

Optimal Entanglement Criterion for Mixed Quantum States

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We develop a strong and computationally simple entanglement criterion. The criterion is based on an elementary positive map Φ which operates on state spaces with even dimension $N \geq 4$. It is shown that Φ detects many entangled states with a positive partial transposition (PPT) and that it leads to a class of optimal entanglement witnesses. This implies that there are no other witnesses which can detect more entangled PPT states. The map Φ yields a systematic method for the explicit construction of high-dimensional manifolds of bound entangled states.

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Entanglement and quantum inseparability are key features of quantum mechanics which are connected to the tensor product structure of the state spaces of composite systems. A mixed state ρ of a bipartite system, for instance, is defined to be separable or classically correlated if it can be written as a convex linear combination of uncorrelated product states, i.e., if it can be represented in the form $\rho = \sum_i p_i \rho_1^i \otimes \rho_2^i$, where $\{p_i\}$ is a probability distribution and the ρ_1^i, ρ_2^i are density matrices describing states of the first and the second subsystem, respectively [1]. States which cannot be written in this way are called inseparable or entangled. Much effort in quantum information theory has been devoted to the problems of the characterization, the classification, and the quantification of mixed state entanglement [2,3]. Although considerable progress has been made in recent years (see, e.g., Refs. [4]), we are still far away from a true understanding of many aspects of these problems.

A problem of central importance in entanglement theory is the development of computationally efficient criteria which allow us to decide whether or not a given state is entangled. Peres [5] has developed a very strong entanglement criterion which is known as the criterion of positive partial transposition (PPT). It states that a necessary condition for a given state ρ to be separable is that its partial transpose is a positive operator. Usually, one writes this condition as $(I \otimes T)\rho \geq 0$, where T denotes the transposition of operators in a chosen basis and I is the identity map, indicating that the transposition is carried out only on the second part of the composite system. The PPT condition represents a necessary and sufficient separability criterion for certain low-dimensional systems [6], but it is only necessary in higher dimensions. Hence, there are generally entangled PPT states which belong to the class of bound entangled states [7].

The transposition T is a distinguished example of a positive but not completely positive map. This means that T maps all positive operators on the subsystems to positive operators, while there exist states ρ of the combined system for which $(I \otimes T)\rho$ has negative eigenvalues.

There are many other maps with this property. The significance of positive maps in entanglement theory is provided by a fundamental theorem established in Ref. [6]. This theorem states that a necessary and sufficient condition for a state ρ to be separable is that $(I \otimes \Lambda)\rho$ is positive for any positive map Λ . Hence, a given state is separable if and only if it remains positive under the application of all positive maps to one of its local parts.

By virtue of the PPT criterion, the development of appropriate separability criteria reduces to the construction of those positive maps which are able to detect entangled PPT states. Such maps are called nondecomposable [8] because they cannot be written as a sum of a completely positive map and of the composition of a completely positive map with the transposition map. However, this formulation does not lead to a simple operational entanglement criterion since the general structural characterization of positive maps is an unsolved mathematical problem. In particular, the explicit construction of nondecomposable positive maps turns out to be an extremely difficult task.

Here, we develop a universal nondecomposable positive map Φ which operates on the states of any state space with even dimension $N \geq 4$. The map Φ is composed of elementary operations and yields a very strong separability criterion which is particularly efficient for the identification of entangled PPT states. We show that Φ detects many entangled states in arbitrary dimensions which are neither detected by the PPT criterion nor by the strong realignment criterion [9,10].

It is known that positive maps are in one-to-one correspondence to certain observables called entanglement witnesses [11]. The map Φ constructed here has the remarkable property that it automatically leads for all N to entanglement witnesses which have the property of being *optimal*. This means that there are no other witnesses which are finer, i.e., which are able to identify more entangled PPT states. Moreover, we develop a systematic method for the explicit construction of high-dimensional manifolds of bound entangled states for arbitrary N .

We consider an N -state system with Hilbert space \mathbb{C}^N . Without loss of generality, we will regard \mathbb{C}^N as the state space of a particle with spin j , where $N = 2j + 1$. The corresponding basis states are denoted by $|j, m\rangle$, where $m = -j, -j + 1, \dots, +j$. Since we assume that N is even, the spin j must be half-integer valued.

An important ingredient of our separability criterion is the symmetry transformation of the time reversal which is described by an antiunitary operator θ [12]. As for any antiunitary operator, we can write $\theta = V\theta_0$, where θ_0 denotes the complex conjugation in the chosen basis $|j, m\rangle$, and V is a unitary operator. In the spin representation introduced above, the matrix elements of V are given by $\langle j, m' | V | j, m \rangle = (-1)^{j-m} \delta_{m', -m}$. For even N this matrix is not only unitary but also skew symmetric, i.e., we have $V^T = -V$, where T denotes the transposition. It follows that $\theta^2 = -I$, which leads to

$$\langle \varphi | \theta \varphi \rangle = 0. \quad (1)$$

This relation expresses a well-known property of the time reversal transformation θ which will play a crucial role in the following: For any state vector $|\varphi\rangle$ of the spin- j particle the time-reversed state $|\theta\varphi\rangle$ is orthogonal to $|\varphi\rangle$. This is a distinguished feature of even-dimensional state spaces, because unitary and skew-symmetric matrices do not exist in state spaces with odd dimension.

The action of the time reversal transformation on an operator B on \mathbb{C}^N can be expressed by

$$\vartheta B = \theta B^\dagger \theta^{-1} = V B^T V^\dagger. \quad (2)$$

This defines a linear map ϑ which transforms any operator B into its time-reversed operator ϑB . For example, if we take the spin operator \hat{j} of the particle, Eq. (2) gives the spin flip transformation $\vartheta \hat{j} = -\hat{j}$. According to the second relation in Eq. (2) the map ϑ is unitarily equivalent to the transposition map. Hence, the PPT criterion is equivalent to the condition that the partial time reversal ϑ_2 is positive:

$$\vartheta_2 \rho \equiv (I \otimes \vartheta) \rho \geq 0.$$

We define a linear map Φ which acts on operators B on \mathbb{C}^N as follows:

$$\Phi B = (\text{Tr} B) I - B - \vartheta B. \quad (3)$$

It will be demonstrated below that this map is positive but not completely positive. Hence, it yields the following necessary condition for separability:

$$\Phi_2 \rho \equiv (I \otimes \Phi) \rho \geq 0. \quad (4)$$

To motivate definition (3) we recall that in another separability criterion, known as reduction criterion [13,14], one uses the positive map defined by $\Lambda B = (\text{Tr} B) I - B$. Comparing this definition with Eq. (3), we see that $\Phi = \Lambda - \vartheta$. Hence, not only the map Λ of the reduction criterion and the time reversal ϑ are positive, but also their

difference $\Phi = \Lambda - \vartheta$. The criterion (4) can therefore be restated as $\Lambda_2 \rho - \vartheta_2 \rho \geq 0$. If ρ is a PPT state, i.e., if $\vartheta_2 \rho \geq 0$ we subtract a positive operator from $\Lambda_2 \rho$ when evaluating condition (4), which sharpens the condition of the reduction criterion considerably. For this reason the inequality (4) can be expected to yield a very strong separability criterion which is particularly suited to recognize the entanglement of PPT states.

It is easy to prove the positivity of the map Φ defined by Eq. (3). We have to show that for any positive operator B also the operator ΦB is positive. This statement is obviously equivalent to the statement that the operator $\Phi(|\varphi\rangle\langle\varphi| \otimes |\varphi\rangle\langle\varphi|)$ is positive for any normalized state vector $|\varphi\rangle$. Using definition (3) we find

$$\Phi(|\varphi\rangle\langle\varphi|) = I - |\varphi\rangle\langle\varphi| - |\theta\varphi\rangle\langle\theta\varphi| \equiv I - \Pi.$$

Because of Eq. (1) the operator Π introduced here represents an orthogonal projection operator which projects onto the subspace spanned by $|\varphi\rangle$ and $|\theta\varphi\rangle$. It follows that also $\Phi(|\varphi\rangle\langle\varphi|)$ is a projection operator and, hence, that it is positive for any normalized state vector $|\varphi\rangle$. This proves our claim. Note that for $N = 2$ the projection Π is identical to the unit operator such that Φ is equal to the zero map in this case. For this reason we restrict ourselves to the cases of even $N \geq 4$.

To show that the map Φ is not completely positive we consider the tensor product space $\mathbb{C}^N \otimes \mathbb{C}^N$ of two spin- j particles. The total spin of the composite system will be denoted by J . According to the triangular inequality J takes on the values $J = 0, 1, \dots, 2j = N - 1$. The projection operator which projects onto the manifold of states corresponding to a definite value of J will be denoted by P_J . In particular, P_0 represents the one-dimensional projection onto the maximally entangled singlet state $J = 0$. We define a Hermitian operator W by applying the tensor extension of Φ to the singlet state:

$$\begin{aligned} W &\equiv N(I \otimes \Phi) P_0 \\ &= -(N - 2)P_0 + 2P_2 + 2P_4 + \dots + 2P_{2j-1}. \end{aligned} \quad (5)$$

In the second line we have used definition (3), the fact that the sum of the P_J is equal to the unit operator, the relation $\text{Tr}_2 P_0 = I/N$ (Tr_2 denotes the partial trace taken over subsystem 2), and the formula [15]

$$\vartheta_2 P_0 = \frac{1}{N} F = -\frac{1}{N} \sum_{J=0}^{2j} (-1)^J P_J, \quad (6)$$

where F denotes the swap operator which is defined by $F|\varphi_1\rangle \otimes |\varphi_2\rangle = |\varphi_2\rangle \otimes |\varphi_1\rangle$. We infer from Eq. (5) that the operator W has the negative eigenvalue $-(N - 2)$ corresponding to the singlet state $J = 0$. Therefore, W is not positive and the map Φ is not completely positive.

Next we show that the criterion (4) detects entangled PPT states for all even $N \geq 4$. To this end, it is again useful to employ the operator W defined by Eq. (5). Since Φ is

positive, but not completely positive, W is an entanglement witness [6,16]. We recall that an entanglement witness is a Hermitian operator which satisfies $\text{Tr}\{W\sigma\} \geq 0$ for all separable states σ , and $\text{Tr}\{W\rho\} < 0$ for at least one entangled state ρ , in which case we say that W detects ρ . A witness W is called nondecomposable if it can detect entangled PPT states [11]. We prove that there are always entangled PPT states ρ which are detected by the witness defined in Eq. (5), i.e., for which $\text{Tr}\{W\rho\} < 0$. In other words, our witness W is nondecomposable. This implies that also Φ is nondecomposable and that the stronger criterion (4) always detects entangled PPT states.

Consider the following one-parameter family of states:

$$\rho(\lambda) = \lambda P_0 + (1 - \lambda)\rho_0, \quad 0 \leq \lambda \leq 1. \quad (7)$$

These normalized states are mixtures of the singlet state P_0 and of the state

$$\rho_0 = \frac{2}{N(N+1)} P_S = \frac{2}{N(N+1)} \sum_{J \text{ odd}} P_J$$

which is proportional to the projection P_S onto the subspace of states which are symmetric under the swap operation. Note that ρ_0 is a separable state which belongs to the class of Werner states [1]. Since P_S can be written as a sum over the projections P_J with odd J , we immediately get, with the help of Eq. (5),

$$\text{Tr}\{W\rho(\lambda)\} = -\lambda(N-2).$$

Hence, we find that $\text{Tr}\{W\rho(\lambda)\} < 0$ for $\lambda > 0$. We conclude that all states of the family (7) corresponding to $\lambda > 0$ are entangled, and that ρ_0 is the only separable state of this family. On the other hand, using the representation $P_S = (I + F)/2$ and Eq. (6) we find

$$\vartheta_2\rho(\lambda) = \frac{1-2\lambda}{N} P_0 + \frac{1}{N} \sum_{j=1}^{2j} \left[(-1)^{j+1} \lambda + \frac{1-\lambda}{N+1} \right] P_j.$$

It is not hard to check by means of this equation that the PPT condition $\vartheta_2\rho(\lambda) \geq 0$ is equivalent to $\lambda \leq 1/(N+2)$. Hence, all $\rho(\lambda)$ with $0 < \lambda \leq 1/(N+2)$ are entangled PPT states which are detected by the witness W . This proves that the witness W and the map Φ are nondecomposable.

The above argument demonstrates that the inequality $\text{Tr}\{W\rho\} \geq 0$ represents a necessary and sufficient separability condition for the family of states (7). Obviously, this criterion cannot be improved by introducing other witnesses which leads to the idea that W is an optimal entanglement witness. To make this idea more precise we introduce the following notations [11]. We denote by D_W the set of all entangled PPT states of the total state space which are detected by some given nondecomposable witness W . A witness W_2 is said to be finer than a witness W_1 if D_{W_1} is a subset of D_{W_2} , i.e., if all entangled PPT states which are detected by W_1 are also detected by W_2 . A given

witness is said to be optimal if there is no other witness which is finer, i.e., if there is no other witness which is able to detect more entangled PPT states. It is a remarkable fact that our witness W is always optimal in this sense.

Theorem.—The operator $W = N(I \otimes \Phi)P_0$ on $\mathbb{C}^N \otimes \mathbb{C}^N$ is a nondecomposable optimal entanglement witness for all even $N \geq 4$.

Proof: The proof is based on results of Lewenstein, Kraus, Horodecki, and Cirac [17]. Following these authors we define for any given entanglement witness W the set Γ_W as the set of all product vectors $|\varphi_1, \varphi_2\rangle \equiv |\varphi_1\rangle \otimes |\varphi_2\rangle$ in $\mathbb{C}^N \otimes \mathbb{C}^N$ for which the expectation value of W is equal to zero, i.e., for which the relation

$$\langle \varphi_1, \varphi_2 | W | \varphi_1, \varphi_2 \rangle = 0 \quad (8)$$

holds. According to Ref. [17] a given nondecomposable entanglement witness W is optimal if the elements of the set Γ_W as well as the elements of the set $\Gamma_{\vartheta_2 W}$ span the total state space $\mathbb{C}^N \otimes \mathbb{C}^N$. In the present case we have $\vartheta_2 W = W$ which follows from the relation $\vartheta\Phi = \Phi$ [see Eq. (3)]. Hence, we only have to show that the elements of Γ_W corresponding to our witness W span the state space of the composite system.

The elements of Γ_W can easily be characterized. We take any normalized product vector $|\varphi_1\rangle \otimes |\varphi_2\rangle$ and use definitions (5) and (3) to evaluate the condition (8):

$$\langle \varphi_1, \varphi_2 | W | \varphi_1, \varphi_2 \rangle = 1 - |\langle \varphi_1 | \varphi_2 \rangle|^2 - |\langle \varphi_1 | \theta \varphi_2 \rangle|^2 = 0.$$

This equation is fulfilled if and only if $|\varphi_1\rangle$ lies in the subspace spanned by the orthogonal vectors $|\varphi_2\rangle$ and $|\theta\varphi_2\rangle$. In particular, all product vectors of the form

$$|\varphi\rangle \otimes |\theta\varphi\rangle \quad \text{or} \quad |\theta\varphi\rangle \otimes |\varphi\rangle \quad (9)$$

belong to Γ_W , where $|\varphi\rangle \in \mathbb{C}^N$ is arbitrary.

Consider now an arbitrary product vector $|\phi_1\rangle \otimes |\phi_2\rangle$, and define $|\varphi_1\rangle = |\theta\phi_1\rangle + |\phi_2\rangle$ and $|\varphi_2\rangle = i|\theta\phi_1\rangle + |\phi_2\rangle$. Then one can easily check the following identity:

$$\begin{aligned} |\phi_1\rangle \otimes |\phi_2\rangle &= -\frac{1}{2} |\theta\varphi_1\rangle \otimes |\varphi_1\rangle - \frac{i}{2} |\theta\varphi_2\rangle \otimes |\varphi_2\rangle \\ &\quad - \frac{1}{2} (1+i) |\phi_1\rangle \otimes |\theta\phi_1\rangle \\ &\quad + \frac{1}{2} (1+i) |\theta\phi_2\rangle \otimes |\phi_2\rangle. \end{aligned}$$

The right-hand side of this identity is a linear combination of four product vectors of the form (9). We conclude that any product vector $|\phi_1\rangle \otimes |\phi_2\rangle$ can be represented as a linear combination of elements of Γ_W . Since any state vector in $\mathbb{C}^N \otimes \mathbb{C}^N$ can of course be written as linear combination of product vectors, this implies that any state vector can be represented as linear combination of elements of Γ_W . In other words, the set Γ_W indeed spans the whole Hilbert space, which proves the theorem.

Because of its optimality the separability criterion (4) can be much stronger than other known separability crite-

ria. Let us illustrate this point by means of the family of states defined by Eq. (7). Each separability criterion recognizes the entanglement of the states $\rho(\lambda)$ with $\lambda^c < \lambda \leq 1$, where λ^c is a certain threshold value depending on the criterion chosen. The weakest criterion is the reduction criterion which gives $\lambda^c = 1/N$. The same result is obtained if one uses the majorization criterion [18] or the quantum Rényi entropy S_∞ [13]. Surprisingly, the realignment criterion, which is known to be able to recognize many entangled PPT states, is not stronger than the reduction criterion in the present case, i.e., we again have $\lambda^c = 1/N$. The PPT criterion is slightly better and yields $\lambda^c = 1/(N+2)$. As shown above, the most efficient criterion is obtained by means of the map Φ which leads to the optimal value $\lambda^c = 0$.

A further instructive example is given by the set of rotationally symmetric states [19] on the state space $\mathbb{C}^4 \otimes \mathbb{C}^4$. These are the states of a system which is composed of two particles with spin $j = 3/2$ and which is invariant under unitary product representations of the group $SU(2)$. As shown in [15] the map Φ detects *all* entangled PPT states in this case, i.e., the inequality $\Phi_2 \rho \geq 0$ taken together with the PPT criterion $\vartheta_2 \rho \geq 0$ represents a necessary *and* sufficient separability condition for all $SU(2)$ -invariant states.

The map Φ is not only useful in detecting entangled PPT states but also provides us with a simple and systematic method of constructing high-dimensional manifolds of such states for arbitrary dimensions N . We take any entangled PPT state ρ_{ppt} which is detected by W , e.g., a PPT state of the family (7). Then

$$\rho = \rho_{\text{ppt}} + \sum_{\alpha} p_{\alpha} |\varphi_1^{\alpha}, \varphi_2^{\alpha}\rangle \langle \varphi_1^{\alpha}, \varphi_2^{\alpha}| \quad (10)$$

is again an (unnormalized) entangled PPT state, where $p_{\alpha} \geq 0$ and the sum is extended over an arbitrary collection of product vectors $|\varphi_1^{\alpha}, \varphi_2^{\alpha}\rangle$ taken from Γ_W . We have a large freedom in the choice of these vectors: The only condition is that for each α the state $|\varphi_1^{\alpha}\rangle$ lies in the subspace which is spanned by $|\varphi_2^{\alpha}\rangle$ and $|\theta\varphi_2^{\alpha}\rangle$. For example, identifying the index α with the quantum number m we can choose $|\varphi_2^{\alpha}\rangle = |j, m\rangle$ and $|\varphi_1^{\alpha}\rangle = |j, m\rangle$ or $|\varphi_1^{\alpha}\rangle = |j, -m\rangle$. Equation (10) then represents a $2N$ -dimensional manifold of entangled PPT states.

Summarizing, we have constructed a universal nondecomposable positive map which leads to a powerful separability criterion and to a class of optimal entanglement witnesses. Our results suggest many further studies and applications. An important issue, for example, is the investigation of the properties of entanglement measures. Recently, Chen, Alberverio, and Fei [20] have derived lower bounds for the concurrence [21] and for the entanglement

of formation [22] by connecting these entanglement measures with the PPT criterion and the realignment criterion. It is very likely that this connection can be extended to the optimal entanglement criterion developed here, which will yield a considerable improvement of the known analytical bounds for entanglement measures.

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