Concurrence in arbitrary dimensions.

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We argue that a complete characterisation of quantum correlations in bipartite systems of many dimensions may require a quantity which, even for pure states, does not reduce to a single number. Subsequently, we introduce multi-dimensional generalizations of concurrence and find evidence that they may provide useful tools for the analysis of quantum correlations in mixed bipartite states. We also introudce *biconcurrence* that leads to a necessary and sufficient condition for separability.

I. INTRODUCTION.

Entanglement plays central role in quantum information theory [1]. Pure state entanglement of bipartite systems is well understood in the sense that the relevant parameters for its optimal manipulation by local operations and classical communication (LOCC) have been identified and analyzed [2], [3]. Many efforts have also been devoted to the study of mixed-state entanglement. There, several possible entanglement measures have been proposed. Among these, entanglement of formation (E_F) [4], [5] attracts much of attention, as it is closely connected with (or, perhaps, equal to) the rate of production of mixed bipartite states out of pure ones by LOCC operations. It is, however, extremely difficult to evaluate E_F , but for the analytical formula for a single copy of an arbitrary state of two qubits obtained by Wootters [6]. Despite efforts, not much progress has been recorded regarding generalization of Wootters' result to the states in more than 2×2 dimensions [7].

Wootters' success in quantifying E_F for two qubits can be attributed to associating E_F with concurrence which is easier to calculate than E_F . Concurrence, as introduced by Hill and Wootters [8], was defined via operation of spin flip. More recently, Rungta et al. [9] made an attempt to generalize the notion of concurrence to pure bipartite states in arbitrary dimensions by introducing operation of universal state inversion [10]. Their universal inverter generalizes spin flip to a transformation which brings pure state $|\psi\rangle$ into the maximally mixed state in the subspace orthogonal to $|\psi\rangle$. In the same way that the spin flip generates concurrence for a pair of qubits, the universal inverter generates a number which generalizes concurrence for joint pure states of pairs of quantum systems of arbitrary dimensions. Generalized in this way, concurrence measures entanglement of pure bipartite states in terms of the purity of their marginal density operators.

As one knows [3], a complete characterization of quantum correlations in bipartite systems of many dimensions may require a quantity which, even for pure states, does not reduce to a single number [11]. Take, e.g., two pure states represented by vectors $\psi = (|11\rangle + |22\rangle)/2$ and $\phi = a\psi + b|33\rangle$, with $a = \sqrt{x}$ and $b = \sqrt{1-x}$, where $x \approx 0.2271$ is a root of $x^x [2(1-x)]^{1-x} = 1$. The two states have the same entanglement E_F of 1 ebit, nevertheless they have different Schmidt numbers and, consequently, it is impossible to locally convert one into the other.

In this contribution, we argue than that a suitable generalization of spin flip to more dimensions should produce a multi-dimensional analogue of concurrence rather than a single number. Such a concurrence would then describe not only the amount of entanglement but also its structure, e.g., the size (the number of dimensions) of the entangled spaces on each side. The concurrence for pure states is thus a matrix acting on the antisymmetric subspace of the total Hilbert space of two systems. Having that, one can follow Wootters and generalize the concept to mixed states by introducing a matrix of preconcurrence. The elements of this matrix are matrices in their own right and at the end, the matrix is often difficult to analyze. At least partially, the difficulties can be associated with the matrix dependence on the choice of the local bases. Therefore, we also generalize the concept of concurrence in a somewhat different direction. We abandon the requirement for preconcurrence to be a second order object in the state's ensemble. For this price we can define a fourth order object, *biconcurrence* matrix. It is independent of the local unitaries and allows us to reformulate separability problem in terms of the main diagonal of the matrix. Biconcurrence is a very simple function of ensemble of density matrix and has many symmetries. Therefore, the obtained necessary and sufficient separability condition seems to be the most promising one from algebraic point of view.

The generalization of pre-concurrence which satisfies our criterion is presented in section II. Then, in section III we give an example to show how our multi-dimensional pre-concurrence can be used for analysis of separability in arbitrary dimensions. There, we also discuss possible limitation of such analysis. Subsequently, in Sec. IV we introduce biconcurrence and formulate the necessary and sufficient condition for separability in terms of its elements. Finally, in section V we present a brief discussion of the results.

II. SPIN FLIP AND CONCURRENCE.

A. Pure states.

For pure states of two qubits, a spin flip transforms vector v in a 2-dimensional vector space into vector \tilde{v} equally long and orthogonal to v. In a bipartite system, a spin flip means that Alice performs a spin flip on her qubit and Bob on his. This gives a particularly simple expression for concurrence:

$$C\left(\psi\right) = \langle \tilde{\psi} | \psi \rangle \tag{1}$$

The spin flip operation and the concurrence which follows are well defined since, in a 2-dim space, there is only one direction which is orthogonal to a given one. One may further notice that concurrence defined in (1) together with the state's normalization allow to determine the eigenvalues of the associated reduced density matrix and, via these, the pure state's entanglement. The eigenvalues are the squares of the moduli of the singular values λ_1 and λ_2 of a 2×2 matrix $[\psi]$ of the coefficients defining the state in the standard basis:

$$\left|\psi\right\rangle = \sum_{i,j} \psi_{i,j} \left|i\right\rangle_A \otimes \left|j\right\rangle_B \tag{2}$$

The singular values are then related to the concurrence via

$$C = 2\lambda_1\lambda_2 = 2 \det\left(\left[\psi\right]\right)$$

In general, in a *d*-dimensional space there are d-1 dimensions orthogonal to a given direction. These can be represented by a d-1 antisymmetric form. From this point of view, performing a spin flip on a bipartite state means constructing a double d-1 form (one side for Alice and one side for Bob) locally dual to the double one-form representing the state vector $|\psi\rangle$. Concurrence can then be associated with the contraction of the form representing $|\psi\rangle$ with the form representing $\langle \tilde{\psi} |$. The contraction gives a double (d-2)-form which is equivalent to a double 2-form and can be represented by a $\binom{d}{2} \times \binom{d}{2}$ matrix with the following elements:

$$C_{i_1 \wedge j_1; i_2 \wedge j_2} = 2\left(\psi_{i_1, i_2} \,\psi_{j_1, j_2} - \psi_{i_1, j_2} \,\psi_{j_1, i_2}\right) \tag{3}$$

These elements are easily identified as twice the two-dimensional minors of matrix $[\psi]$. They describe the two-state contributions to the bipartite entanglement.

Regarding their structure, matrices C form a vector space with a natural trace norm:

$$\left|C\right|^{2} = Tr\left(C C^{\dagger}\right) = \sum_{i \wedge j, k \wedge l} \left|C_{i \wedge j; k \wedge l}\right|^{2}$$

$$\tag{4}$$

Having constructed the concurrence matrix, one may proceed in the same spirit and construct higher dimensional minors of $[\psi]$ (up to the Schmidt number). They will represent those contributions to the bipartite entanglement which embrace local subspaces of higher dimensions. We believe that, in principle, these concurrences of order higher than two may be important for the quantification of entanglement even if the separability of a pure state is determined by the lowest order (i.e. 2) concurrence. Clearly, a pure state (2) in arbitrary dimensions is separable iff [C] = 0.

B. Mixed states.

In order to further generalize the concept of concurrence to multidimensional mixed states, we follow Wootters and introduce (pre)concurrence as follows. Given a decomposition of state ρ into pure, unnormalized states,

$$\varrho = \sum_{\mu} |\psi^{\mu}\rangle \langle \psi^{\mu}| \tag{5}$$

we define pre-concurrences

$$C_{i_{1}\wedge j_{1};i_{2}\wedge j_{2}}^{\mu\nu} = \psi_{i_{1},i_{2}}^{\mu}\psi_{j_{1},j_{2}}^{\nu} - \psi_{i_{1},j_{2}}^{\mu}\psi_{j_{1},i_{2}}^{\nu} + \psi_{i_{1},i_{2}}^{\nu}\psi_{j_{1},j_{2}}^{\mu} - \psi_{i_{1},j_{2}}^{\nu}\psi_{j_{1},i_{2}}^{\mu}$$

$$(6)$$

The pre-concurrences can be regarded as a set of $\binom{d}{2} \times \binom{d}{2}$ matrices in μ and ν or, equivalently, as one matrix in μ

and ν with vector-like elements living in a $\binom{d}{2} \times \binom{d}{2}$ dimensional space. To systematize this picture, it may also be convenient to view C as an operator in the tensor product of two spaces. The first, \mathcal{H}_{∞} is the antisymmetric subspace of the space $C^d \otimes C^d$ the state acts on. Thus $\mathcal{H}_{\infty} = \mathcal{C}^{\lceil \epsilon - \lceil \ell \epsilon \rceil}$. The space $\mathcal{H}_{\mathcal{F}}$ is the space of "lists" of vectors for decomposition of the state. In principle we should allow this space to be infinite-dimensional, as one can consider infinite decompositions. However, it is likely that dimension d^4 is enough (for example, a separable state can be certainly decomposed into no more than d^4 product states [15]; similarly, there always exists an optimal decomposition for entanglement of formation containing no more than d^4 components [12]).

Matrix C viewed as operator acting on $\mathcal{H}_1 \otimes \mathcal{H}_2$ has simple transformation rules under (i) change of decomposition (ii) local unitary transformations of the state. Operations of type (i) transform the preconcurrence matrix according to:

$$C^{\mu'\nu'} = \sum_{\mu \ \nu} U^{\mu'\mu} C^{\mu\nu} U^{\nu'\nu}$$
(7)

with U being a unitary matrix changing the decomposition of the state into pure states [20]. This transformation can be represented as:

$$C \quad \to \quad C' = I \otimes UCI \otimes U^T \tag{8}$$

where subscript T stands for transposition. Similarly, a unitary transformation of the local bases

$$|e_{i_1} \otimes f_{i_2}\rangle = \sum_{k_1 \ k_2} \left| \hat{e}_{k_1} \otimes \hat{f}_{k_2} \right\rangle V_{k_1 i_1} \ W_{k_2 i_2}$$
(9)

(matrices V and W unitary) changes the components of the elements of $C^{\mu\nu}$ according to

$$\hat{\mathbf{C}}_{\mathbf{i}_{1}\wedge\mathbf{j}_{1};\mathbf{i}_{2}\wedge\mathbf{j}_{2}}^{\mu\nu} = \sum_{k_{1}l_{1}k_{2}l_{2}} V_{i_{1}k_{1}}V_{j_{1}l_{1}}W_{i_{2}k_{2}}W_{j_{2}l_{2}} \ \mathbf{C}_{\mathbf{k}_{1}\wedge\mathbf{l}_{1};\mathbf{k}_{2}\wedge\mathbf{l}_{2}}^{\mu\nu}
= \sum_{k_{1}< l_{1};k_{2}< l_{2}} (V_{i_{1}k_{1}}V_{j_{1}l_{1}} - V_{i_{1}l_{1}}V_{j_{1}k_{1}}) (W_{i_{2}k_{2}}W_{j_{2}l_{2}} - W_{i_{2}l_{2}}W_{j_{2}k_{2}}) \mathbf{C}_{\mathbf{k}_{1}\wedge\mathbf{l}_{1};\mathbf{k}_{2}\wedge\mathbf{l}_{2}}^{\mu\nu}$$
(10)

which can be represented as

$$C \to \hat{C} = (V \otimes W) \otimes I C (V^T \otimes W^T) \otimes I$$
(11)

III. CONCURRENCE AND SEPARABILITY.

The preconcurrence matrix defined in the previous section sheds some interesting light on the separability of mixed states. Obviously, a given bipartite state ρ is separable iff there is a decomposition for which all the diagonal elements $C^{\mu\mu}$ are zero vectors. The non-separable states can then be divided into two classes:

- a) the states which allow for such a pair of local bases that for at least one $\kappa_0 = i_1^0 \wedge j_1^0; i_2^0 \wedge j_2^0$, no transformation (7) can zero the diagonal of $C^{\mu\nu}_{\kappa_0}$.
- b) the states where for every single component $\kappa = i_1 \wedge j_1$; $i_2 \wedge j_2$, there exist a decomposition with all the diagonal elements $C_{\mu}^{\mu\mu}$ to zero (different decompositions for different multi-indexes κ). This property must hold irrespective of the choice of the local bases.

The states in class (a) contain 2-qubit entanglement and as such are distillable [13]. Class (b), on the other hand contains all the bound entangled (BE) states [14,15]. Indeed, two qubit entangled states are distillable hence a BE state cannot contain two-qubit entanglement. A known open question in this context is if class (b) is equivalent to the BE states or if it is strictly larger. In Ref. [14] it was shown that a state ρ is distillable iff for some number k the state $\rho^{\otimes k}$ has two-qubit entanglement. Call such state k-copy pseudo distillable (according to notation of Ref. [16]). The question if the set of BE states is equal to class (b) can be then rephrased as: does k-copy pseudo distillability imply 1-copy pseudo distillability. In principle it might happen that the property of having two-qubit entanglement is not additive: 1 copy would not contain it, but two or more copies would. For some Werner states there is strong evidence that this is the case [16,17]. In Ref. [18] a possible equivalence of the considered sets was connected with some "binarization" of conditional information in cryptography based on mixed quantum states.

In this context, our preconcurrence matrix allows for a simple argument which shows that rank 2 states are either separable or 1-copy pseudo distillable (for the original proof of non-existence of bound entangled states of rank 2 see [19]).

A. Rank-2 states are either separable or 1-copy pseudo distillable.

Rank-2 states have 2×2 preconcurrence matrices. A state which has a decomposition where all the matrices are of the form

$$C_1 = \begin{bmatrix} 0 & x \\ x & 0 \end{bmatrix} \tag{12}$$

is separable. A candidate for a non-separable and not 1-copy pseudo-distillable state must have at least two essentially different preconcurrence matrices. In a decomposition where one of the matrices is of the form (12), there must be another one

$$\tilde{C}_2 = e^{i\varphi} \begin{bmatrix} a \ e^{i\alpha} & b \\ b & -a \ e^{-i\alpha} \end{bmatrix}$$
(13)

with all the parameters real and $a \neq 0$. This form is necessary since otherwise it would be impossible for transformation (7) to make the diagonal of \tilde{C}_2 zero. Moreover, a simple phase adjustment in the decomposition of the state can bring α and φ to zero, without changing \tilde{C}_1 's diagonal. With such an adjustment the second matrix becomes

$$C_2 = \begin{bmatrix} a & b \\ b & -a \end{bmatrix}$$
(14)

with both a and b real. Now, a change of the local bases which (up to a normalizing factor) produces

$$C_2' = C_2 + i \begin{bmatrix} 0 & |x| \\ |x| & 0 \end{bmatrix}$$

shows that the state contains 2-qubit entanglement, i.e., it is distillable. Indeed, C'_2 is of form (13) with real non-zero a and complex b. Such a matrix has two singular values of different moduli. Consequently, no transformation (7) can reduce its trace to zero. This implies 2-qubit entanglement.

As a corollary to the above argument, one may notice that a rank-2 state is separable iff there exists a 2-state decomposition of the state which simultaneously diagonalizes all the C_{κ} matrices so that all the matrices are of the essentially the same form

$$C_{\kappa} = \begin{bmatrix} x_{\kappa} & 0\\ 0 & -x_{\kappa} \end{bmatrix}$$
(15)

Indeed, if separability requires existence of a decomposition where, irrespectively of the choice of the local bases, all the C_{κ} 's are of form (12), then transformation (7) with

$$U = U_q = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1\\ -1 & 1 \end{bmatrix}$$
(16)

transforms them into (15).

Analysis of separability of states of rank higher than two appears to be more difficult. In particular, an attempt to follow Wootters' minimization procedure for the expectation value of the concurrence's norm is not simple since there is no guarantee that transformation (8) can diagonalize matrix C (notice that the elements of C are vectors while the elements of U are numbers. One can, nevertheless, diagonalize $D = Tr_{\mathcal{H}_{\infty}}CC^{\dagger}$. This leads to some simplifications in special cases, like when diagonal D implies diagonal C. Nevertheless, at the moment, we do not have any general results for states of rank higher than 2.

IV. BICONCURRENCE.

Bearing in mind the difficulties, one may try to look at the generalized concurrence from a somewhat different perspective. For two qubits, preconcurrence can be viewed as a bilinear form $C(\psi, \phi)$ which distinguishes between product vectors and entangled vectors. It satisfies the following crucial condition:

Condition 1. $C(\psi, \psi) = 0$ if and only if ψ is a product vector.

In passing, one may note that a form which satisfies condition 1 cannot be linear in one argument and anti-linear in the other, since a linear-antilinear form can be written as

$$C(\psi,\phi) = \langle \psi | A\phi \rangle,\tag{17}$$

where A is a linear operator acting on space \mathcal{H} . However, form (17) which vanishes on all the product vectors, vanishes everywhere, thus violating condition 1. Consequently, the form must be bi-linear (or bi-antilinear, it does not matter which). In this context, Wootters' concurrence defines a good form for $\mathcal{H} = \mathcal{C}^{\in} \otimes \mathcal{C}^{\in}$. It reads

$$C(\psi,\phi) = \langle \psi | \phi \rangle \tag{18}$$

Wootters' preconcurrence matrix is then simply

$$C^{\mu\nu}(\varrho) = C(\psi_{\mu}, \psi_{\nu}) \tag{19}$$

Unfortunately, as it follows from Ref. [9], in higher dimensions there does not exist a bi-linear form satisfying Condition 1. A possible way to generalize Wootters concurrence can then be to look for a 4-argument form $B(\psi, \phi, \kappa, \theta)$ which would satisfy

Condition 1'. $B(\psi) \equiv B(\psi, \psi, \psi, \psi) = 0$ iff ψ is a product vector. A possible form satisfying Condition 1', linear in two arguments and antilinear in the two other is closely related to Rungta et al. concurrence [9] and to our preconcurrence matrix. For instance, one can take a slightly simplified version of concurrence in [9] as a departure point, and define

$$B(\psi) = -\langle \psi | I \otimes \Lambda(|\psi\rangle \langle \psi|) | \psi \rangle.$$
⁽²⁰⁾

where Λ is the positive map used in the reduction criterion of separability [21]: $\Lambda(A) = Tr(A)I - A$

One finds that $B(\psi) = 1 - \text{Tr}\rho^2$, where ρ is a reduction of ψ . It is then clear that **B** satisfies the condition 1'. The corresponding bi-concurrence matrix is then

$$B^{\mu\nu mn} = B(\psi_{\mu}, \psi_{\nu}, \psi_{m}, \psi_{n}) = -\langle \psi_{\mu} | I \otimes \Lambda(|\psi_{\nu}\rangle \langle \psi_{m}|) | \psi_{n}\rangle.$$
⁽²¹⁾

After some algebra this can be rewritten as

$$B^{\mu\nu mn} = \langle \psi_{\mu} | \psi_{\nu} \rangle \langle \psi_{m} | \psi_{n} \rangle - Tr \left[[\psi_{\mu}]^{\dagger} [\psi_{\nu}] [\psi_{m}]^{\dagger} [\psi_{n}] \right]$$
(22)

which is nothing else than a partial contraction of a product of preconcurrence matrix with its complex conjugation.

$$B^{\mu\nu\ mn} = \frac{1}{4} \sum_{i \wedge j, k \wedge l} C^{n\nu}_{i \wedge j; k \wedge l} \cdot \left(C^{m\mu}_{i \wedge j; k \wedge l} \right)^* \tag{23}$$

Bi-concurrence is invariant under local unitary rotations of the state. Changes in the state's decomposition, on the other hand, transform bi-concurrence as follows

$$\tilde{B}^{\mu\nu mn} = \sum_{\alpha,\beta,a,b} (U^{\mu\alpha})^* (U^{ma})^* B^{\alpha\beta ab} U^{\nu\beta} U^{nb}.$$
(24)

If we treat the matrix \mathbf{B} as an operator acting on tensor product of Hilbert spaces with Greek (Latin) indices for first (second) space, we obtain

$$\tilde{\mathbf{B}} = U^* \otimes U^* \mathbf{B} (\mathbf{U}^*)^{\dagger} \otimes (\mathbf{U}^*)^{\dagger}$$
(25)

One can see that the matrix B contains the whole information about possible separability of state ρ . Moreover, irrespective of the decomposition, the elements on the main diagonal of B are real and non-negative. Therefore, in terms of biconcurrence, separability is equivalent to the existence of such a unitary U that in eq. (25)

$$tr(\mathbf{B}) = 0 \tag{26}$$

The lower-case tr is here understood as the sum of the elements on the main diagonal:

$$tr\tilde{\mathbf{B}} = \sum_{\mu} \tilde{B}^{\mu\mu\mu\mu}.$$
(27)

Note that the elements $\tilde{B}^{\mu\mu\mu\mu}$ are always nonnegative. Therefore it suffices to minimize (26)over unitaries U and check whether the minimum vanishes.

Within the picture of B acting on product Hilbert space one can express the condition as follows

$$\min_{U} Tr(U \otimes UPU^{\dagger} \otimes U^{\dagger}B) = 0, \tag{28}$$

where $P = \sum_{i} |ii\rangle \langle ii|$ with $|ij\rangle$ being standard product basis.

The condition (26) seems to be quite simple, and we hope that it will lead to a more operational condition for separability.

V. CONCLUSIONS.

In conclusion, we argue that the multidimensional generalizations of concurrence which we have introduced in this contribution put the question of determination of separability of bipartite quantum states in a somewhat new perspective.

First, we introduced a concept of preconcurrence matrix. The matrix was designed to distinguish between the contributions to the entanglement which embrace pairs of different two dimensional subspaces of the bipartite system. In this way, our preconcurrence matrix contained all the information necessary to identify separability of a given state. Nevertheless, its dependence on the particular choice of the local basis made it rather difficult to analyze in detail, but in a rather restricted class of cases.

Therefore, we also generalized the concept of concurrence in another direction and abandoned the requirement for it to be a second order object in the state's ensemble. We arrived at the concept of biconcurrence matrix. This matrix is of the fourth order in the state's ensemble, however, for this price it is invariant under local unitaries. Biconcurrence can be easily derived from a given bipartite state directly. It can also be constructed by a suitable contraction out of our preconcurrence matrix. The resulting separability condition is probably the easiest possible one from the algebraic point of view.

Regarding a complete characterization of entanglement, on the other hand, our generalizations of concurrence matrix may not be enough. The main reason for this is that in order to specify the singular values of $[\psi]$, in addition to the length of the preconcurrence defined in eq. (4), one needs the lengths of all its tri-, ..., d-linear analogues. We hope to return to this point in the nearest future.

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