Concurrence of Mixed Multipartite Quantum States

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We propose generalizations of concurrence for multipartite quantum systems that can distinguish qualitatively distinct quantum correlations. All introduced quantities can be evaluated efficiently for arbitrary mixed sates.

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Quantum correlations display one of the crucial—and arguably the least understood—qualitative differences between classical and quantum systems. While we start to develop some kind of intuition for nonclassical correlations which arise in quantum systems composed of two subsystems, our comprehension remains rather strained when we deal with a larger number of constituents. This qualitative difference between bi- and multipartite quantum systems originates—among others—from the fact that in bipartite quantum systems there are no qualitatively different quantum correlations, i.e., any state ϱ can be prepared with local operations and classical communication (LOCC), starting out from a maximally entangled state. Therefore, the entanglement of bipartite states can be well characterized by a single scalar quantity, such as, e.g., the entanglement of formation [1]. In multipartite systems this is no more true. For example, the label "maximally entangled" can be justified for both GHZ [2] and *W* states, though none of them can be prepared from the other using only LOCC [3]. Hence, they are characterized by qualitatively different, inequivalent quantum correlations.

Also the very definition of multipartite separability and entanglement requires some refinement as compared to bipartite systems: An *N*-partite system is described by a Hilbert space $\mathcal{H}$ that decomposes into a direct product of *N* subspaces $\mathcal{H} = \mathcal{H}_1 \otimes \ldots \otimes \mathcal{H}_N$, where the dimension of the space $\mathcal{H}_i$ will be denoted by n_i. A multipartite state acting on $\mathcal{H}$ is separable [4], if it can be written as a convex sum of direct products of subsystem states

$$\varrho = \sum_i p_i \varrho_1^{(i)} \otimes \ldots \otimes \varrho_N^{(i)} = \sum_i p_i \bigotimes_{j=1}^{N} \varrho_j^{(i)}, \qquad p_i > 0. \quad (1)$$

In such a state all correlations between any of the subsystems are of classical nature, and can be described in terms of the classical probabilities p_i. However, the tensorial structure of $\mathcal{H}$ holds room for qualitatively distinct quantum correlations which go beyond the classical framework. A state is *biseparable*, if it can be written as a convex sum of states which each decompose into a direct product of at least two factors. This definition can be immediately generalized to *m separability* ($m \leq N$), which provides a fine graduation of states according to their different degrees of separability.

In general, it is an open problem to decide on the degree of separability of a given state ϱ. Some substantial progress has been achieved with entanglement witnesses [5,6], which allow us to distinguish some multipartite entangled states from biseparable ones. Though, their use also has two severe drawbacks: some *a priori* knowledge on the considered state is required, in order to construct a suitable witness—and there is no general prescription for such construction. Moreover, a witness can give reliable information only if it actually does detect the considered state—if not, this can either be due to the fact that the witness is not well adapted for the given state, or that the state simply does not contain the quantum correlations seeked for. A secure answer is only obtained if all (infinitely many) different witnesses are consulted.

In the present Letter, we follow an alternative route, by formulating a general recipe for the characterization of targeted separability properties of arbitrary mixed *N*-partite states. No *a priori* knowledge on the state under scrutiny will be needed here. Our approach is built upon suitable generalizations of the concurrence of bipartite quantum states, and on recently derived [7], in general tight [8], lower bounds thereof.

Let us start with a novel definition of pure state concurrence which is different from the ones familiar from the published literature [9,10], though comprises these as special cases. A simple definition on the level of pure states is an indispensable prerequisite for the treatment of mixed states, which we are finally aiming at.

By analogy to the expectation value of an observable, the expectation value of a suitably chosen linear, Hermitean operator comes to mind as a simple choice. However, there is none such that all expectation values with respect to entangled states are strictly positive, whereas they vanish for all separable states—so that entanglement can be identified unambiguously. Though we will see that the expectation value of linear, Hermitean operators $\mathcal{A}$ with respect to *two* copies of a pure state can capture entanglement properties very well, which provides a solid basis for generalizations for multipartite mixed states.

So which operators $\mathcal{A}$ serve our purpose? Of course, concurrence needs to be invariant under local unitaries. Since this must hold for any state, it is natural to require that $\mathcal{A}$ itself bears this invariance property. The projectors $P_-^{(i)}$ and $P_+^{(i)}$ onto the antisymmetric and symmetric subspaces $\mathcal{H}_i \wedge \mathcal{H}_i$ and $\mathcal{H}_i \odot \mathcal{H}_i$ of $\mathcal{H}_i \otimes \mathcal{H}_i$ [11] ($i = 1, \ldots, N$ labels the individual subsystems) exhibit the desired invariance property, since any local unitary transformation $\mathcal{U}_i \otimes \mathcal{U}_i$ on $\mathcal{H}_i \otimes \mathcal{H}_i$ commutes with the exchange of both copies. Hence, they can be used as elementary building blocks of $\mathcal{A} = \bigotimes_{j=1}^N P_{s_j}^{(j)}$ ($s_j = \pm$), which immediately inherits their invariance with respect to local unitaries. Thus, we can define a generalized concurrence of a pure, N-partite state $|\Psi\rangle$ as

$$c(\Psi) = \sqrt{\langle\Psi| \otimes \langle\Psi|\mathcal{A}|\Psi\rangle \otimes |\Psi\rangle}, \tag{2}$$

where $\mathcal{A}$ acts on $\bigotimes_{i=1}^N \mathcal{H}_i \otimes \mathcal{H}_i$ [12], as shown schematically in Fig. 1.

The above expression for $\mathcal{A}$ in terms of products of $P_\pm^{(i)}$ allows us to tailor Eq. (2) such as to address specific types of correlations, as follows from inspection of the action of $P_\pm^{(i)}$ on a twofold copy $|\xi^{(i)}\rangle \otimes |\xi^{(i)}\rangle \in \mathcal{H}_i \otimes \mathcal{H}_i$ of a one-party state: Since any such twofold copy is symmetric, the expectation value of $P_-^{(i)}$ vanishes identically, whereas the corresponding expression for $P_+^{(i)}$ gives unity. Now, consider an N-partite state that separates into a one-party state (let us take subsystem N, for simplicity) and a state of the remaining $N-1$ subsystems. If $\mathcal{A}$ in Eq. (2) comprises the term $P_-^{(N)}$, the corresponding concurrence necessarily vanishes, thus highlighting the vanishing entanglement between subsystem N and the rest. If, instead, one chooses to incorporate the term $P_+^{(N)}$ in Eq. (2), the respective concurrence will be sensitive to $(N-1)$-partite correlations between the $N-1$ first subsystems. This argument can be iterated recursively down to bipartite correlations, such that the original concurrence [9,10] of bipartite systems emerges with the specific choice $\mathcal{A} = 4P_-^{(1)} \otimes P_-^{(2)}$.

Similarly to the case of bipartite systems, also our presently introduced N-partite concurrences can be generalized for mixed states via their convex roofs,

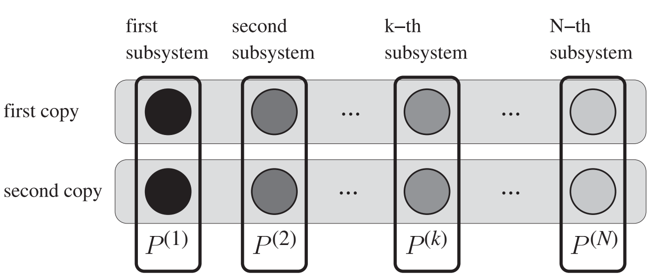

FIG. 1. The concurrence of a pure state $|\Psi\rangle$ is defined in terms of two copies (shown schematically as gray boxes) of $|\Psi\rangle$, and of an operator $\mathcal{A}$ acting on them. $\mathcal{A}$ is composed of projectors $P^{(i)}$ acting on the two copies of subsystem i only (shown as circles in different gray scales).

$$c(\varrho) = \inf \sum_i c(\psi_i), \tag{3}$$

where the infimum is to be taken among all sets of properly normalized N-partite states such that $\varrho = \sum_i |\psi_i\rangle\langle\psi_i|$. Given one such set—e.g., the spectral decomposition $\{|\phi_i\rangle\}$ of ϱ—all legitimate decompositions can be constructed as linear combinations $|\psi_i\rangle = \sum_j V_{ij}|\phi_j\rangle$, with the additional constraint that the complex prefactors V_{ij} define a left unitary matrix, i.e., $\sum_i V_{ij}^* V_{ik} = \delta_{jk}$ [13]. The above optimization over decompositions into pure states is thus equivalent to an optimization over left unitary transformations, acting on the tensor $\hat{\mathcal{A}}$, with elements $\hat{\mathcal{A}}_{jk}^{lm} = \langle\phi_j| \otimes \langle\phi_k|\mathcal{A}|\phi_l\rangle \otimes |\phi_m\rangle$ [7,14].

Since left unitary transformations define a high dimensional, continuous set, the explicit evaluation of Eq. (3) tends to be rather cumbersome for a general mixed state. However, techniques which were devised to ease that task in the bipartite case [7] can be generalized in a straightforward manner, because the algebraic structure of the above N-partite concurrences (2) is strictly identical to the bipartite definition: $\mathcal{A}$ and therefore also $\hat{\mathcal{A}}$ is Hermitean and positive, which allows the decomposition $\hat{\mathcal{A}}_{jk}^{lm} = \sum_\alpha T_{jk}^\alpha (T_{lm}^\alpha)^*$, in terms of the matrices $T_{jk}^\alpha = \langle\phi_j| \otimes \langle\phi_k|\chi^\alpha\rangle$, which in turn are defined via the spectral decomposition $\mathcal{A} = \sum_\alpha |\chi_\alpha\rangle\langle\chi_\alpha|$. Analogous to [7] one can invoke the Cauchy-Schwarz inequality and the triangle inequality and bound the concurrence of an arbitrary mixed state from below by

$$c(\varrho) = \inf_V \sum_i \sqrt{\sum_\alpha |[VT^\alpha V^T]_{ii}|^2} \geq \inf_V \sum_i |[V\tau V^T]_{ii}|, \tag{4}$$

with $\tau = \sum_\alpha z_\alpha T^\alpha$; and the inequality holds for an arbitrary set of complex numbers z_α, such that $\sum_\alpha |z_\alpha|^2 = 1$ [7].

Without loss of generality, we can assume the number of factors $P_-^{(i)}$ in the explicit representation of $\mathcal{A}$ to be even, since otherwise the concurrence vanishes identically [15]. Therefore, any $|\chi_\alpha\rangle$ is symmetric with respect to the exchange of the two copies of $\mathcal{H}$, and thus, the matrices T^α are complex symmetric. Consequently, the infimum on the right-hand side of Eq. (4) can be evaluated algebraically [9,16], and the explicit solution in terms of the singular values λ_j (labeled in decreasing order) of τ reads $\lambda_1 - \sum_{j>1}\lambda_j$. The choice of the prefactors z_α—that determine τ—can be optimized numerically in order to approach the optimal lower bound. Furthermore, a purely algebraic, and in most cases excellent [17,18], approximation for $c(\varrho)$ can be obtained by substituting τ by the matrix τ^{qp} with elements $\tau_{ij}^{qp} = \langle\phi_1| \otimes \langle\phi_1|\mathcal{A}|\phi_i\rangle \otimes |\phi_j\rangle / \sqrt{\langle\phi_1| \otimes \langle\phi_1|\mathcal{A}|\phi_1\rangle \otimes |\phi_1\rangle}$. Herein, $|\phi_1\rangle$ is the eigenvector associated with the largest eigenvalue in the spectral decomposition of ϱ.

The above does not only apply to the discrete set of concurrences discussed so far, but also to the following continuous interpolation between them: Instead of a single direct product of projectors onto symmetric and antisymmetric subspaces, one may equally well consider convex combinations thereof,

$$\mathcal{A} = \sum_{\substack{\mathcal{V}\{s_i=\pm\} \\ \prod_{i=1}^{N} s_i=+}} p_{\{s_i\}} \bigotimes_{j=1}^{N} P_{s_j}^{(j)}, \qquad p_{\{s_i\}} \geq 0, \tag{5}$$

where $\mathcal{V}\{s_i = \pm\}$ represents all possible variations of an N string of the symbols $+$ and $-$, and the summation is restricted to contributions with an even number of projectors onto antisymmetric subspaces. Hence, through the arbitrariness of the choice of the $p_{\{s_i\}}$, there is actually a continuous family of concurrences, and we leave the interpretation of such N-particle concurrences for arbitrary $p_{\{s_i\}}$ as an open (and intriguing) question.

However, a discrete subset of N-partite concurrences has a transparent physical interpretation, and precisely allows us to distinguish different categories of multipartite entanglement. As an illustration, let us focus on some examplary tripartite and four-partite concurrences, which target at specific types of multipartite quantum correlations (see also Table I), in the remainder of the present Letter. Note that contenting ourselves with pure states, does not imply any restriction, since the concept of convex roofs guarantees that all properties on the level of pure states immediately convey to mixed states, as, e.g., also utilized in [18].

Biseparability with respect to specific partitions of tripartite states is easily detected by $c_1^{(3)}$, with $\mathcal{A} = 4P_+^{(1)} \otimes P_-^{(2)} \otimes P_-^{(3)}$ in Eq. (5) above, and, analogously, by $c_2^{(3)}$, with $\mathcal{A} = 4P_-^{(1)} \otimes P_+^{(2)} \otimes P_-^{(3)}$, and by $c_3^{(3)}$, with $\mathcal{A} = 4P_-^{(1)} \otimes P_-^{(2)} \otimes P_+^{(3)}$. Whereas $c_1^{(3)}$ and $c_2^{(3)}$ vanish identically for biseparable states like $|\psi\rangle = |\varphi^{(12)}\rangle \otimes |\zeta^{(3)}\rangle$, $c_3^{(3)}$ reduces to the bipartite concurrence of $|\varphi^{(12)}\rangle$, i.e., $c_3^{(3)}(\psi) = c(\varphi^{(12)})$. Thanks to the above construction (3) as a convex roof, these properties also pertain to mixed states. Note, however, that $c_3^{(3)}(\varrho)$ for a biseparable mixed state ϱ is *not* equivalent to $c(\mathrm{Tr}_3\varrho)$: Whereas the latter expression gives the bipartite correlation of ϱ only for a product state $\varrho = \rho^{(12)} \otimes \sigma^{(3)}$, $c_3^{(3)}$ is significantly more powerful, and performs the same task for any state with arbitrary classical correlations between $\mathcal{H}_3$ and the combined system of $\mathcal{H}_1$ and $\mathcal{H}_2$, i.e., for states alike $\sum_i p_i \rho_i^{(12)} \otimes \sigma_i^{(3)}$, $p_i \geq 0$. Arbitrary quantum correlations can be accounted for by C_3 with $p_{+--} = p_{-+-} = p_{--+} = 4$ and $p_{+++} = 0$ in Eq. (5), which vanishes only for completely separable states. For any biseparable state its value is given by the bipartite concurrence of the remaining entangled part.

Similarly, different degrees of separability are also captured in larger systems. For example, concurrences like $c_{ij}^{(4)}$, with $\mathcal{A} = 16P_{s_1}^{(1)} \otimes P_{s_2}^{(2)} \otimes P_{s_3}^{(3)} \otimes P_{s_4}^{(4)}$, $s_i = s_j = +$, and $s_k = -$ for $i \neq k \neq j$, determine with respect to which bipartite partition a mixed four-partite state is separable, and reduce to the bipartite (tripartite) concurrences of the entangled remainder.

Moreover, there is also the concurrence $c^{(4)}$, defined through $\mathcal{A} = 16P_-^{(1)} \otimes P_-^{(2)} \otimes P_-^{(3)} \otimes P_-^{(4)}$, that characterizes separability properties independent of any pairing of subsystems: $c^{(4)}$ vanishes for any state where at least one subsystem is uncorrelated with all other system components. In particular, for GHZ-like states $|\Psi_{\mathrm{GHZ}}\rangle = \sum_i \sqrt{\lambda_i}|iiii\rangle$, $c^{(4)}$ yields nonvanishing values, see Table I, whereas it vanishes for W states, as it is in accord with observations that in tripartite systems W states contain only bipartite correlations [19]. For two-level systems, $c^{(4)}$ can be used as a measure of the usefulness of a given state for multiparticle teleportation [20], and, since $\mathcal{A}$ is of rank one, Eq. (4) not only provides a lower bound, but rather the exact concurrence of arbitrary mixed states.

As a last example, we would like to focus on the N-partite generalization C_N of C_3, with $p_{\{s_i\}} = 4$ for all $\{s_i\}$ in Eq. (5), except for $p_{+\ldots+} = 0$. Defined for systems with an arbitrary number N of subsystems, C_N can be shown [21] to be monotonously decreasing under LOCC operations, such that it does not only allow to access separability properties, but also is an entanglement monotone [22]. As already pointed out in [18], C_N can—like any of the concurrences defined in Eq. (2)—be expressed in terms of all reduced density matrices ϱ_i

$$C_N(\Psi) = 2^{1-N/2}\sqrt{(2^N - 2)\langle\Psi|\Psi\rangle - \sum_i \mathrm{Tr}\varrho_i^2}, \tag{6}$$

TABLE I. Some examplary tripartite and four-partite concurrences for biseparable and GHZ-like states. For biseparable states, the concurrences $c_i^{(3)}$ $(i = 1, 2, 3)$, $c_{12}^{(4)}$, and $c_{34}^{(4)}$ either vanish or reduce to the bipartite (tripartite) concurrence of the remaining entangled part ($|\varphi^{(12)}\rangle$, $|\varphi^{(13)}\rangle|\varphi^{(23)}\rangle$, $|\varphi^{(123)}\rangle$or $|\zeta^{(34)}\rangle$) of $|\psi\rangle$, with $\eta(\phi) = \sqrt{1 - c(\phi)^2/4}$. C_4 vanishes for all states where at least one particle is uncorrelated with the other system components.

$\|\psi\rangle \in \otimes_{i=1}^3 \mathcal{H}_i$	$c_1^{(3)}(\psi)$	$c_2^{(3)}(\psi)$	$c_3^{(3)}(\psi)$	$C_3(\psi)$	$\|\psi\rangle \in \otimes_{i=1}^4 \mathcal{H}_i$	$c_{12}^{(4)}(\psi)$	$c_{34}^{(4)}(\psi)$	$C_4(\psi)$
$\|\varphi^{(12)}\rangle \otimes \|\zeta^{(3)}\rangle$	0	0	$c(\varphi^{(12)})$	$c(\varphi^{(12)})$	$\|\varphi^{(123)}\rangle \otimes \|\zeta^{(4)}\rangle$	0	$2c_3^{(3)}(\varphi^{(123)})$	0
$\|\varphi^{(13)}\rangle \otimes \|\zeta^{(2)}\rangle$	0	$c(\varphi^{(13)})$	0	$c(\varphi^{(13)})$	$\|\varphi^{(12)}\rangle \otimes \|\zeta^{(34)}\rangle$	$c(\zeta^{(34)})\eta(\varphi^{(12)})$	$c(\varphi^{(12)})\eta(\zeta^{(34)})$	$c(\varphi^{(12)})c(\zeta^{(34)})$
$\|\zeta^{(1)}\rangle \otimes \|\varphi^{(23)}\rangle$	$c(\varphi^{(23)})$	0	0	$c(\varphi^{(23)})$	$\|\Psi_{\mathrm{GHZ}}\rangle$	$2\sqrt{\sum_{i>j}\lambda_i\lambda_j}$	$2\sqrt{\sum_{i>j}\lambda_i\lambda_j}$	$2\sqrt{\sum_{i>j}\lambda_i\lambda_j}$

where the multi-index i runs over all $(2^N - 2)$ subsets of the N subsystems.

Like C_3, C_N only vanishes for completely separable N-partite states. Furthermore, it has the particularly nice property that $C_N(\psi)$ reduces to $C_{N-1}(\varphi)$ for any state $|\psi\rangle$ that factorizes into a product state on one subsystem and on the $(N-1)$-partite remainder $|\varphi\rangle$. This allows us to compare the nonclassical correlations inscribed in multipartite systems of variable size N.

In conclusion, we have seen that a discrete subset of the continuous family of concurrences defined by Eqs. (2) and (5), allows for a selective assessment of the separability properties of mixed multipartite quantum states. Given the lower bound (4), these quantities can be evaluated efficiently [7,17,18], and thus allows us, e.g., to address important questions such as the time evolution and the scaling properties (in terms of the system size) of entanglement in higher dimensional quantum systems [18]—an objective which so far could only be accomplished for the simple 2×2 case [23]. Furthermore, our definition reveals a continuously parametrized identifier of multipartite entanglement, an observation which still awaits its physical or statistical interpretation.

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[12] Note that $\mathcal{A}$ is acting on $\bigotimes_{i=1}^{N} \mathcal{H}_i \otimes \mathcal{H}_i$, whereas $|\Psi\rangle \otimes |\Psi\rangle \in (\bigotimes_{i=1}^{N} \mathcal{H}_i) \otimes (\bigotimes_{i=1}^{N} \mathcal{H}_i)$. Though, the two different spaces are isomorphic, and it is obvious how to identify their corresponding elements.

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