Bipartite entanglement of quantum states in a pair basis

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Even if entanglement is a fundamental tool for quantum technologies, its non ambiguous detection and quantification is still limited to low dimensions or specific classes of states. In this sense every extension beyond such special cases is of the utmost importance. Here, we consider quantum states in arbitrary $d \times d$ dimensions, particularly relevant to quantum optics, written in terms of a pair basis where each state in the subsystem $A$ is paired with only one state in $B$. We extend the class of states for which negativity is a necessary and sufficient measure of entanglement to mixtures of states in a pair basis. In addition, we provide analytical expressions for a tight lower-bound estimation of the entanglement of formation, a central quantity for quantum information applications.

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Quantum entanglement attracts a considerable interest due to its fundamental role as a resource for quantum information processes [14]. For this reason it is necessary to conceive efficient and reliable measures to estimate it [5 8]. While bipartite entanglement in a pure state can be measured using the Von Neumann entropy as well as other entanglement monotones, the problem of its evaluation is still open in the case of a general mixed state. A significant step forward has been done with the proof that the bipartite entanglement in a general mixed state of a system of dimension $2 \times 2$ is suitably quantified by the concurrence [7]. In $d \times d$ dimensions, with $d \geq 3$, a suitable measure has not yet been found except in the presence of special symmetries, like in the case of Werner states [9]. A computable measure in arbitrary dimension is the negativity [10], which can be evaluated for different physical systems [11 12], but in general it represents only a sufficient condition for entanglement.

Here we consider the case of an arbitrary dimension $d$ where the pure states, parted in two subsystems $A$ and $B$, have the form

$$|\Psi\rangle = \sum_{i=1}^{d} c_i |\phi_i\rangle_A \otimes |\chi_i\rangle_B , \quad \sum_{i} |c_i|^2 = 1, \quad (1)$$

namely a projection has been applied into a subspace where every state $\phi_i$ in $A$ is paired with only one state $\chi_i$ in $B$, forming a set of factorized states that we call pair basis. This particular reduction of the Hilbert space occurs in a variety of physical situations, the most remarkable one represented by two-mode Gaussian states in quantum optics [3 13 15], that include twin-beam states, a key element of quantum communication, metrology and sensing. In atomic physics, bosonic atoms trapped in double wells have the same structure as in (1) where the conservation of the total number $N$ imposes that each state $|n\rangle$ of $n$ bosons in one well is paired with the state $|N-n\rangle$ in the other well. Also for electron models in a lattice one may be interested to restrict the total Hilbert space of two-sites to the pair basis $\{|\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\uparrow\uparrow\rangle, |\downarrow\downarrow\rangle\}$, i. e. the sector of zero magnetization and two electrons, thanks to the presence of special quantum numbers.

In this Letter, we address the problem of evaluating the entanglement of mixtures of states written in the pair basis (1), identifying a suitable measure. In addition, we will estimate lower bounds to the entanglement of formation (EOF), a relevant quantity from the perspective of quantum information.

**Pure states** Given the orthonormality of both bases $|\phi_i\rangle_A$ and $|\chi_i\rangle_B$, the Schmidt decomposition of states of the form (1) is just written in the same basis, but with the non negative coefficients $\mu_i = |c_i|$. The Schmidt coefficients $\mu_i$ are the square roots of the eigenvalues of the reduced density matrix $\rho_A = \text{Tr}_B \rho$. It follows that the only factorized states are those for which $c_i = 0$ for every $i$ except one. The entanglement of the pure state $|\Psi\rangle$ is estimated by the von Neumann entropy $S^{(d)}(\rho) = -\sum_{i=1}^{d} \mu_i^2 \log \mu_i^2$. From now on, we shall adopt the short-hand notation $|i,i\rangle$ in place of the pair basis set $|\phi_i\rangle_A \otimes |\chi_i\rangle_B$ used in Eq.(1).

For estimating the entanglement of pure states, in this work we use a generalization of the concurrence that we construct in the following way. First, let us consider the easiest case $d = 2$ with the two elements of the basis $|0,0\rangle$ and $|1,1\rangle$. In the full 4-dimensional space the double spin-flip operation is performed by $\sigma^x \otimes \sigma^y$, and the concurrence is given by the well-known formula $C = |\langle \psi | \sigma^x \otimes \sigma^y | \psi \rangle| = 2 |c_1 c_2|$, where the swap is represented by the single Pauli matrix $\sigma^z$.

As an extension to the $d$-dimensional case we take the sum of the concurrences of every possible pair, that gives the quantity

$$D(\Psi) = 2 \sum_{i<j} |c_i c_j| = (\text{Tr} \sqrt{\rho_A})^2 - 1. \quad (2)$$
Now, in addition to the diagonal part of $P$ to the original Hilbert space of $\rho$, we may consider the operation of partial transposition (LOCC) for every mixed state in arbitrary dimension under local operations and classical communication. The operation of partial transposition is that it represents an entanglement monotone under local operations and classical communication, which is a convex function and is a good measure of entanglement for any mixture and is zero only for factorizable states.

As a matter of fact, the operation of partial transposition introduces non vanishing matrix elements outside the original Hilbert space of $|\Psi\rangle$ in Eq. (1), obtaining

$$\langle i, j | \rho^{T_A} | i', j' \rangle = \delta_{ij}\delta_{c_jc_j'c_j'c_j'}.$$  

Now, in addition to the diagonal part of $\rho$ that is left unchanged, the matrix $\rho^{T_A}$ displays $2 \times 2$ blocks of the form

$$
\begin{pmatrix}
0 & c_j^* c_j \\
c_j^* c_j & 0
\end{pmatrix}
$$

for every pair $i < j$ in the subspace formed by the two basis vectors $|i, j \rangle$ and $|j, i \rangle$. The eigenvalues of such blocks turn out to be pairs of opposite numbers $\pm |c_j c_j|$, signaling the presence of entanglement in virtue of a negative eigenvalue. Thus, the negativity for pure states amounts to

$$N(\Psi) = \sum_{i \neq j} |c_i c_j|.$$  

and is zero only for factorizable states.

**Mixed states** A fundamental property of the negativity is that it represents an entanglement monotone under local operations and classical communication (LOCC) for every mixed state in arbitrary dimension. Specifically, $N(P(\rho)) \leq N(\rho)$ for an arbitrary LOCC $P(\rho)$. Moreover, the negativity is a convex function, i.e., $N(\sum_{i} p_i \rho_i) \leq \sum_{i} p_i N(\rho_i)$, with weights obeying to $\sum_{i} p_i = 1$ and $p_i \geq 0$, $\forall i$.

The extension of Eq. (3) to an arbitrary mixed state $\rho_{ij}$ written in the same pair basis as in Eq. (1), is

$$N(\rho) = \sum_{i < j} |\rho_{ij}|.$$  

which is a good measure of entanglement for any mixture of states in pair basis, since it is a convex function and it vanishes only in absence of off-diagonal terms of $\rho_{ij}$, i.e., for factorizable states. In other words, a necessary and sufficient condition for having entanglement is the non vanishing of negativity, a property which is not valid for general states. In addition, the monotonicity of $N(\rho)$ introduces a ordering in terms of entanglement content. Despite its simplicity, Eq. (4) constitutes an important result, which may reveal of great utility in the evaluation of entanglement in several systems expressable in a pair basis. Along the same line, one can compute the logarithmic negativity $E_N(\rho) = \log \left( \rho^{T_A} \right) = \log(1 + 2 \sum_{i < j} |\rho_{ij}|)$, which bounds the distillable entanglement of $\rho$ [10, 11].

**Entanglement of formation** The EOF $E_f(\rho)$ is defined as the convex roof

$$E_f(\rho) = \min_{\{p_k, \psi_k\}} \sum_{k=1}^{d} p_k S^{(d)}(\psi_k).$$  

that gives the minimum entanglement over all possible decompositions of $\rho = \sum_k p_k |\psi_k\rangle \langle \psi_k|$ into pure states $|\psi_k\rangle$, $k = 1, \ldots, d$, with weights $p_k$. The calculation of $E_f$ for general states is notoriously a formidable task. However, for our class of states we are able to establish some tight lower bounds of $E_f$ of evident use in a variety of applications.

In our case, the task is somewhat facilitated by the crucial property that every single element $|\psi_k\rangle$ of the decomposition must be also restricted to the same pair basis as $\rho$. In fact, the diagonal elements $\langle ij | \rho | ij \rangle = 0$ for $i \neq j$, can only originate from a convex combination of zero diagonal elements $\langle ij | p_k | ij \rangle = 0$, since they are non negative by definition, as well as the weights $p_k$. As a consequence, even the off-diagonal elements of $\rho_{ij}$ that lie outside the pair basis are zero.

The entanglement of any pure state in Eq. (1) is determined by $d - 1$ parameters, the Schmidt weights $\mu_j$, with the normalization condition. As known these coefficients cannot be inferred by the partial trace in the mixed case. Instead, we want to relate them to the off-diagonal entries of $\rho_{ij}$. After relabeling the states in decreasing order, $\mu_1 < \mu_2 < \cdots < \mu_d$ (corresponding to $\Gamma_1 < \Gamma_2 < \cdots < \Gamma_d$), one can write the relations

$$\mu^2_{d} = \frac{1}{2} \left( 1 - \epsilon_{1} \sqrt{1 - 4\Gamma_{d}^2} \right)$$  

with the auxiliary quantities

$$\Gamma_{d}^2 = \mu^2_{d}(1 - \mu^2_{d}) = \sum_{j \neq d} \mu^2_{j} \mu^2_{d} = \sum_{j \neq d} |\rho_{ij}|^2$$  

where the signs $\epsilon_{i}$ are all 1 except for $\epsilon_{1} = -1$ when $|\mu_{1}|^2 > 1/2$. Of course, for pure states the quantities $|\rho_{ij}|^2$ are overdetermined, so there are many ways to take $d - 1$ of them which are independent. One way to avoid such a overdetermination is to consider only the first row of the density matrix, obtaining $\mu^2_{j} = |\rho_{ij}|^2/\mu^2_{j}$, $j = 2, \ldots, d$, and $\mu^2_{1}$ as in Eq. (6). After these considerations, we are able to find a lower bound to the EOF, by means of the following:
Theorem. Given a generic state with density matrix \( \rho \) in the relabeled pair basis with \( \Gamma_1 < \Gamma_2 < \cdots < \Gamma_d \), we have
\[
E_f(\rho) \geq F(\mathbf{x}) \equiv -\sum_{i=1}^{d} \alpha_i^2(\mathbf{x}) \log \alpha_i^2(\mathbf{x})
\]
where
\[
\alpha_1^2 = \frac{1}{2} \left( 1 + \sqrt{1 - 4|x|^2} \right); \quad \alpha_i^2 = \frac{|x_i|^2}{\alpha_1^2}, \; i = 2, \ldots, d
\]
and the components of the vector \( \mathbf{x} \equiv \{\rho_{ii}, \; i = 2, \ldots, d\} \) are the \( d - 1 \) off-diagonal elements in the first row of \( \rho \), which act as independent parameters.

Proof. Let us assume that there exist an optimal decomposition of \( \rho = \sum_k p_k |\psi_k(\mathbf{x})\rangle \langle \psi_k(\mathbf{x})| \) formed by an ensemble of pure states \( \{p_k, |\psi_k(\mathbf{x})\rangle\} \). Clearly, the matrix elements of \( \rho \) are given by the convex sum \( \mathbf{x} = \sum_k p_k \mathbf{x}^k \). The EOF is lower bounded by \( F(\mathbf{x}) \) thanks to
\[
E_f(\rho) = -\sum_k p_k \left( \sum_{i=1}^{d} \alpha_i^2(\mathbf{x}^k) \log \alpha_i^2(\mathbf{x}^k) \right) \\
\geq -\sum_k p_k \left( \sum_{i=1}^{d} \alpha_i^2(\mathbf{x}^k) \log \alpha_i^2(\mathbf{x}^k) \right) \\
= \sum_k p_k F(\mathbf{x}^k) \geq F(\mathbf{x}).
\]

The first inequality has been obtained by observing that for all \( z \in [0, 1] \), we get
\[
\frac{1}{2} \left( 1 + \sqrt{1 - z} \right) \log \left[ \frac{1}{2} \left( 1 + \sqrt{1 - z} \right) \right] \leq \frac{1}{2} \left( 1 - \sqrt{1 - z} \right) \log \left[ \frac{1}{2} \left( 1 - \sqrt{1 - z} \right) \right],
\]
thus eliminating the problem of determining the sign \( c_1 \). The second inequality holds thanks to the convexity of \( F(\mathbf{x}) \) over its domain \( \mathbf{x} : |x|^2 \in [0, \frac{1}{2}] \). After observing that \( F \) depends only on the moduli of the components of \( \mathbf{x} \), we get
\[
\sum_k p_k F(\mathbf{x}^k) = \sum_k p_k F(|x_i^k|^2) \geq F(\{\sum_k p_k |x_i^k|^2\}) \\
\geq F(\{\sum_k p_k \mathbf{x}^k_i|2\}) = F(\mathbf{x}),
\]
where the first inequality comes from the convexity of \( F(\mathbf{v}) \) as a function of a real vector \( \mathbf{v} \), such that \( |\mathbf{v}|^2 \in [0, \frac{1}{2}] \), while the second inequality is a consequence of the triangular relation \( |z + w| \leq |z| + |w| \), with \( z, w \in \mathbb{C} \) and the monotonicity of \( F(\mathbf{v}) \) with respect to any of its components. The latter property can be easily proven by calculating \( \nabla F(\mathbf{v}) \) and checking it is non negative for \( |\mathbf{v}|^2 \in [0, \frac{1}{2}] \). For showing that \( F(\mathbf{v}) \) is convex it is sufficient to calculate the Hessian \( H_F(\mathbf{v}) \) and check that its eigenvalues are non negative within the domain. This task is rather cumbersome to perform analytically due to the presence of trascendental functions; however it can be inspected numerically in low dimension. In \( d = 3 \) we can represent graphically the function \( F(\mathbf{v}) \) and check its concavity (See Fig. 1). We have numerically verified the positivity of \( H_F(\mathbf{v}) \) up to \( d = 10 \) for thousands of sample states. Conjecturing that the property of convexity holds for every \( d \), the theorem is proven in every dimension. \( \square \)

A step further in the seek of lower bounds for the EOF can be made by defining the function \( G(\mathbf{x}) \) in a similar way as \( F(\mathbf{x}) \) in Eqs. [5] and [8], but with
\[
\alpha_1^2 = \frac{1 + \sqrt{1 - 4|x_1|^2}}{2}, \\
\alpha_i^2 = \frac{1 + \sqrt{1 - 4|x_i|^2}}{2}, \; i = 2, \ldots, d
\]
where \( x_i \equiv \{\rho_{ii}, \; i = 2, \ldots, d\} \) and \( x_l \equiv \{\rho_{ii}, \; i = 2, \ldots, d\} \). In this new defini-
is no unique correspondence between negativity and entropy for $d > 2$. However, one may introduce a convex function $s(N)$, that for any $N$ is not larger than the minimum entropy $S_{\min}^{(d)}(N) = \min_{|\psi_k\rangle} S^{(d)}(\psi_k)$ in the manifold of all states $|\psi_k\rangle$ with a given negativity $N$. Such an optimization problem has been solved in Ref. [17], with solution

$$s(x) = \begin{cases} H_2(\gamma) + (1 - \gamma) \log(d - 1), & N \in \left[0, \frac{3}{2} - \frac{2}{d} \right] \\ \frac{2N + 1 - x}{d - 1} \log(d - 1) + \log d, & N \in \left[\frac{3}{2} - \frac{2}{d}, \frac{d - 1}{2} \right] \end{cases}$$

where

$$\gamma(N) = \frac{1}{d} \left[ \sqrt{2N + 1} + \sqrt{(d - 1)(d - 2N - 1)} \right]^2.$$ 

By assuming first to know the optimal decomposition $\{p_k, |\psi_k\rangle\}$ that gives the minimum in Eq. (5), one can apply the inequalities

$$E_f(\rho) \geq \sum_k p_k \min_{|\psi_k\rangle} S^{(d)}(\psi_k) \geq \sum_k p_k s(N(\psi_k))$$

$$\geq s \left( \sum_k p_k N(\psi_k) \right) \geq s(N(\rho)), \quad (11)$$

thanks to the convexity of both $s$ and $N$. It is clear that the function $s(N(\rho))$ sets a lower bound to the EOF of $\rho$. The advantage of introducing the function $s$ is to establish a 1-1 relationship between negativity and EOF, like in the two-qubit case. On the one hand, this lower bound to EOF is exact for isotropic states [17] and in our case work very well for states where the off-diagonal terms assume very similar values. On the other hand, $F$ and $G$ set better lower bounds for states where few $\Gamma_j$’s dominate over the others. In particular, in large dimensions when $d \gg N$, the leading term $s(N) \approx (2N - 1)d^{-1} \log d$ goes to zero, which is of course a very low estimation of EOF for a state with a finite $N$.

After having identified the above quantities, it is clear that the best estimation of the EOF is given by $\max F(\rho), G(\rho), s(\rho)$ for an arbitrary state $\rho$. In Fig. 3 we show a comparative plot of the three lower bounds $F$, $G$, and $s$ for some randomly generated states, ordered according to their negativity. We can see that the lower bound $G$ tends to dominate as the dimension is increased, while $s$ is a good estimation of EOF for states close to the maximally entangled one.

**Conclusions** In this Letter, we have extended the family of states for which the negativity is a necessary and sufficient condition for entanglement. We have considered density matrices given by mixtures of pure states written in the paired form of Eq. (1), a class of states that occurs in a variety of relevant physical situations. We have also found new lower bounds improving the estimation of the EOF with respect to other quantities known in the literature. We believe that in future works, the ideas here outlined for determining the functions $F$ and

![Figure 2](image2.png)  
**Figure 2:** The average entanglement (horizontal axis) is plotted against the function $G$ (vertical axis) for several density matrices $\rho$ in various dimensions $d$. Each point is calculated from a set of randomly generated pure states, combined with random weights. The fact that all the points lie below the bisector line, constitutes a stochastic demonstration that $G$ is a lower bound to the EOF. The sample states are not completely random but are built by choosing decompositions close to the optimal one (see text).

![Figure 3](image3.png)  
**Figure 3:** The maximum between the lower bounds to the EOF in various dimensions $d$. Circles (blue), squares (red) and rhombs (yellow) represent $F(\rho)$, $G(\rho)$ and $s(\rho)$, respectively. The sample states $\rho$ are arranged according to their negativity $N$ (horizontal axis). For reference, we have plotted the curve $s(N)$. 

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$G$ may be extended to the completely general case.

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