $\epsilon > 0$, because $R(P) = K(\delta)$ and therefore, since $R(\delta)$ does not contain any $|\psi^{<k}\rangle$ by the definition of edge state, $K(P)$ cannot contain any $|\psi^{<k}\rangle$ either. This implies:

Lemma 1. Given an k -edge state δ , then

$$W = P - \frac{\epsilon}{c} C \quad (2)$$

is a k -SW that detects δ .

The simplest choice of P and C consists in taking projections onto $K(\delta)$ and the identity operator, respectively. As we will see below, this choice provides a canonical form for a k -SW.

Proposition 2. Any k -Schmidt witness can be written in the canonical form:

$$W = \tilde{W} - \epsilon \mathbb{1}, \quad (3)$$

such that $R(\tilde{W}) = K(\delta)$, where δ is a k -edge state and $0 < \epsilon \leq \inf_{|\psi\rangle \in S_{k-1}} \langle\psi|\tilde{W}|\psi\rangle$.

Proof. Assume W is an arbitrary k -SW so W has at least one negative eigenvalue. Construct $W + \epsilon \mathbb{1} = \tilde{W}$, so \tilde{W} is a positive operator, but it does not have a full rank, $K(\tilde{W}) \neq \emptyset$ (by continuity this construction is always possible). But $\langle\psi^{<k}|\tilde{W}|\psi^{<k}\rangle \geq \epsilon > 0$ since W is a k -SW, ergo no $|\psi^{<k}\rangle \in K(\tilde{W})$. ■

Let us now introduce some additional notations.

Definition 5. A k -Schmidt witness W is tangent to S_{k-1} at ρ if \exists a state $\rho \in S_{k-1}$ such that $\text{Tr}(W\rho) = 0$.

Observation 1. The state ρ is of Schmidt class $k-1$ iff for all k -SW's tangent to S_{k-1} , $\text{Tr}(W\rho) \geq 0$.

Proof (see [17]). (Only if) if ρ is of class k , then from the Hahn-Banach theorem, there exists a k -SW W that detects it. We can subtract $\epsilon \mathbb{1}$ from W , making $W - \epsilon \mathbb{1}$ tangent to S_{k-1} at some σ , but then $\text{Tr}[\rho(W - \epsilon \mathbb{1})] < 0$. ■

We will now discuss the optimization of a Schmidt witness. As proposed in [17(a)] an entanglement witness W is optimal if there exists no other EW that detects more states than it. The same definition can be applied to Schmidt witnesses. We say that a Schmidt number k witness W_2 is finer than a Schmidt number k witness W_1 , if W_2 detects more states than W_1 . Analogously, we define a Schmidt number k witness W to be optimal when there exists no finer witness than itself. Let us define the set of $|\psi^{<k}\rangle$ for which the expectation value of the Schmidt number k witness W vanishes:

$$T_W = \{|\psi^{<k}\rangle\langle\psi^{<k}|W|\psi^{<k}\rangle = 0\}, \quad (4)$$

i.e., the set of pure tangent states of Schmidt rank $<k$. W is an optimal k -SW iff $W - \epsilon P$ is not a k -SW, for any positive operator P . If the set T_W spans the whole Hilbert space, then W is an optimal k -SW. If T_W does not span $\mathcal{H}_A \otimes \mathcal{H}_B$, then we can optimize the witness by subtracting from it a positive operator P , such that $PT_W = 0$. For $k=3$, for instance, this is possible, provided $\inf_{|e_1\rangle, |e_2\rangle \in \mathcal{H}_A} [P_{e_1 e_2}^{-1/2} W_{e_1 e_2} P_{e_1 e_2}^{-1/2}]_{\min} > 0$, where for any X acting on $\mathcal{H}_A \otimes \mathcal{H}_B$

$$X_{e_1 e_2} = \begin{bmatrix} \langle e_1 | X | e_1 \rangle & \langle e_1 | X | e_2 \rangle \\ \langle e_2 | X | e_1 \rangle & \langle e_2 | X | e_2 \rangle \end{bmatrix}, \quad (5)$$

acts in $C^2 \otimes \mathcal{H}_B$, and $[X]_{\min}$ denotes its minimal eigenvalue (see [17]). An example of an optimal witness of Schmidt number k in $C^m \otimes C^m$ is given by

$$W = \mathbb{1} - \frac{m}{k-1} \mathcal{P}, \quad (6)$$

where \mathcal{P} is a projector onto a maximally entangled state $|\Psi_+\rangle = \sum_{i=0}^{m-1} |ii\rangle / \sqrt{m}$. The k -positive map corresponding to Eq. (6) has been discussed in [7]. For $k=3$ and $m \geq 3$, the partial transpose of Eq. (6) provides an example of a one-copy nondistillable state with nonpositive partial transpose [19]. Note that W is decomposable, i.e., $W = \tilde{P} + \tilde{Q}^{TA}$, where $\tilde{P}, \tilde{Q} \geq 0$, and therefore it cannot detect any PPTES [17(a)]. This can be seen by rewriting Eq. (6) as $W = [1 - 1/(k-1)]\mathbb{1} + 2P_a^{TA}/(k-1)$, where P_a^{TA} is the partially transposed projector onto the antisymmetric subspace of $C^m \otimes C^m$.

Let us now focus on the case $C^3 \otimes C^3$ (two qutrits). We summarize below the following observations:

(i) Any 2-SW (entanglement witness) has the form $W = Q - \epsilon \mathbb{1}$, where $K(Q)$ does not contain any product vector, i.e., $r(Q) \geq 5$ [21(b)].

(ii) Any 3-SW has the form $W = Q - \epsilon \mathbb{1}$, where $r(Q) = 8$. This follows from the fact that any two-dimensional subspace of $C^3 \otimes C^3$ contains a vector of Schmidt rank 2. Note that thus we have $W = \tilde{Q} - \epsilon P$, where P is a projector on a vector $|\Psi^3\rangle$ of Schmidt rank 3 orthogonal to $R(Q)$, and $\tilde{Q} = Q - \epsilon \mathbb{1}_Q$ is positive [$\mathbb{1}_Q$ denotes the projector on $R(Q)$].

(iii) Let A be a local transformation in Alice's space that transforms the maximally entangled state $|\Psi_+\rangle$ to $|\Psi^3\rangle$, and let the Schmidt coefficients of $|\Psi^3\rangle$ be $a_1 \geq a_2 \geq a_3 > 0$. We can write $W = \tilde{Q} + (\lambda_{\min} - \epsilon)\mathbb{1} - \lambda_{\min} A A^\dagger / 3 + 2\lambda_{\min} (A P_a A^\dagger)^{TB} / 3$, with $\lambda_{\min} = [Q]_{\min}$. This implies that if $(\lambda_{\min} - \epsilon)\mathbb{1} - \lambda_{\min} A A^\dagger / 3$ is positive definite, i.e., $\lambda_{\min}(1 - a_1^2) \geq \epsilon$, then W is decomposable. On the other hand, we observe that for $|\Psi^2\rangle$ such that $|\langle \Psi^2 | \Psi^3 \rangle|^2 = a_1^2 + a_2^2$, we have $0 \leq \langle \Psi^2 | W | \Psi^2 \rangle \leq \lambda_{\max} a_3^2 - \epsilon$, where $\lambda_{\max} = [Q]_{\max}$. In turn, these two observations imply:

Lemma 2. If $\lambda_{\max} / \lambda_{\min} \leq 1 + a_2^2 / a_3^2$, then W is decomposable.

Note that if W does not fulfill the assumption of this Lemma, it is very likely that it can be transformed using

local transformations to fulfill it. These observations allow us to formulate the following conjecture:

Conjecture 1. In $C^3 \otimes C^3$ all PPT entangled states have Schmidt number 2, i.e., all Schmidt witnesses of class 3 are decomposable.

Evidence. Obviously, it suffices to prove the conjecture for the edge states. First we prove it rigorously for rank-4 edge states, such as those constructed from unextendible product bases [22(a)], chessboard states of Ref. [22(b)], and generalized Choi matrices [22(c)].

Lemma 3. All PPT entangled states of rank 4 have Schmidt number 2 [23].

Proof. If $r(\delta) = 4$ then there exists a product vector $|e_1, f\rangle \in K(\delta)$ [21(b)]. From $\delta^{TA} \geq 0$ we see that $|e_1^*, f\rangle \in K(\delta^{TA})$. Let $|e_i\rangle$, $i=1,2,3$ form an orthonormal basis in \mathcal{H}_A . We have then $\langle e_1 | \delta | e_i, f \rangle = 0$ for $i=2,3$. Thus, $\delta | e_2, f \rangle = |\Psi^2\rangle = |e_2, g\rangle + |e_3, h\rangle$, i.e., $|\Psi^2\rangle$ has Schmidt rank 2. We can write then $\delta = \delta' + \Lambda |\Psi^2\rangle \langle \Psi^2|$, where $\delta' \geq 0$, $\Lambda^{-1} = \langle \Psi^2 | \delta^{-1} | \Psi^2 \rangle = \langle \Psi^2 | e_2, f \rangle$. Note that $r(\delta') = 3$, and $\delta' | e_i, f \rangle = 0$ for $i=1,2$, while $\delta' | e_3, f \rangle = (\delta - \Lambda |\Psi^2\rangle \langle \Psi^2|) | e_3, f \rangle = |\Phi^2\rangle = |e_2, \tilde{g}\rangle + |e_3, \tilde{h}\rangle$, and $|\Phi^2\rangle$ has at most Schmidt rank 2. This allows us to write $\delta' = \delta'' + \tilde{\Lambda} |\Phi^2\rangle \langle \Phi^2|$, where $\delta'' \geq 0$, $r(\delta'') = 2$, and $\delta'' | e_i, f \rangle = 0$ for $i=1,2,3$. But, that means that δ'' acts in a 3×2 space (orthogonal to $|f\rangle$ in \mathcal{H}_B), ergo δ'' (and therefore δ' and δ) have Schmidt number 2. ■

From [21] we know that the edge states in $C^3 \otimes C^3$ have ranks $r(\delta) + r(\delta^{TA}) \leq 13$. Considering pairs $(r(\delta), r(\delta^{TA}))$, we observe:

Lemma 4. Typically, for any decomposable W , tangent to the set of PPTES at the edge state δ with $(r(\delta), r(\delta^{TA})) = (5,7), (5,8), (6,6), (6,7), (7,6)$, or $(8,5)$, for any $\epsilon > 0$, the nondecomposable witness $W_\epsilon = W - \epsilon \mathbb{1}$ is not a Schmidt witness of S_3 , i.e., there exists a vector $|\Psi^2\rangle$ of Schmidt rank 2, such that $\langle \Psi^2 | W_\epsilon | \Psi^2 \rangle < 0$.

To prove it, we first write $W = P + Q^{TA}$, with $P, Q \geq 0$, where $R(P) = K(\delta)$, $R(Q) = K(\delta^{TA})$ [17]. We then consider $|\Psi\rangle = |e_1, f_1\rangle + \beta |e_2, f_2\rangle$, such that $P|\Psi\rangle = 0$, $Q|e_i, f_i\rangle = 0$ for $i=1,2$. Then, $\langle \Psi | W | \Psi \rangle = 2 \operatorname{Re}(\beta \langle e_2^*, f_1 | W | e_1^*, f_2 \rangle)$. Choosing the phase of β appropriately, we can always get $\langle \Psi | W | \Psi \rangle \leq 0$, i.e., $W - \epsilon \mathbb{1}$ cannot be a 3-SW. Let us check if such $|\Psi\rangle$ exists. The set of $|\Psi\rangle$'s can be parametrized by nine complex parameters. The vector $|\Psi\rangle$ has to fulfill $L = r(P) + 2r(Q) = 27 - r(\delta) - 2r(\delta^{TA})$ equations, and one inequality for the phase of β . Obviously, $L < 9$ for $(r(\delta), r(\delta^{TA})) = (5,7), (5,8), (6,7)$, and $(7,6)$, so that we expect to have an infinite family of solutions, and in particular those with the desired phase of β . While examples of edge states with ranks $(5,8), (5,7)$ are not known, the Horodecki matrix of Ref. [24], and the matrix from the α family of states of Ref. [16(b)] with $\alpha=4$ have ranks $(6,7)$. We have checked that for those matrices the desired $|\Psi\rangle$ exists. For $(r(\delta), r(\delta^{TA})) = (6,6)$, and $(8,5)$, $L=9$ and we expect a finite number of solutions, but still some of them fulfilling the requirements for β . We conclude that if a Schmidt witness of the class 3 were nondecomposable, then it could not be of the form $W = P + Q^{TA} - \epsilon \mathbb{1}$, where P is supported on $R(\delta)$ and Q on $R(\delta^{TA})$, for δ of the category considered in Lemma

4. The only possibility is that $(r(\delta), r(\delta^{TA})) = (5,5), (5,6), (6,5)$, or $(7,5)$. To investigate these cases we prove:

Observation 2. For any edge state δ with $r(\delta) + r(\delta^{TA}) \leq 13$, there exists an edge state $\tilde{\delta}$ with $r(\tilde{\delta}) + r(\tilde{\delta}^{TA}) = 13$ arbitrarily close to δ (in any norm).

Proof. Let us consider for instance the case $(5,5)$. We can add to δ an infinitesimally small separable state composed of two projectors on product vectors from $R(\delta)$ and two from $R(\delta^{TA})$, making the resulting state ρ of the category $(7,7)$. For such a state there exists a finite number of product vectors $|e, f\rangle \in R(\delta)$, $|e^*, f\rangle \in R(\delta^{TA})$. We subtract a projector on one such vector, keeping the remainder non-negative and PPT [21]. We choose a vector different from the ones used to construct δ . Generically, the resulting state will be arbitrarily close to δ , but will have ranks $(6,7)$, or $(7,6)$. ■

From Observation 2 we get that if δ with ranks $r(\delta)$

$+ r(\delta^{TA}) \leq 13$ did not belong to S_2 , then there would be a state $\tilde{\delta}$ with $r(\tilde{\delta}) + r(\tilde{\delta}^{TA}) = 13$ arbitrarily close to δ , which would not belong to S_2 neither. But, that contradicts Lemma 4. In effect, if Lemma 4 is rigorous, then the conjecture is true.

Summarizing, we have presented a general characterization of witnesses of Schmidt number k , and the methods of optimizing them. The results allow us to provide strong evidence that all bound entangled states with positive partial transpose in two qutrit systems have Schmidt number 2, i.e., can be prepared using a two qubit entangled state, local operations, and classical communication.

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