Classification of Mixed Three-Qubit States

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We introduce a classification of mixed three-qubit states, in which we define the classes of separable, biseparable, *W*, and Greenberger-Horne-Zeilinger states. These classes are successively embedded into each other. We show that contrary to pure *W*-type states, the mixed *W* class is not of measure zero. We construct witness operators that detect the class of a mixed state. We discuss the conjecture that all entangled states with positive partial transpose (PPTES) belong to the *W* class. Finally, we present a new family of PPTES "edge" states with maximal ranks.

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The rapidly increasing interest in quantum information processing has motivated the detailed study of entanglement. Whereas entanglement of pure bipartite systems is well understood, the classification of mixed states according to the degree and character of their entanglement is still a matter of intensive research (see [1]). It was soon realized that the entanglement of pure tripartite quantum states is not a trivial extension of the entanglement of bipartite systems [2,3]. Recently, the first results concerning the entanglement of pure tripartite systems have been achieved [4–6]. There, the main goal has been to generalize the concept of the Schmidt decomposition to three-party systems [4,5], and to distinguish classes of locally inequivalent states [6]. The knowledge of mixed tripartite entanglement is much less advanced (see, however, [7–9]).

In this Letter we introduce a classification of the whole space of mixed three-qubit states into different entanglement classes. We provide a method to determine to which class a given state belongs (tripartite witnesses). We also discuss the characterization of entangled states that are positive under partial transposition (PPTES). Finally, we introduce a new family of PPTES for mixed tripartite qubits.

Our proposal to classify mixed tripartite-qubit states is done by specifying compact convex subsets of the space of all states, which are embedded into each other. This idea vaguely resembles the classification of bipartite systems by their Schmidt number [9–11]. However, as shown later our classification does *not* follow the Schmidt number [9]. Also in this respect, entanglement of tripartite systems differs genuinely from the one of bipartite quantum systems.

Before presenting our results concerning mixed states, we briefly review some of the recent results on pure three-qubit states. Any three-qubit vector (pure state) can be written as

$$|\psi_{\mathrm{GHZ}}\rangle = \lambda_0|000\rangle + \lambda_1 e^{i\theta}|100\rangle + \lambda_2|101\rangle$$
$$+ \lambda_3|110\rangle + \lambda_4|111\rangle, \qquad (1)$$

where $\lambda_i \geq 0$, $\sum_i \lambda_i^2 = 1$, $\theta \in [0, \pi]$, and $\{|0\rangle, |1\rangle\}$ denotes an orthonormal basis in Alice's, Bob's, and Charlie's spaces, respectively [4]. Apart from separable and biseparable pure states, there exist also two different types

of locally inequivalent entangled vectors: the so-called Greenberger-Horne-Zeilinger (GHZ) type [2] and *W* type [6]. Vectors belonging to GHZ and *W* types cannot be transformed into each other by local invertible and, in particular, local unitary [12] operations. Generically, a vector described by Eq. (1) is of the GHZ type, while *W* vectors can be written as

$$|\psi_W\rangle = \lambda_0|000\rangle + \lambda_1|100\rangle + \lambda_2|101\rangle + \lambda_3|110\rangle. \quad (2)$$

W vectors form a set of measure zero among all pure states [6]. Also, given a *W* vector one can always find a GHZ vector as close to it as desired by adding an infinitesimal λ_4 term to the right-hand side of Eq. (2). Furthermore, the so-called tangle, τ, introduced in [13], can be used to detect the type, since $\tau(|\psi_W\rangle) = 0$ [6].

Mixed states of three-qubit systems can be classified generalizing the classification of pure states. To this aim we define the following (see Fig. 1): (i) the class S of separable states, i.e., those that can be expressed as a convex sum of projectors onto product vectors; (ii) the class B of biseparable states, i.e., those that can be expressed as a convex sum of projectors onto product and bipartite entangled vectors (A-BC, B-AC, and C-AB); (iii) the class W of W states, i.e., those that can be expressed as a convex sum
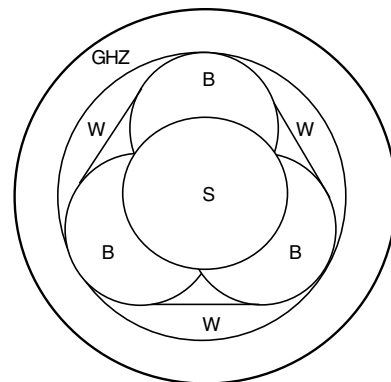

FIG. 1. Schematic structure of the set of all three-qubit states. *S*: separable class; *B*: biseparable class (convex hull of biseparable states with respect to any partition); *W* class and GHZ class.

of projectors onto product, biseparable, and W-type vectors; (iv) the class GHZ of GHZ states, i.e., the set of all physical states. All these sets are convex and compact, and satisfy $S \subset B \subset W \subset$ GHZ. States in S are not entangled. No genuine three-party entanglement is needed to prepare entangled states in the subset $B\backslash S$. The formation of entangled states in $W\backslash B$ requires W-type vectors with three-party entanglement, but zero tangle, which is an entanglement monotone decreasing under local operations and classical communication [6]. Finally, the class GHZ contains all types of entanglement, and, in particular, GHZ-type vectors are needed to prepare states from GHZ$\backslash W$. The introduced classes are invariant under local unitary or invertible nonunitary operations, while local POVM's can transform states only from a "higher" to a "lower" class.

Notice that since GHZ vectors can be expressed as the sum of only two product vectors, i.e., $|\text{GHZ}\rangle = (|000\rangle + |111\rangle)/\sqrt{2}$, whereas the minimum number of product terms forming a W vector is three [4,6], as in the state $|W\rangle = (|100\rangle + |010\rangle + |001\rangle)/\sqrt{3}$, our scheme may seem somehow counterintuitive. Indeed, for bipartite systems, states with lower Schmidt number, i.e., lower number of product terms in the Schmidt decomposition, are embedded into the set of states with higher Schmidt number [10]. One is tempted to extend this classification to tripartite systems as $S \subset B \subset$ GHZ $\subset W$, where now W is the set of all states. However, such generalization is evidently wrong, because the set of GHZ states in such classification cannot be closed.

Having established the structure of the set of mixed three-qubit states, we show how to determine to which class a given state ρ belongs. To this aim, we use the approach developed previously in the construction and optimization of witness operators [11,14,15].

We denote the range of ρ by $R(\rho)$, its rank by $r(\rho)$, its kernel by $K(\rho)$, and the dimension of $K(\rho)$ by $k(\rho)$. Following the approach of the best separable approximation [16], one can decompose any state ρ as a convex combination of a W-class state and a remainder δ,

$$\rho = \lambda_W \rho_W + (1 - \lambda_W)\delta, \qquad (3)$$

where $0 \le \lambda_W \le 1$, and $R(\delta)$ does not contain any W vector. Maximization of λ_W leads to the best W approximation of ρ. Notice that only for ρ belonging to the GHZ$\backslash W$ class, this decomposition is nontrivial, i.e., $\lambda_W \neq 1$. Also, $r(\delta) = 1$, since any subspace spanned by two linearly independent GHZ vectors contains at least one pure state with zero tangle. Therefore, any W approximation must have the form

$$\rho = \lambda_W \rho_W + (1 - \lambda_W)|\psi_{\text{GHZ}}\rangle\langle\psi_{\text{GHZ}}|. \qquad (4)$$

Similarly, one can express ρ in the best biseparable approximation as

$$\rho = \lambda_B \rho_B + (1 - \lambda_B)\delta, \qquad (5)$$

where now $R(\delta)$ must not contain any biseparable states,

i.e., $r(\delta) < 4$, since any N-dimensional subspace of the $2 \times N$ space contains at least one product vector [17].

We use the above decompositions to construct operators that detect the desired subset (see [15]). In analogy to entanglement witnesses and Schmidt witnesses we term these operators tripartite witnesses. The existence of witness operators is a consequence of the Hahn-Banach theorem, which states that a point outside a convex compact set is separated from that set by a hyperplane. The equation $\text{Tr}(\mathcal{W}\rho) = 0$ describes such a hyperplane, and one calls $\mathcal{W}$ a witness operator. For example, in our setting, a W witness is an operator $\mathcal{W}_W$ such that $\text{Tr}(\mathcal{W}_W \rho_B) \ge 0$ holds $\forall\ \rho_B \in B$, but for which there exists a $\rho_W \in W\backslash B$ such that $\text{Tr}(\mathcal{W}_W \rho_W) < 0$.

Any GHZ witness (W witness) has the canonical form $\mathcal{W} = Q - \epsilon\mathbb{1}$, where Q is a positive operator which has no W-type (B-type) vectors in its kernel; thus $k(Q) = 1$ [$k(Q) < 4$] [11,15]. An example of a GHZ witness is

$$\mathcal{W}_{\text{GHZ}} = \frac{3}{4}\mathbb{1} - P_{\text{GHZ}}, \qquad (6)$$

where P_{GHZ} is the projector onto $|\text{GHZ}\rangle$. The value 3/4 corresponds to the maximal squared overlap between $|\text{GHZ}\rangle$ and a W vector. This construction guarantees that $\text{Tr}(\mathcal{W}_{\text{GHZ}}\rho_W) \ge 0$ for any W state, and since $\text{Tr}(\mathcal{W}_{\text{GHZ}}P_{\text{GHZ}}) < 0$, there is a GHZ$\backslash W$ state which is detected by $\mathcal{W}_{\text{GHZ}}$. The maximal overlap is obtained as follows: due to the symmetry of $|\text{GHZ}\rangle$ we need to consider only W vectors that are symmetric under the exchange of any of the three qubits [18]. Therefore, we have to consider all local trilateral rotations of $|\psi_W\rangle = \kappa_0|000\rangle + \kappa_1(|100\rangle + |010\rangle + |001\rangle)$, where κ_0, κ_1 are real and $\kappa_0^2 + 3\kappa_1^2 = 1$. Because of the symmetry, such rotations can be parametrized for all parties as $|0\rangle \to \alpha|0\rangle + \beta|1\rangle$, $|1\rangle \to \beta^*|0\rangle - \alpha^*|1\rangle$, with $|\alpha^2| + |\beta^2| = 1$. Thus, the overlap $\langle\text{GHZ}|\psi_W\rangle$ is a function of six parameters with two constraints, and can be maximized using Lagrange multipliers. An optimal choice of parameters is $\kappa_0 = 0$, $\kappa_1 = 1/\sqrt{3}$, and $\beta = -\alpha = 1/\sqrt{2}$. This leads to $|\langle\text{GHZ}|\psi_W\rangle|^2_{\text{max}} = 3/4$.

Analogously, we can construct a W witness as

$$\mathcal{W}_{W_1} = \frac{2}{3}\mathbb{1} - P_W, \qquad (7)$$

where P_W is now the projector onto a vector $|W\rangle$, and 2/3 corresponds to the maximal squared overlap between $|W\rangle$ and a B vector. Another example of a W witness is

$$\mathcal{W}_{W_2} = \frac{1}{2}\mathbb{1} - P_{\text{GHZ}}, \qquad (8)$$

where now 1/2 is the maximal squared overlap between $|\text{GHZ}\rangle$ and a B type vector [19]. The W vector that has maximal overlap with $|\text{GHZ}\rangle$ is detected by $\mathcal{W}_{W_2}$.

The tripartite witness $\mathcal{W}_{W_2}$ allows one to prove that the class of mixed $W\backslash B$ states is not of measure zero: consider the family of states in $C^2 \otimes C^2 \otimes C^2$ given by the convex

sum of the identity and a projector onto a W-type vector that maximizes the squared overlap with $|GHZ\rangle$,

$$\rho = \frac{1-p}{8}\mathbb{1} + pP_W. \qquad (9)$$

Obviously, the states (9) belong at most to W. The range for the parameter p, in which $\mathcal{W}_{W_2}$ detects ρ, i.e., $\mathrm{Tr}(\mathcal{W}_{W_2}\rho) < 0$, is found to be $3/5 < p \leq 1$, and is bigger than the one found by using $\mathcal{W}_{W_1}$. Taking any p which has a finite distance to the border of this interval, i.e., $p - 3/5 > \Delta$ and $1 - p > \Delta$, it is always possible to find a finite region around ρ which still belongs to the $W \backslash B$ class. This can be seen by considering

$$\tilde{\rho} = (1-\epsilon)\left[\frac{1-p}{8}\mathbb{1} + pP_W\right] + \epsilon\sigma, \qquad (10)$$

where σ is an *arbitrary* density matrix, which covers all directions of possible deviations from ρ in the operator space. In the worst case σ is orthogonal to P_{GHZ}, so that $\mathrm{Tr}(P_{\mathrm{GHZ}}\sigma) = 0$, and therefore $\mathrm{Tr}(\mathcal{W}_{W_2}\tilde{\rho}) = (1-\epsilon)\mathrm{Tr}(\mathcal{W}_{W_2}\rho) + \epsilon/2$. As long as the relation $\epsilon < (5p - 3)/(5p + 1)$ holds, the corresponding state $\tilde{\rho}$ is still detected by $\mathcal{W}_{W_2}$. Moreover, one can also find a finite ϵ' such that if $\epsilon < \epsilon'$, then $\tilde{\rho}$ is in the W class. The bound ϵ' is obtained, for instance, by demanding that $(1-\epsilon')(1-p)\mathbb{1}/8 + \epsilon'\sigma$ is biseparable. The intersection of the two intervals gives a finite range for ϵ where the state $\tilde{\rho}$ is in the $W \backslash B$ class. This proves that the set of mixed $W \backslash B$ states contains a ball, i.e., is not of measure zero.

We discuss now some possible consequences of our results for PPTES of three qubits, for which the partial transposes ρ^{T_A}, ρ^{T_B}, and ρ^{T_C} are positive. Any of these states can be decomposed as

$$\rho = \lambda_S\rho_S + (1 - \lambda_S)\delta, \qquad (11)$$

where ρ_S is a separable state and δ is an edge state [20]. We conjecture that *PPTES cannot belong to the GHZ\W class*; i.e., they are at most in the W class. This conjecture is true for states that have edge states with low ranks in the above decomposition. It was shown in [17] that for bipartite systems in $C^2 \otimes C^N$, the rank of PPTES must be larger than N, and if $r(\rho) \leq N$ and $\rho^{T_A} \geq 0$, then the state ρ is separable. Thus, any PPTES of three qubits with $r(\rho) \leq 4$ is biseparable with respect to any partition; examples of such states are the UPB states from Ref. [7].

For the case of higher ranks we can give some support only for our conjecture. We proceed as in [11], and observe first that it suffices to prove the conjecture for the edge states. For these states, the sum of ranks satisfies $r(\delta) + r(\delta^{T_A}) + r(\delta^{T_B}) + r(\delta^{T_C}) \leq 28$ [20]. Any PPT entangled state can be detected only by a nondecomposable entanglement witness, which in the case of tripartite systems has the canonical form $\mathcal{W}_{nd} = \mathcal{W}_d - \epsilon\mathbb{1}$ where $\mathcal{W}_d = P + \sum Q_X^{T_X}$ is a decomposable operator

with $P, Q_X \geq 0$, $R(P) = K(\delta)$, $R(Q_X) = K(\delta^{T_X})$ for some edge state δ, and $X = A, B, C$ [20]. We restrict ourselves to edge states with the maximal sum of ranks, i.e., states δ with $[r(\delta), r(\delta^{T_A}), r(\delta^{T_B}), r(\delta^{T_C})] = [8, 8, 7, 5], [8, 8, 6, 6], [8, 7, 7, 6], [7, 7, 7, 7]$ and permutations. Indeed, if the conjecture is true for these states, it will be true for all edge states, and thus for all PPTES, since the edge states with maximal sum of ranks are dense in the set of all edge states [11]. We conjecture that for the case of edge states with maximal sum of ranks it is always possible to find a pure W-type vector, $|\phi_W\rangle$, such that for any nondecomposable witness $\mathcal{W}_{nd}$ of δ, $\langle\phi_W|\mathcal{W}_d|\phi_W\rangle \leq 0$, so that $\langle\phi_W|\mathcal{W}_{nd}|\phi_W\rangle < 0$. That means $\mathcal{W}_{nd}$ *cannot* be a GHZ witness, so the edge state δ belongs to the W class. If this holds for any δ it implies that all PPTES belong to the W class.

Any W vector can be obtained by local invertible operations applied to $|W\rangle$, i.e., can be written as

$$|\phi_W\rangle = \alpha_A|e_2, f_1, g_1\rangle + \alpha_B|e_1, f_2, g_1\rangle + \alpha_C|e_1, f_1, g_2\rangle. \qquad (12)$$

We denote

$$\begin{aligned}
|\Phi_A\rangle &= |e_2^*, f_1, g_1\rangle, \\
|\Psi_A\rangle &= \alpha_B|e_1^*, f_2, g_1\rangle + \alpha_C|e_1^*, f_1, g_2\rangle, \\
|\Phi_B\rangle &= |e_1, f_2^*, g_1\rangle, \\
|\Psi_B\rangle &= \alpha_A|e_2, f_1^*, g_1\rangle + \alpha_C|e_1, f_1^*, g_2\rangle, \\
|\Phi_C\rangle &= |e_1, f_1, g_2^*\rangle, \\
|\Psi_C\rangle &= \alpha_A|e_2, f_1, g_1^*\rangle + \alpha_B|e_1, f_2, g_1^*\rangle.
\end{aligned} \qquad (13)$$

In order to fulfill the condition $\langle\phi_W|\mathcal{W}_d|\phi_W\rangle \leq 0$ we demand that $Q_X|\Phi_X\rangle = 0$; $P|\phi_W\rangle = 0$, and $Q_X|\Psi_X\rangle = 0$ for $X = A, B, C$. The latter four conditions form four linear homogeneous equations for the α_X's, whose solutions exist if two 3×3 determinants vanish. Together with the first three conditions this gives at most five equations in the case $r(\delta) < 8$, and six equations in the worst case $r(\delta) = 8$, for the six complex parameters characterizing $|e_i\rangle$, $|f_i\rangle$, and $|g_i\rangle$, with $i = 1, 2$. For $r(\delta) < 8$ [$r(\delta) = 8$] one expects here a one complex parameter (finite, but large) family of solutions. At the same time $\langle\phi_W|\mathcal{W}_d|\phi_W\rangle = 2\mathrm{Re}\sum_X \alpha_X\langle\Psi_X^{*_X}|Q_X^{T_X}|\Phi_X^{*_X}\rangle$, (where $|\Phi^{*_X}\rangle$ denotes partial complex conjugation with respect to X), i.e., is a Hermitian form of α_X's, whose diagonal elements vanish, since $|\Psi_X\rangle$ does not depend on α_X. Employing the freedom of choosing the solutions from the family, one expects to find at least one with $\langle\phi_W|\mathcal{W}_d|\phi_W\rangle \leq 0$. In this way we obtain the W vector we were looking for. For the cases $[6, 8, 8, 6]$ and $[5, 8, 8, 7]$, a similar argument indeed shows that there should exist a biseparable state, $|\psi_B\rangle$, such that $\langle\psi_B|\mathcal{W}_{nd}|\psi_B\rangle < 0$. Note that the above method of searching $|\psi_W\rangle$ ($|\psi_B\rangle$) for a given δ, if successful, provides a sufficient condition for δ to belong to the W class (B class).

Finally, we present an example for a PPTES entangled edge state with ranks $[7,7,7,7]$. We introduce

$$\rho = \frac{1}{n} \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & a & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & b & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & c & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{c} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{b} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{a} & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \quad (14)$$

with $a, b, c > 0$ and $n = 2 + a + 1/a + b + 1/b + c + 1/c$. The basis is $\{000, 001, 010, 011, 100, 101, 110, 111\}$. This density matrix has a positive partial transpose with respect to each subsystem. One sees immediately that $r(\rho) = r(\rho^{T_A}) = r(\rho^{T_B}) = r(\rho^{T_{AB}}) = 7$. In order to check that ρ is a PPT entangled edge state, one has to prove that it is impossible to find a product vector $|\phi\rangle \in R(\rho)$, such that at the same time $|\phi^{*X}\rangle \in R(\rho^{T_X})$ for $X = A, B, C$. This, indeed, is not possible, as one readily concludes by looking at the kernels directly: one cannot find a product vector $|\phi\rangle$ that is orthogonal to $|000\rangle - |111\rangle$, whereas at the same time $|\phi^{*_A}\rangle \perp |011\rangle - c|100\rangle$, $|\phi^{*_B}\rangle \perp |010\rangle - b|101\rangle$, and $|\phi^{*_C}\rangle \perp |001\rangle - a|110\rangle$, unless the condition $ab = c$ is fulfilled. Thus, for generic a, b, c we have found a family of bound PPT entangled edge states of three qubits with maximal sum of ranks. By direct inspection we observe that ρ fulfills our conjecture, and is biseparable with respect to any partition. It can be written, e.g., as a sum of separable projectors and a B state acting in the 2×2 subspace spanned by Alice's space and the vectors $|00\rangle$ and $|11\rangle$ in Bob's-Charlie's space.

To summarize, we show that the set of density matrices for three qubits has an "onion" structure (see Fig. 1) and contains convex compact subsets of states belonging to the separable S, biseparable B, W and GHZ classes, respectively. We provide the canonical form of witness operators for the GHZ and W classes, and give the first examples of such witnesses. The study of the family of tripartite states given in Eq. (9) allows us to prove that the W class is not of measure zero. We conjecture and give some evidence that all PPTES of three-qubit systems do not require GHZ-type pure states for their formation. We formulate a sufficient condition which allows us to check constructively if a state belongs to the W class (B class). Finally, we present a family of PPT entangled edge states of three qubits with maximal sum of ranks.

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