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 generic mixed state by constructing a Schmidt number witness that detects 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 two qutrit systems have Schmidt number 2.

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 detect the presence of entanglement in a given state [3,4], and also to characterize multiple 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. The Schmidt decomposition is the representation of $|\psi\rangle$ by means of an expansion (with minimal number of terms) in an orthogonal product basis. The Schmidt rank is the number of non-vanishing terms in such an expansion. This decomposition gives a clear insight on 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: which is the minimum number of degrees of freedom that must be entangled in order to prepare them. We present strong evidence that all PPTES in $3 \times 3$ 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 $k$ in the range $2 \leq k \leq M$. Before going into the details of 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 $\rho$ was introduced by the Horodeckis [11] in terms of PM's. Their criterion asserts that a state $\rho$ acting on a composite Hilbert space $H_A \otimes H_B$ is separable iff the tensor product of any positive map acting on $A$ and the identity acting on $B$ (or vice versa) maps $\rho$ 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). An entanglement witness $W$ is an observable that reveals the entanglement of some entangled state $\rho$, i.e. $W$ is such that $\text{Tr}(W\sigma) \geq 0$ for all separable $\sigma$, but $\text{Tr}(W\rho) < 0$. The Hahn-Banach theorem implies that a state $\rho$ 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 non positive partial transposition (termed NPPT). However, given a PPT entangled state (PTTES), i.e. a state with bound entanglement [16], 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 which are needed to detect all entangled states, has been presented in [17].

In this paper we extend the notion of entanglement witnesses (EW) to Schmidt number $k$ witnesses ($k$-SW), where $k \geq 2$. To this aim we define an observable which is non-negative for all $\rho$ of Schmidt number $k - 1$, and negative for at least one $\rho$ of Schmidt number $k$. Following [17], we express such operators in their canonical form, and show how to optimize them. As a result we obtain novel insight in the structure of the set of PPT-bound entangled states and in the minimum number of degrees of freedom that must be entangled in order to prepare them. We present strong evidence that all PPTES in $2 \times k$ systems have Schmidt number $k-1$. 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 $k$ in the range $2 \leq k \leq M$. Before going into the details of
respectively, we observe that $K$ matrix is nondistillable) state. and a so-called density matrix of class $S$. Sets of increasing Schmidt number are embedded into each other, i.e. $S_1 \subset S_2 \subset \ldots S_k \subset S_M$. In particular, $S_1$ is the set of separable states (i.e. those that can be written as a convex combination of product states); $S_2$ is 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. Notice that detecting inseparability is, thus, equivalent to searching between the two parties being entangled, etc. Notice that detecting inseparability is, thus, equivalent to searching 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 $\rho^F_1$ is detected by a 2-SW (3-SW) then $\rho$ is a distillable (1-copy nondistillable) state.

To determine which is the Schmidt number of a density matrix $\rho$ 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 $\delta$ [20]:

**Proposition 1** Any state of class $k$, $\rho_k$, can be written as a convex combination of a density matrix of class $k-1$ and a so-called $k$-edge state $\delta$:

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

(1)

where the $k$-edge state $\delta$ 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 $\rho$ 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 $\lambda \leq \langle\psi^{<k}|\rho^{-1}|\psi^{<k}|^{-1}$ (see [20]). The idea behind this decomposition is that the edge state $\delta$ contains all the information concerning the Schmidt number $k$ of the density matrix $\rho_k$. This edge state, however, has a low rank and is much easier to handle than the generic matrix $\rho_k$.

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

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

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

Therefore, the problem of finding Schmidt witnesses for arbitrary density matrices can be reduced to finding Schmidt witnesses for the edge states. Let us now define a $k$-Schmidt witness (k-SW):

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

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

Let $\delta$ be a $k$-edge state, $C$ an arbitrary positive operator such that $\text{Tr}(BC) > 0$, and $P$ a positive operator whose range fulfills $R(P) = K(\delta)$. We define $\epsilon \equiv \inf_{|\psi\rangle \in S_{k-1}} \langle \psi|P|\psi\rangle$ and $\epsilon \equiv \sup_{|\psi\rangle \in S_{k-1}} \langle \psi|C|\psi\rangle$ and required $\epsilon > 0$. Note that $\epsilon > 0$, because $R(P) = K(\delta)$ and therefore, since $R(\delta)$ does not contain any $|\psi^{<k}\rangle$ by the definition of edge state, $K(\rho)$ cannot contain any $|\psi^{<k}\rangle$ either. This implies:

**Lemma 1** Given an $k$-edge state $\delta$, then

$$W_1 = P - \frac{\epsilon}{C}$$

(2)

is a $k$-SW which detects $\delta$.

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 us with a canonical form for a $k$-SW. In order to show that, let us first introduce some additional notations.

**Definition 5** A $k$-Schmidt witness $W$ is tangent to $S_{k-1}$ at $\rho$ if there exists a state $\rho \in S_{k-1}$ such that $\text{Tr}(W\rho) = 0$. 
The state $\rho$ is of Schmidt class $k-1$ iff for all k-SW’s tangent to $S_k$, Tr$(W\rho) \geq 0$.

**Proof** (See [17]): (only if) Suppose that $\rho$ is of class $k$. From Hahn-Banach theorem, there exists a k-SW $W$, that detects it. We can subtract $\epsilon 1$ from $W$, making $W - \epsilon 1$ tangent to $S_{k-1}$ at some $\sigma$, but then Tr$(\rho (W - \epsilon 1)) < 0$.

**Observation 2** If a $(k+1)$-Schmidt witness $W$ is tangent to $S_k$ at $\rho \in S_k$, then for any decomposition of the form (1) the equality Tr$(W \delta) = 0$ holds.

We can now write the canonical form of a Schmidt witness:

$$W = \bar{W} - \epsilon 1,$$

where $\bar{W}$ is a $(k+1)$-witness tangent to $S_k$ at some $\rho$, such that $R(\bar{W}) = K(\delta)$ where $\delta$ is a $k$-edge state, and $\epsilon \leq \inf |\psi\rangle \in S_{k-1} \langle \psi|W|\psi\rangle$. As before, $\epsilon > 0$ by construction.

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 $k$-Schmidt witness $W_2$ is finer than a $k$-Schmidt witness $W_1$, if $W_2$ detects more states than $W_1$. Analogously, we define a $k$-Schmidt witness $W$ to be optimal when there exists no finer witness than itself.

We will now discuss the optimisation of a Schmidt witness. Let us define the set of $|\psi^{<k}\rangle$ for which the expectation value of the k-Schmidt witness vanishes:

$$T_W = \{|\psi^{<k}\rangle \in S_{k-1} \text{ s.t. } \langle \psi^{<k}|W|\psi^{<k}\rangle = 0\},$$

i.e. the set of pure tangent states of Schmidt rank $< k$. $W$ is an optimal k-SW iff $W - \epsilon I$ is 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 $H_A \otimes H_B$, then we can optimize the witness by subtracting from it a positive operator $P$, such that $PT_W = 0$. This is possible, provided

$$inf_{|e_1\rangle,|e_2\rangle \in H_A / P_{e_1 e_2}^{1/2}W_{e_1 e_2}P_{e_1 e_2}^{-1/2}|min > 0,}$$

acts in $H_A \otimes H_B$, and $[X]_{min}$ is its minimal eigenvalue (see [17]).

An example of an optimal witness of Schmidt number $k$ in $H_m \otimes H_m$ is given by

$$W = 1 - \frac{m}{k+1}P$$

where $P$ 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 (6) has been discussed in [7]. For $k = 3$ and $m \geq 3$, the partial transpose of (6) provides an example of a one copy non–distillable state with non-positive partial transpose [19]. Note that $W$ is decomposable, i.e. $W = \tilde{P} + \tilde{Q}^T$, where $\tilde{P}, \tilde{Q} \geq 0$, and therefore it cannot detect any PPTES [17](a). This can be seen by rewriting (6) as $W = (1 - 1/k)I + 2PT_3/k$, where $PT_3$ is the partially transposed projector onto the antisymmetric subspace of $H_m \otimes H_m$.

Let us now focus on the case $H_3 \otimes H_3$ (two qutrits). We summarize below the following observations:

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

ii) Any 3-SW has the form $W = Q - e 1$, where $r(Q) = 8$. This follows from the fact that any 2-dimensional subspace of $H_3 \otimes H_3$ contains a vector of Schmidt rank 2. Note that thus we have $W = \tilde{Q} - e P$, where $P$ is a projector on a vector $|\Psi^3\rangle$ of Schmidt rank 3 orthogonal to $R(Q)$, and $\tilde{Q} = Q - e I_Q$ is positive ($I_Q$ 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 $W = \tilde{Q} + (\lambda_{min} - \epsilon) 1 - \lambda_{min} A^A A^B / 3 + 2 \lambda_{min} (A^A A^B)^T / 3$, with $\lambda_{min} = |Q|_{min}$. This implies that if $(\lambda_{min} - \epsilon) 1 - \lambda_{min} A^A A^B / 3$ is positive definite, i.e. $\lambda_{min} (1 - a_i^2) \geq \epsilon$, then $W$ is decomposable. On the other hand, we observe that for $|\Psi^3\rangle$ such that $|\Psi^3|_{min}^2 = a_1^2 + a_2^2$, we have $0 \leq |\Psi^2|^2 / |\Psi^3|^2 \leq \lambda_{max} a_i^2 - \epsilon$, 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 $H_3 \otimes H_3$ 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 [17](a). 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.

**Proof:** If $r(\delta)=4$ then there exists a product vector $|e_1, f\rangle \in K(\delta) [21]$. From $\delta^{T_A} \geq 0$ we see that $|e_i, f\rangle \in K(\delta^{T_A})$. Let $|e_i\rangle$, $i = 1, 2, 3$ form an orthonormal basis in $H_A$. We have then $\langle e_i|\delta|e_i, f\rangle = 0$ 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 $\Lambda^2 = |\Psi^2|\langle\delta^{T_A}|\Psi^2\rangle = |\Psi^2|\langle e_2|, f\rangle$. Note that $r(\delta') = 3$, and $\delta'|e_i, f\rangle = 0$ for $i = 1, 2, 3$. While $\delta'|e_3, f\rangle = (\delta - \Lambda|\Psi^2\rangle\langle\Psi^2|)|e_3, f\rangle = |\Phi^2\rangle = |e_2, g\rangle + |e_3, h\rangle$. 


where \( \vec{\Phi} \) has Schmidt rank 2. This allows us to write \( \vec{\delta}' = \vec{\delta}'' + \Lambda [\vec{\Phi}] \langle \vec{\Phi}^2 \rangle \), where \( \vec{\delta}'' \geq 0 \), \( r(\vec{\delta}'') = 2 \), and \( \vec{\delta}''(e_i, f_i) = 0 \) for \( i = 1, 2, 3 \). But, that means that \( \vec{\delta}'' \) acts in a 5 \( \times \) 2 space (orthogonal to \( |f_i \rangle \) in \( \mathcal{H}_B \)), ergo \( \vec{\delta}' \) (and therefore \( \delta' \) and \( \delta \)) have Schmidt number 2. □

The edge states in \( \mathcal{H}_3 \otimes \mathcal{H}_3 \) have ranks \( r(\delta) + r(\delta^{T_A}) \leq 13 \) [21]. Let us consider pairs \((\vec{\delta}, \vec{\delta}^{T_A})\). We have

**Lemma 4** Typically, for any decomposable EW, \( W \) tangent to the set of PPTES at the edge state \( \vec{\delta} \) with \( \langle \vec{\delta} | r(\vec{\delta}) = r(\vec{\delta}^{T_A}) = (5, 7), (5, 8), (6, 6), (6, 7), (7, 6) \), or (8, 5), for any \( \epsilon > 0 \), the non–decomposable witness \( W_\epsilon = W - \epsilon \mathbb{1} \) is not a Schmidt witness of \( S_3 \), i.e., there exist 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 \( W = P + Q^{T_A} \), with \( P, Q \geq 0 \), where \( R(P) = K(\delta), R(Q) = K(\delta^{T_A}) \) [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, \( \langle \Psi | W | \Psi \rangle = 2 \text{Re}(\beta (e_2^*, f_1 W |e_1^*, f_2 \rangle) \). Choosing the phase of \( \beta \) 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 forms a 9 dimensional complex manifold. The vector \( |\Psi\rangle \) has to fulfill \( L = r(P) + 2r(Q) = 27 - r(\delta) - 2r(\delta^{T_A}) \) equations, and one inequality for the phase of \( \beta \). Obviously, \( L < 9 \) for \( (r(\delta), r(\delta^{T_A})) \in (5, 7), (5, 8), (6, 7), (7, 6) \), so that we expect to have an infinite family of solutions, and in particular those with the desired phase of \( \beta \). While examples of edge states with ranks \((5, 8), (5, 7)\) are not known, the Horodecki matrix of Ref. [23], and the matrix from the \( \alpha \)-family of states of Ref. [16] with \( \alpha = 4 \) have ranks \((6, 7)\). We have checked that for those matrices the desired \( |\Psi\rangle \) exists. For \( (r(\delta), r(\delta^{T_A})) \in (6, 6), (8, 5) \), \( L = 9 \) and we expect a finite number of solutions, but still some of them fulfilling the requirements for \( \beta \). We conclude that if a Schmidt witness of the class 3 was non-decomposable, then it could not be of the form \( W = P + Q^{T_A} - \epsilon \mathbb{1} \), where \( P \) is supported on \( R(\delta) \) and \( Q \) on \( R(\delta^{T_A}) \), for \( \delta \) of the category considered in Def3. The only possibility is that \( (r(\delta), r(\delta^{T_A})) \in (5, 5), (5, 6), (6, 5), \) or \( (7, 5) \).

To investigate these cases we prove:

**Observation 3** For any edge state \( \delta \) with \( r(\delta) + r(\delta^{T_A}) \leq 13 \), there exists an edge state \( \tilde{\delta} \) with \( r(\tilde{\delta}) + r(\tilde{\delta}^{T_A}) = 13 \) arbitrarily close to \( \delta \) in the sense of an operator norm.

**Proof:** Let us consider for instance the case \((5, 5)\). We can add to \( \delta \) an infinitesimally small separable state composed of 2 projectors on product vectors from \( R(\delta) \) and 2 from \( R(\delta^{T_A}) \), making the resulting state \( \rho \) of the category \((7, 7)\). For such state there exists a finite number of product vectors \( |e_i, f_i \rangle \in R(\delta), |e^*, f \rangle \in R(\delta^{T_A}) \). 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 \( \delta \). Generically, the resulting state will be arbitrarily close to \( \delta \), but will have ranks \((6, 7), \) or \((7, 6)\). □

From Lemma (3) we immediately get that if \( \delta \) with ranks \( r(\delta) + r(\delta^{T_A}) \leq 13 \) does not belong to \( S_2 \), then there would be a state with ranks \( \delta \) with \( r(\delta) + r(\delta^{T_A}) = 13 \) arbitrarily close to \( \delta \), which, according to the Hahn–Banach theorem would not belong to \( S_2 \) neither. But, that contradicts the Obs. 3. In effect, if Obs. 3 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. The results can be generalized to higher dimensional systems.

We thank I. Cirac, P. Horodecki, B. Kraus, M. Nielsen and M. Plenio for discussions. This work has been supported by the DFG (SFB 407 and Schwerpunkt “Quanteninformationsverarbeitung”), the ESF PESC Programme on Quantum Information, and Besnasque Center for Science Workshop 2000.

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[14] Given an operator \( X \) and an orthonormal basis
\{\langle k | \rangle_B \}_{k=1}^N \in H_B$, one defines the partial transpose of $X$ with respect to $B$ in that basis as follows: $X^{TB} = \sum_{k, k' = 1}^N \langle k' | B \rangle \langle k | X \rangle_B \langle k | B \rangle \langle k' |$. We say that $\rho$ has a positive partial transposition (PPT) if $\rho^{TB} \geq 0$. Note that this property is basis-independent.