Tight bounds on the concurrence of quantum superpositions

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The entanglement content of superpositions of quantum states is investigated based on a measure called *concurrence*. Given a bipartite pure state in arbitrary dimension written as the quantum superposition of two other such states, we find simple inequalities relating the concurrence of the state to that of its components. We derive an exact expression for the concurrence when the component states are biorthogonal and provide elegant upper and lower bounds in all other cases. For quantum bits, our upper bound is tighter than the previously derived bound [N. Linden *et al.*, Phys. Rev. Lett. **97**, 100502 (2006)].

I. INTRODUCTION

Consider a quantum state $|\Psi\rangle$ of two parties, Alice and Bob, written as the superposition of two arbitrary states

$$|\Psi\rangle = \alpha|\phi\rangle + \beta|\varphi\rangle, \tag{1}$$

with $|\alpha|^2 + |\beta|^2 = 1$. We are interested in the relation between the entanglement of $|\Psi\rangle$ and that of $|\phi\rangle$ and $|\varphi\rangle$. This problem was recently addressed by Linden, Popescu, and Smolin in Ref. [1], where an upper bound on the entanglement of $|\Psi\rangle$ was derived using the *entanglement of formation* $E_f(\Psi)$ as a measure of entanglement—i.e., the von Neumann entropy of the reduced state of either party. When Alice and Bob hold two-dimensional quantum systems (qubits), the entanglement of formation $E_f(\Psi)$ completely characterizes the entanglement of the pure state $|\Psi\rangle$. However, for higher-dimensional systems (and in the case of a finite number of copies), the measure of entanglement is not unique and $E_f(\Psi)$ alone is not sufficient to completely describe the entanglement of a bipartite pure state. With a pair of three-dimensional systems, for example, one can find states that have the same value of $E_f(\Psi)$, but different Schmidt numbers, and hence cannot be transformed to each other by local operations and classical communications [2]. Although the two states have the same amount of entanglement, as measured by the number of singlet states needed (asymptotically) to prepare them, the nature of this entanglement is quite different. Indeed, one can argue that for a pair of d-dimensional systems, the structure of entanglement depends on $d-1$ independent Schmidt coefficients; hence, a complete description would require $d-1$ independent measures of entanglement [3].

In this paper, we pursue the study of the entanglement of quantum superpositions based on a measure of entanglement other than $E_f(\Psi)$. This study is thus particularly interesting in dimensions higher than 2. In Ref. [1], an exact solution to this problem was derived in the special case where the two component states are biorthogonal. In this scenario, one may ask whether such an exact solution can also be obtained with other measures of entanglement. In addition, in the cases where the component states are orthogonal (but not biorthogonal) or even arbitrary, can we derive new upper bounds, as was done for $E_f(\Psi)$ in [1], but also lower bounds? These questions are of great importance since a good characteriza-

tion of the entanglement of a superposition clearly requires knowledge of both upper and lower bounds. Furthermore, one would like to know whether one can extract a common structure for the bounds based on different measures of entanglement as this would highlight the mechanism underlying the entanglement of superpositions and hence improve our understanding of entanglement itself.

In what follows, we shall address these various issues based on another widely used measure of entanglement, so-called *concurrence* [4]. For two-level systems, which are studied in Sec. II, this quantity is in one-to-one correspondence with $E_f(\Psi)$ so that our results can be directly compared to those of Ref. [1]. We shall see that our derived upper bound is generally tighter than that of Ref. [1], while it can also be supplemented with a lower bound so that we get strong constraints on the allowed values for the entanglement of superpositions. In Sec. III, we shall generalize our analysis to the case of a pair of d-level systems with any d and derive simple upper and lower bounds for arbitrary states. The special cases of biorthogonal and orthogonal component states will also be treated, and an exact solution will again be given in the former case. As emphasized above, the derived upper and lower bounds yield new constraints to the entanglement of superpositions in d dimensions, which are complementary to those of Ref. [1].

Very recently, the problem of finding bounds on the concurrence of superpositions has also been addressed in Ref. [5]. Since it is based on matrix notations for pure states, this approach gives, however, quite complicated bounds, which, in addition, assume prior knowledge of parameters such as the rank of the superposition state or the largest eigenvalues of the component states. The usefulness of such bounds is then very questionable as it may become equally simple to compute directly the entanglement of the superposition state $|\Psi\rangle$ itself. To be sensible, the bounds should only depend on the entanglement of the component states $|\phi\rangle$ and $|\varphi\rangle$ as well as on simple parameters such as the coefficients α and β or the scalar product $\langle\phi|\varphi\rangle$ between the component states.

II. SUPERPOSITION OF BIPARTITE PURE STATES IN DIMENSION 2

Let us first consider the simplest scenario of Alice and Bob both having a qubit as it will help us gain some useful

intuition. For qubits, the definition of the concurrence makes use of the *spin-flip* transformation S acting on a single qubit,

$$|\tilde{\psi}\rangle = S(|\psi\rangle) = \sigma_y K(|\psi\rangle) = \sigma_y |\psi^*\rangle, \qquad (2)$$

where K denotes complex conjugation; that is, $|\psi^*\rangle$ is the complex conjugate of $|\psi\rangle$ when it is expressed in the eigenbasis of σ_z. Here, σ_i denote the Pauli matrices. With this notation, the concurrence reads [4]

$$C(\Psi) = |\langle\Psi|\tilde{\Psi}\rangle| = |\langle\Psi|\sigma_y \otimes \sigma_y|\Psi^*\rangle| \qquad (3)$$

and it corresponds, physically, to the overlap between the state and its image under a spin flip of both qubits. Note that the spin flip of both qubits can also be interpreted as complex conjugation in the so-called "magic" basis introduced in Ref. [4]. Note also that the concurrence is usually defined for normalized quantum states. In the case of an unnormalized state $|\Psi\rangle$, the meaningful quantity is actually the concurrence of $|\Psi'\rangle = |\Psi\rangle/\|\Psi\|$, the normalized version of $|\Psi\rangle$. For two-level systems, the concurrence has the interesting property of being directly related to the entanglement of formation through

$$E_f(\Psi) = h\left(\frac{1 + \sqrt{1 - C^2(\Psi)}}{2}\right), \qquad (4)$$

where $h(x)$ is the binary entropy function [4]. This simple formula will make it possible to connect our results to those of Ref. [1].

Introducing relation (1) in definition (3), we can write the concurrence of the superposition as

$$C(\Psi) = |(\alpha^*)^2\langle\phi|\sigma_y \otimes \sigma_y|\phi^*\rangle + (\beta^*)^2\langle\varphi|\sigma_y \otimes \sigma_y|\varphi^*\rangle$$
$$+ (\alpha^*\beta^*)(\langle\phi|\sigma_y \otimes \sigma_y|\varphi^*\rangle + \langle\varphi|\sigma_y \otimes \sigma_y|\phi^*\rangle)|. \quad (5)$$

A. Orthogonal states

First we note that when $|\phi\rangle$ and $|\varphi\rangle$ are biorthogonal, the problem boils down to the trivial solution $C(\Psi) = 2|\alpha\beta|$. The easiest interesting scenario is when the two component states are orthogonal (but not necessarily biorthogonal)—that is, $\langle\phi|\varphi\rangle = 0$. This condition implies that we can construct an orthonormal basis $\{|\phi\rangle, |\varphi\rangle, |\xi_1\rangle, |\xi_2\rangle\}$ such that the coefficients of any normalized state in this basis will sum to 1—i.e., $\forall|\psi\rangle$,

$$|\langle\phi|\psi\rangle|^2 + |\langle\varphi|\psi\rangle|^2 + |\langle\xi_1|\psi\rangle|^2 + |\langle\xi_2|\psi\rangle|^2 = 1. \qquad (6)$$

This is true in particular for the two spin-flipped states $|\tilde{\phi}\rangle = \sigma_y \otimes \sigma_y|\phi^*\rangle$ and $|\tilde{\varphi}\rangle = \sigma_y \otimes \sigma_y|\varphi^*\rangle$, and hence

$$|\langle\varphi|\sigma_y \otimes \sigma_y|\phi^*\rangle| \leq \sqrt{1 - C^2(\phi)},$$

$$|\langle\phi|\sigma_y \otimes \sigma_y|\varphi^*\rangle| \leq \sqrt{1 - C^2(\varphi)}. \qquad (7)$$

In addition, since $\sigma_y K = -K\sigma_y$, one can easily check that both left-hand sides of (7) are equal. We thus derive the useful relation

$$|\langle\phi|\sigma_y \otimes \sigma_y|\varphi^*\rangle| = |\langle\varphi|\sigma_y \otimes \sigma_y|\phi^*\rangle| \leq \sqrt{1 - \delta^2}, \qquad (8)$$

where $\delta = \max(C(\phi), C(\varphi))$.

Proposition 1: *upper bound*. Let Alice and Bob have a qubit, and let $|\phi\rangle$ and $|\varphi\rangle$ be orthogonal; the concurrence of the superposition $|\Psi\rangle = \alpha|\phi\rangle + \beta|\varphi\rangle$, with $|\alpha|^2 + |\beta|^2 = 1$, satisfies

$$C(\Psi) \leq |\alpha|^2 C(\phi) + |\beta|^2 C(\varphi) + 2|\alpha\beta|\sqrt{1 - \delta^2}, \qquad (9)$$

where $\delta = \max(C(\phi), C(\varphi))$.

Proof. Successive application of the triangle inequality (TI) $|x+y| \leq |x| + |y|$ to Eq. (5), followed by the introduction of relation (8) together with the definition of the concurrence of $|\phi\rangle$ and $|\varphi\rangle$, directly leads to the upper bound (9). ∎

Proposition 2: *lower bound*. Under the same conditions and with the same definition of δ, the concurrence of the superposition satisfies

$$C(\Psi) \geq ||\alpha|^2 C(\phi) - |\beta|^2 C(\varphi)| - 2|\alpha\beta|\sqrt{1 - \delta^2}. \qquad (10)$$

Proof. This time, we make use of the inverse triangle inequality (ITI) $|x+y| \geq ||x| - |y||$. First, we apply it to Eq. (5) and separate between the first two and last two terms of the right-hand side. Next, we remember that the absolute difference of two positive terms is always greater than their difference—i.e., $||x| - |y|| \geq |x| - |y|$. We can then express our bound by applying ITI again to the first of these positive terms and TI to the second. Finally, we inject relation (8) and the definition of the concurrence of $|\phi\rangle$ and $|\varphi\rangle$ into this last expression to obtain the lower bound (10). ∎

Let us comment on our results until now. First, this approach based on the concurrence is fruitful in the sense that, for two-dimensional systems, it makes it possible to derive both an upper and a lower bound on the entanglement of a superposition. Second, these bounds can be saturated. Consider, for example, the states

$$|\Psi_1\rangle = \alpha_1|\Phi^+\rangle + \beta_1|01\rangle,$$

$$|\Psi_2\rangle = \alpha_2|\Phi^+\rangle + \beta_2|\Phi^-\rangle, \qquad (11)$$

with α_i and β_i real, and $|\Phi^\pm\rangle = 1/\sqrt{2}(|00\rangle \pm |11\rangle)$. One can easily check that $C(\Psi_1)$ exactly saturates the upper bound (9), while $C(\Psi_2)$ exactly saturates the lower bound (10). Finally, when translated to a bound on the entanglement of formation via relation (4), our upper bound (9) typically gives stronger constraints than those derived in Ref. [1]. This is illustrated in Fig. 1 for two orthogonal randomly generated states $|\phi\rangle = -0.264|00\rangle + 0.528|01\rangle + 0.487|10\rangle - 0.643|11\rangle$ and $|\varphi\rangle = -0.034|00\rangle + 0.675|01\rangle - 0.734|10\rangle + 0.010|11\rangle$.

B. Arbitrary states

When the two component states are not orthogonal, the superposition (1) is not normalized. We can nevertheless derive bounds on the concurrence of the normalized version of this superposition—i.e., $|\Psi'\rangle = |\Psi\rangle/\|\Psi\|$—using the same method as before. Note that relation (8) does not hold anymore. However, we can always introduce an orthonormal basis—say, $\{|\phi\rangle, |\xi_1\rangle, |\xi_2\rangle, |\xi_3\rangle\}$—such that $|\varphi\rangle = \lambda|\phi\rangle + \sqrt{1 - \lambda^2}|\xi_1\rangle$ with $\lambda = |\langle\phi|\varphi\rangle|$. Again, the coefficients of any normalized state $|\Psi\rangle$ written in this basis will sum to 1. Expressing $|\xi_1\rangle$ in terms of $|\phi\rangle$ and $|\varphi\rangle$, and after some straight-
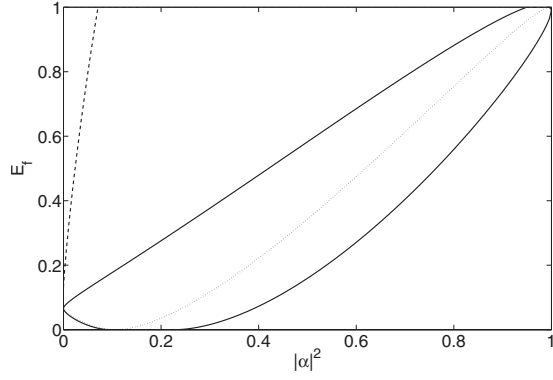
FIG. 1. Entanglement of formation of $|\Psi\rangle = \alpha|\phi\rangle + \beta|\varphi\rangle$, with $|\phi\rangle$ and $|\varphi\rangle$ being two random orthogonal states defined in the text. The dotted line is the exact value of $E_f(\Psi)$, while the two solid lines correspond to the upper and lower bounds derived from relations (9) and (10). The dashed line is the upper bound of Ref. [1]. All variables are dimensionless.

forward calculations, this normalization condition becomes

$$|\langle\phi|\Psi\rangle|^2 + |\langle\varphi|\Psi\rangle|^2 \le (1-\lambda^2) + 2\lambda|\langle\phi|\Psi\rangle||\langle\varphi|\Psi\rangle|. \quad (12)$$

In particular, for $|\tilde{\phi}\rangle = \sigma_y \otimes \sigma_y|\phi^*\rangle$ and $|\tilde{\varphi}\rangle = \sigma_y \otimes \sigma_y|\varphi^*\rangle$, the condition leads to

$$|\langle\varphi|\sigma_y \otimes \sigma_y|\phi^*\rangle| \le \sqrt{1 - [C(\phi) - |\langle\phi|\varphi\rangle|]^2},$$

$$|\langle\phi|\sigma_y \otimes \sigma_y|\varphi^*\rangle| \le \sqrt{1 - [C(\varphi) - |\langle\phi|\varphi\rangle|]^2}. \quad (13)$$

Noting again that the two left-hand-side terms are equal, we obtain

$$|\langle\phi|\sigma_y \otimes \sigma_y|\varphi^*\rangle| = |\langle\varphi|\sigma_y \otimes \sigma_y|\phi^*\rangle| \le \sqrt{1 - \delta^2}, \quad (14)$$

with $\delta = \max(|C(\phi) - |\langle\phi|\varphi\rangle||, |C(\varphi) - |\langle\phi|\varphi\rangle||)$.

Proposition 3: arbitrary states. When $|\phi\rangle$ and $|\varphi\rangle$ are arbitrary normalized states, the concurrence of the normalized version of the superposition $|\Psi\rangle = \alpha|\phi\rangle + \beta|\varphi\rangle$ with $|\alpha|^2 + |\beta|^2 = 1$ obeys the upper and lower bounds

$$\|\Psi\|^2 C(\Psi') \le |\alpha|^2 C(\phi) + |\beta|^2 C(\varphi) + 2|\alpha\beta|\sqrt{1-\delta^2},$$

$$\|\Psi\|^2 C(\Psi') \ge ||\alpha|^2 C(\phi) - |\beta|^2 C(\varphi)| - 2|\alpha\beta|\sqrt{1-\delta^2},$$
$$(15)$$

where $\delta = \max(|C(\phi) - |\langle\phi|\varphi\rangle||, |C(\varphi) - |\langle\phi|\varphi\rangle||)$.

Proof. We first realize that $C(\Psi') = |\langle\Psi'|\sigma_y \otimes \sigma_y|\Psi'\rangle| = |\langle\Psi|\sigma_y \otimes \sigma_y|\Psi\rangle|/\|\Psi\|^2$; then, proceed exactly as before using Eq. (14) instead of Eq. (8). ∎

III. SYSTEMS OF ARBITRARY DIMENSION

Although the concurrence was initially introduced to measure the entanglement of a pair of qubits, it has since been generalized to pairs of quantum systems of arbitrary dimension d. The first generalization, based on the notion of conjugations, is due to Uhlmann [6]. However, this approach was later shown to lead to a definition of concurrence that

cannot serve as a basis for a general measure of entanglement [7]. We will thus use in what follows the definition of the generalized concurrence introduced by Rungta *et al.* [7], sometimes known as *I concurrence*. This definition makes use of a superoperator called the *universal inverter*, which naturally extends the idea of spin flip to d-dimensional quantum systems or qudits (the extension of the spin flip to more than two dimensions had also been studied in the context of the reduction criterion for separability in Refs. [8,9]). On a qudit state ρ, the action of the universal inverter is given by

$$S_d(\rho) = \nu_d(I - \rho), \quad (16)$$

where ν_d is a positive constant. Thus, the universal inverter maps a pure qudit state $|\Psi\rangle$ onto a multiple of the maximally mixed state in the subspace orthogonal to $|\Psi\rangle$. As argued in [7], in order to have a meaningful definition of the concurrence, consistent with the expression of the concurrence for qubits, one should choose the scaling factor ν_d equal to one. However, ν_d is sometimes chosen equal to $1/(d-1)$ [10] and we will briefly discuss this possibility at the end of this section. With $\nu_d = 1$, as we assume in what follows, the universal inverter is a trace-increasing positive superoperator, which preserves Hermiticity. The corresponding generalized concurrence for a bipartite pure state $|\Psi\rangle$ of d-dimensional quantum systems is given by

$$C(\Psi) = \sqrt{\langle\Psi|S_d \otimes S_d(|\Psi\rangle\langle\Psi|)|\Psi\rangle}. \quad (17)$$

Let us now briefly state some useful properties of the superoperator $\Lambda_d = S_d \otimes S_d$ with $\nu_d = 1$, as defined in Refs. [8,9], since they will be used repeatedly in what follows. Since the universal inverter is a positive operator which preserves Hermiticity, so is Λ_d. Nevertheless, Λ_d is *not* completely positive. In fact, one can prove that it can be decomposed as a completely positive map Λ_d^{CP} supplemented with the transpose—or time reversal—map T—i.e., $\Lambda_d = \Lambda_d^{CP}T$ [9]. Its action on an arbitrary operator σ is given by

$$\Lambda_d(\sigma) = \text{Tr}(\sigma)I \otimes I - \sigma_A \otimes I - I \otimes \sigma_B + \sigma, \quad (18)$$

where $\sigma_A = \text{Tr}_B(\sigma)$ and $\sigma_B = \text{Tr}_A(\sigma)$ are the reduction of the operator σ on A and B, respectively [8,9]. The map Λ_d is trace increasing as

$$\text{Tr}[\Lambda_d(\sigma)] = (d-1)^2\text{Tr}(\sigma). \quad (19)$$

Finally, one can easily check that expressions such as $\text{Tr}[\rho\Lambda_d(\sigma)]$ are symmetric with respect to the interchange between σ and ρ—that is,

$$\text{Tr}[\rho\Lambda_d(\sigma)] = \text{Tr}[\sigma\Lambda_d(\rho)]. \quad (20)$$

Now, coming back to the generalized concurrence in dimension d, we note first that by expressing relation (18) in the case of a pure state $\sigma = |\Psi\rangle\langle\Psi|$, we can rewrite the concurrence as

$$C(\Psi) = \sqrt{2[1 - \text{Tr}(\rho_A^2)]}. \quad (21)$$

Hence, the concurrence ranges from 0 for separable states to $\sqrt{2(d-1)/d}$ for maximally entangled ones. Next, to address the problem of the concurrence of superpositions, we can plug Eq. (1) into the definition (17) of the concurrence, or

actually the square of the concurrence (to get rid of the unnecessary square root). We can develop this expression, resulting in a simple yet lengthy summation over 16 different terms. Out of these 16 terms, many are identical as can be proven using relation (20): for example,

$$
\begin{aligned}
\langle\phi|\Lambda_d(|\phi\rangle\langle\varphi|)|\phi\rangle &= \mathrm{Tr}[|\phi\rangle\langle\phi|\Lambda_d(|\phi\rangle\langle\varphi|)] \\
&= \mathrm{Tr}[|\phi\rangle\langle\varphi|\Lambda_d(|\phi\rangle\langle\phi|)] \\
&= \langle\varphi|\Lambda_d(|\phi\rangle\langle\phi|)|\phi\rangle.
\end{aligned}
\tag{22}
$$

In addition, one can also show that $\langle\phi|\Lambda_d(|\phi\rangle\langle\varphi|)|\varphi\rangle$ $=\langle\varphi|\Lambda_d(|\phi\rangle\langle\phi|)|\varphi\rangle$ holds, as well as its counterpart $\langle\varphi|\Lambda_d(|\varphi\rangle\langle\phi|)|\phi\rangle=\langle\phi|\Lambda_d(|\varphi\rangle\langle\varphi|)|\phi\rangle$. To do so, first develop both sides using the expression (18) for Λ_d, write $|\phi\rangle$ and $|\varphi\rangle$ in a given basis—say, the Schmidt basis of $|\phi\rangle$ for simplicity—and then prove that all four terms are identical. We finally obtain a general expression for the square of the concurrence of a superposition state,

$$
\begin{aligned}
C^2(\Psi) &= |\alpha|^4 C^2(\phi) + |\beta|^4 C^2(\varphi) + 4|\alpha\beta|^2\langle\varphi|\Lambda_d(|\phi\rangle\langle\phi|)|\varphi\rangle \\
&\quad + 2|\alpha|^2[\alpha^*\beta\langle\phi|\Lambda_d(|\phi\rangle\langle\phi|)|\varphi\rangle + \alpha\beta^*\langle\varphi|\Lambda_d(|\phi\rangle\langle\phi|) \\
&\quad \times|\phi\rangle] + 2|\beta|^2[\alpha^*\beta\langle\phi|\Lambda_d(|\varphi\rangle\langle\varphi|)|\varphi\rangle + \alpha\beta^*\langle\varphi|\Lambda_d(|\varphi\rangle \\
&\quad \times\langle\varphi|)|\phi\rangle] + [(\alpha^*\beta)^2\langle\phi|\Lambda_d(|\varphi\rangle\langle\phi|)|\varphi\rangle \\
&\quad + (\alpha\beta^*)^2\langle\varphi|\Lambda_d(|\phi\rangle\langle\varphi|)|\phi\rangle].
\end{aligned}
\tag{23}
$$

A. Biorthogonal states

When the two component states $|\phi\rangle$ and $|\varphi\rangle$ are biorthogonal, that is, when

$$
\mathrm{Tr}_A[\mathrm{Tr}_B(|\phi\rangle\langle\phi|)\mathrm{Tr}_B(|\varphi\rangle\langle\varphi|)] = 0,
$$

$$
\mathrm{Tr}_B[\mathrm{Tr}_A(|\phi\rangle\langle\phi|)\mathrm{Tr}_A(|\varphi\rangle\langle\varphi|)] = 0,
\tag{24}
$$

an exact expression for the entanglement of a superposition can be derived based on the entanglement of formation; see Ref. [1]. As stated in the following theorem, one can also find an exact value for the concurrence of the superposition.

Theorem 1: biorthogonal states. If $|\phi\rangle$ and $|\varphi\rangle$ satisfy conditions (24) and if $|\alpha|^2+|\beta|^2=1$, then the concurrence of the superposition $|\Psi\rangle=\alpha|\phi\rangle+\beta|\varphi\rangle$ is given by

$$
C(\Psi) = \sqrt{|\alpha|^4 C^2(\phi) + |\beta|^4 C^2(\varphi) + 4|\alpha\beta|^2}.
\tag{25}
$$

Proof. In addition to conditions (24), we also note that the reductions on A and B of the operators $|\phi\rangle\langle\varphi|$ and $|\varphi\rangle\langle\phi|$ are equal to zero. Hence, one can easily check, using relation (18), that all the terms of Eq. (23) are zero except for the first three. The equality follows from the fact that $\langle\varphi|\Lambda_d(|\phi\rangle\times\langle\phi|)|\varphi\rangle=1$ when the states are biorthogonal [as can be checked by Eq. (18) again]. ∎

B. Orthogonal states

Let us now consider the less restrictive case of $|\phi\rangle$ and $|\varphi\rangle$ being orthogonal but not necessarily biorthogonal. As we will prove in the next theorem, one can derive a simple upper

bound which nicely generalizes the upper bound (9) that we had found for qubits.

Theorem 2: upper bound. Let Alice and Bob each have a qudit, and let $|\phi\rangle$ and $|\varphi\rangle$ be orthogonal states, the concurrence of the superposition $|\Psi\rangle=\alpha|\phi\rangle+\beta|\varphi\rangle$ with $|\alpha|^2+|\beta|^2=1$ satisfies

$$
C(\Psi) \leq |\alpha|^2 C(\phi) + |\beta|^2 C(\varphi) + 2|\alpha\beta|.
\tag{26}
$$

Proof. First, remember that the map Λ_d, while it is not completely positive, can be written as the transpose map T followed by a completely positive map Λ_d^{CP}—i.e., $\Lambda_d=\Lambda_d^{\mathrm{CP}}T$. Since Λ_d^{CP} is completely positive, it has an operator-sum representation based on a set of operators $\{A_k\}$. Hence, for an arbitrary operator σ, the action of Λ_d can be written as

$$
\Lambda_d(\sigma) = \Lambda_d^{\mathrm{CP}}(T(\sigma)) = \sum_k A_k\sigma^T A_k^\dagger,
\tag{27}
$$

where the operators A_k satisfy $\Sigma_k A_k A_k^\dagger=(d-1)^2 I$ according to Eq. (19). We can now make use of this decomposition to bound the different terms of Eq. (23). Considering $\langle\phi|\Lambda_d(|\varphi\rangle\langle\phi|)|\varphi\rangle$, for example, one can prove that

$$
\begin{aligned}
|\langle\phi|\Lambda_d(|\varphi\rangle\langle\phi|)|\varphi\rangle| &= \left|\sum_k \langle\phi|A_k|\phi^*\rangle\langle\varphi^*|A_k^\dagger|\varphi\rangle\right| \\
&\leq \sum_k |\langle\phi|A_k|\phi^*\rangle||\langle\varphi^*|A_k^\dagger|\varphi\rangle| \\
&\leq \sqrt{\sum_k |\langle\phi|A_k|\phi^*\rangle|^2}\sqrt{\sum_k |\langle\varphi^*|A_k^\dagger|\varphi\rangle|^2} \\
&= \sqrt{\langle\phi|\Lambda_d(|\phi\rangle\langle\phi|)|\phi\rangle}\sqrt{\langle\varphi|\Lambda_d(|\varphi\rangle\langle\varphi|)|\varphi\rangle} \\
&= C(\phi)C(\varphi),
\end{aligned}
\tag{28}
$$

where in the first line we have made use of relation (27) and expressed the transposition in a fixed basis of the operator $|\varphi\rangle\langle\phi|$ as $(|\varphi\rangle\langle\phi|)^T=|\phi^*\rangle\langle\varphi^*|$. The second and third lines follow, respectively, from the triangle inequality and Holder's inequality (see, e.g., [11]). The last two equalities result from Eq. (27) again and the definition of the concurrence of $|\phi\rangle$ and $|\varphi\rangle$. We can repeatedly use the same argument on the other terms and prove

$$
|\langle\varphi|\Lambda_d(|\phi\rangle\langle\varphi|)|\phi\rangle| \leq C(\phi)C(\varphi)
$$

$$
|\langle\phi|\Lambda_d(|\phi\rangle\langle\phi|)|\varphi\rangle| \leq C(\phi)\sqrt{\langle\varphi|\Lambda_d(|\phi\rangle\langle\phi|)|\varphi\rangle}
$$

$$
|\langle\varphi|\Lambda_d(|\phi\rangle\langle\phi|)|\phi\rangle| \leq C(\phi)\sqrt{\langle\varphi|\Lambda_d(|\phi\rangle\langle\phi|)|\varphi\rangle}
$$

$$
|\langle\varphi|\Lambda_d(|\varphi\rangle\langle\varphi|)|\phi\rangle| \leq C(\varphi)\sqrt{\langle\varphi|\Lambda_d(|\phi\rangle\langle\phi|)|\varphi\rangle}
$$

$$
|\langle\phi|\Lambda_d(|\varphi\rangle\langle\varphi|)|\varphi\rangle| \leq C(\varphi)\sqrt{\langle\varphi|\Lambda_d(|\phi\rangle\langle\phi|)|\varphi\rangle}.
\tag{29}
$$

Finally, all we need to do is to bound $C^2(\Psi)$ by the sum of the modulus of each of the terms of Eq. (23) and then bound each term individually by use of the previous relations. This gives

$$C^2(\Psi) \le [|\alpha|^2 C(\phi) + |\beta|^2 C(\varphi) + 2|\alpha\beta|\sqrt{\langle\varphi|\Lambda_d(|\phi\rangle\langle\phi|)|\varphi\rangle}]^2. \quad (30)$$

The conclusion follows from the value of $\langle\varphi|\Lambda_d(|\phi\rangle \times \langle\phi|)|\varphi\rangle$, which can be bounded using Eq. (18)—that is,

$$\langle\varphi|\Lambda_d(|\phi\rangle\langle\phi|)|\varphi\rangle = 1 - \mathrm{Tr}_A(\rho_\phi^A \rho_\varphi^A) - \mathrm{Tr}_B(\rho_\phi^B \rho_\varphi^B) \le 1, \quad (31)$$

where $\rho_\phi^{A,B} = \mathrm{Tr}_{B,A}(|\phi\rangle\langle\phi|)$ and $\rho_\varphi^{A,B} = \mathrm{Tr}_{B,A}(|\varphi\rangle\langle\varphi|)$. ∎

Let us make a few comments at this point. First, it is interesting to see how the structure of our upper bound closely resembles the one derived for the entanglement of formation in [1]. Both bounds are the sum of two terms: the first one is the average of the entanglement of $|\phi\rangle$ and $|\varphi\rangle$ (up to a factor), and the second one is a function of α and β only, which takes its maximum value when $\alpha = \beta$.

Another comment we should make is related to the definition of the I concurrence. Although the upper bound (26) resembles much the bound that we have derived for qubits, Eq. (9), the third term lacks the correction factor in δ that we had deduced from Eq. (8). To understand this difference, remember that the universal inverter is defined up to a scaling factor ν_d. As noted in Ref. [7], the definition of a generalized measure of entanglement such as the concurrence requires ν_d to be independent of the dimension; otherwise, the concurrence could be changed simply by adding an extra dimension that is not used to one of the subsystems. Unfortunately, this leads to a universal inverter which is not trace preserving, and with the choice $\nu_d = 1$, the condition (8) becomes

$$\sqrt{\langle\varphi|\Lambda_d(|\phi\rangle\langle\phi|)|\varphi\rangle} \le \sqrt{(d-1)^2 - \delta^2}. \quad (32)$$

This bound becomes useless whenever $d > 2$, which explains the discrepancy between (9) and (26). If, on the other hand, we had chosen $\nu_d = 1/(d-1)$ to make the universal inverter trace preserving (at the expense of an ill-defined I concurrence), relation (8) would still be valid for $d > 2$ and our upper bound (9) would hold regardless of the dimension. Thus, with respect to our chosen definition of the I concurrence, our upper bound for qudits is consistent with the bound we had previously derived for qubits.

Let us now derive a lower bound for the concurrence of the superposition of orthogonal states, generalizing the bound obtained for qubits, Eq. (10). To do so, a natural approach would be to start again from Eq. (23) and apply the inverse triangle inequality to separate between the first three terms, which are always positive, and the rest of the expression, which can take negative values. This negative part could then be upper bounded by repeated uses of the triangle inequality, followed by the introduction of relations (29) to bound the norm of each term separately. Unfortunately, this approach would lead to a rather bad and complicated bound. However, as stated in the next theorem, one can nevertheless find a simple yet meaningful bound by use of a different approach.

Theorem 3: lower bound. Let Alice and Bob each have a qudit, and let $|\phi\rangle$ and $|\varphi\rangle$ be orthogonal; the concurrence of the superposition $|\Psi\rangle = \alpha|\phi\rangle + \beta|\varphi\rangle$, with $|\alpha|^2 + |\beta|^2 = 1$ satisfies

$$C(\Psi) \ge ||\alpha|^2 C(\phi) - |\beta|^2 C(\varphi)| - 2|\alpha\beta|(1 + \delta), \quad (33)$$

where $\delta = \min(|\frac{\beta}{\alpha}|C(\varphi), |\frac{\alpha}{\beta}|C(\phi))$.

Proof. First, we note that Eq. (1) can be rewritten as

$$|\phi\rangle = \frac{\alpha^*}{|\alpha|^2}|\Psi\rangle - \frac{\alpha^*\beta}{|\alpha|^2}|\varphi\rangle. \quad (34)$$

Next, we make use of the fact that the bound (30) was derived based solely on the properties of the map Λ_d and on the normalization condition $\|\Psi\| = 1$. We did not make explicit use of the orthogonality of $|\phi\rangle$ and $|\varphi\rangle$; nor did we use the condition $|\alpha|^2 + |\beta|^2 = 1$ in the derivation. It follows that the bound (30) can be applied to Eq. (34), that is,

$$C(\phi) \le \frac{1}{|\alpha|^2}C(\Psi) + \frac{|\beta|^2}{|\alpha|^2}C(\varphi) + 2\frac{|\beta|}{|\alpha|^2}\sqrt{\langle\Psi|\Lambda_d(|\varphi\rangle\langle\varphi|)|\Psi\rangle},$$

from which we deduce

$$C(\Psi) \ge |\alpha|^2 C(\phi) - |\beta|^2 C(\varphi) - 2|\beta|\sqrt{\langle\Psi|\Lambda_d(|\varphi\rangle\langle\varphi|)|\Psi\rangle}. \quad (35)$$

Furthermore, we can plug Eq. (1) into $\langle\Psi|\Lambda_d(|\varphi\rangle\langle\varphi|)|\Psi\rangle$ in order to bound the last term of the right-hand side of Eq. (35), that is,

$$\langle\Psi|\Lambda_d(|\varphi\rangle\langle\varphi|)|\Psi\rangle = |\alpha|^2\langle\phi|\Lambda_d(|\varphi\rangle\langle\varphi|)|\phi\rangle + |\beta|^2\langle\varphi|\Lambda_d(|\varphi\rangle\langle\varphi|)$$
$$\times|\varphi\rangle + 2\,\mathrm{Re}[|\alpha\beta^*|\langle\varphi|\Lambda_d(|\varphi\rangle\langle\varphi|)|\phi\rangle]$$
$$\le [|\alpha|\sqrt{\langle\phi|\Lambda_d(|\varphi\rangle\langle\varphi|)|\phi\rangle} + |\beta|C(\varphi)]^2$$
$$\le [|\alpha| + |\beta|C(\varphi)]^2, \quad (36)$$

where we have bounded the real part of the complex number by its modulus and used the third relation of (29) to obtain the first inequality. The last line follows directly from Eq. (31). Thus, we get

$$C(\Psi) \ge |\alpha|^2 C(\phi) - |\beta|^2 C(\varphi) - 2|\alpha\beta|\left(1 + \left|\frac{\beta}{\alpha}\right|C(\varphi)\right). \quad (37)$$

Alternatively, we can express $|\varphi\rangle$ as a superposition of $|\Psi\rangle$ and $|\phi\rangle$ instead of starting from Eq. (34), which would result into the dual relation

$$C(\Psi) \ge |\beta|^2 C(\varphi) - |\alpha|^2 C(\phi) - 2|\alpha\beta|\left(1 + \left|\frac{\alpha}{\beta}\right|C(\phi)\right). \quad (38)$$

Combining these two bounds (37) and (38) and noticing that $|\alpha|^2 C(\phi) - |\beta|^2 C(\varphi) > 0$ is equivalent to $|\frac{\beta}{\alpha}|C(\varphi) < |\frac{\alpha}{\beta}|C(\phi)$ leads to Eq. (33). ∎

We do not know whether Eq. (33) is the best possible lower bound and suspect that a more appropriate expression, if it exists, would probably have the correction factor δ equal to zero as it would then generalize the bound obtained for qubits. Nevertheless, our bound has the desired shape and is close to this guessed optimal when δ is small—that is, when
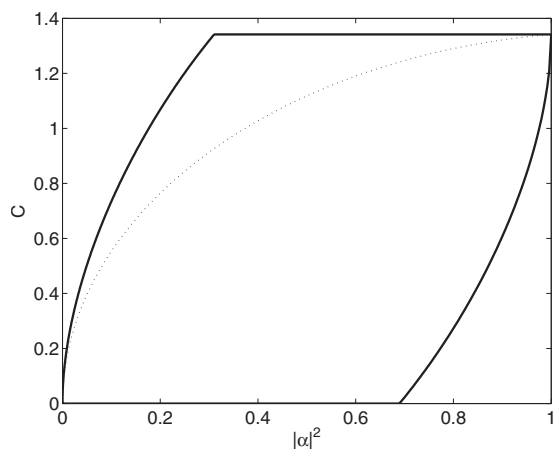
FIG. 2. Concurrence of $|\Psi\rangle = \alpha|\phi\rangle + \beta|\varphi\rangle$, with $|\phi\rangle$ and $|\varphi\rangle$ as defined in the text. The dotted line is the exact value of $C(\Psi)$, while the two solid lines correspond to the upper and lower bounds derived from relations (26) and (33). All variables are dimensionless.

the concurrence of one of the superposed state is small or when the superposition is strongly unbalanced—i.e., $|\alpha| \gg |\beta|$ or $|\beta| \gg |\alpha|$. As a last comment, let us note that this lower bound is useful (i.e., provides a value above zero) whenever

$$C(\phi) > 3\left|\frac{\beta}{\alpha}\right|^2 C(\varphi) + 2\left|\frac{\beta}{\alpha}\right| \qquad (39)$$

or

$$C(\varphi) > 3\left|\frac{\alpha}{\beta}\right|^2 C(\phi) + 2\left|\frac{\alpha}{\beta}\right|. \qquad (40)$$

In Fig. 2, we illustrate the upper and lower bounds for the case of two orthogonal component states in dimension $d = 10$—namely,

$$|\phi\rangle = \frac{1}{10}\sum_{i,j=0}^{9}|i,j\rangle,$$

$$|\varphi\rangle = \frac{1}{\sqrt{10}}\sum_{i=0}^{9}(-1)^i|i,i\rangle. \qquad (41)$$

In general, we notice that the bounds in high dimensions are less constraining than for $d=2$. This is natural as for a larger dimension, the set of states with a given value of the concurrence gets larger; hence, the range of possible values for the concurrence of the superposition of two states with a fixed concurrence becomes wider.

C. Arbitrary states

Let us show finally that the previous theorems can be nicely generalized to the completely general situation of the component states $|\phi\rangle$ and $|\varphi\rangle$ being arbitrary.

Theorem 4: arbitrary states. Let $|\phi\rangle$ and $|\varphi\rangle$ be normalized but arbitrary, and let $|\alpha|^2 + |\beta|^2 = 1$; the concurrence of $|\Psi'\rangle$, the normalized version of the superposition $|\Psi\rangle = \alpha|\phi\rangle + \beta|\varphi\rangle$, satisfies

$$\|\Psi\|^2 C(\Psi') \le |\alpha|^2 C(\phi) + |\beta|^2 C(\varphi) + 2|\alpha\beta|\sqrt{1 + |\langle\phi|\varphi\rangle|^2}$$

$$\|\Psi\|^2 C(\Psi') \ge \left||\alpha|^2 C(\phi) - |\beta|^2 C(\varphi)\right| - 2|\alpha\beta|(\sqrt{1 + |\langle\phi|\varphi\rangle|^2} + \delta), \qquad (42)$$

where $\delta = \min(|\frac{\beta}{\alpha}|C(\varphi), |\frac{\alpha}{\beta}|C(\phi))$.

Proof. First, we note that $\|\Psi\|^4 C^2(\Psi') = \langle\Psi|\Lambda_d(|\Psi\rangle\times\langle\Psi|)|\Psi\rangle$. Next, we remember that the derivation of theorems 2 and 3 was mostly based on the property of the map Λ_d only, for a normalized state $|\Psi\rangle$. In particular, Eqs. (30) and (35) as well as the dual of the latter equation were derived without explicitly assuming $|\phi\rangle$ and $|\varphi\rangle$ to be orthogonal. One can thus easily check that these inequalities hold provided that $C(\Psi)$ is replaced by $\|\Psi\|^2 C(\Psi')$. Furthermore, when $|\langle\phi|\varphi\rangle| \ne 0$, Eq. (31) should be replaced by

$$\langle\varphi|\Lambda_d(|\phi\rangle\langle\phi|)|\varphi\rangle \le 1 + |\langle\phi|\varphi\rangle|^2, \qquad (43)$$

as can be deduced from Eq. (18). Combining these relations directly leads to Eq. (42). ∎

IV. CONCLUSION

We have investigated the concurrence of the quantum superposition of two bipartite pure states in arbitrary dimension. The concurrence being an entanglement measure that is distinct from the entanglement of formation in dimensions higher than 2, our study complements that of Ref. [1]. We have derived simple relations between the concurrence of the superposition state and the concurrence of its two component states. When the scalar product of these two states is known, our method provides both a lower and an upper bound on the concurrence of the superposition state. These bounds take particularly simple forms when this scalar product is zero—i.e., when the two component states are orthogonal. In dimension 2, we have checked that our upper bound is typically tighter than the bound of Ref. [1]. Finally, in the special case where the component states are biorthogonal, we have derived an exact expression for the concurrence of the superposition.

Note added. Recently, a related paper on the entanglement of quantum superpositions has appeared, where the generalization to a multipartite setting and an arbitrary entanglement witness is considered [12]. Some of the results obtained there are in perfect agreement with ours.

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