# LEWENSTEIN-SANPERA DECOMPOSITION OF A GENERIC $2\otimes 2$ DENSITY MATRIX BY USING WOOTTERS'S BASIS

S. J. AKHTARSHENAS<sup>a,b,c</sup> and M. A. JAFARIZADEH<sup>a,b,c</sup>
<sup>a</sup> Department of Theoretical Physics and Astrophysics, Tabriz University

Tabriz 51666, Iran

<sup>b</sup> Institute for Studies in Theoretical Physics and Mathematics

Tehran 19395-1795, Iran

<sup>c</sup> Research Institute for Fundamental Sciences

Tabriz 51666, Iran

E-mail: akhtarshenas@tabrizu.ac.ir jafarizadeh@tabrizu.ac.ir

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An analytical expression for optimal Lewenstein-Sanpera (L-S) decomposition of a generic two qubit density matrix is given. By evaluating the L-S decomposition of Bell decomposable states, the optimal decomposition for arbitrary full rank state of two qubit system is obtained via local quantum operations and classical communications (LQCC). In Bell decomposable case the separable state optimizing L-S decomposition, minimize the von Neumann relative entropy as a measure of entanglement. The L-S decomposition for a generic two-qubit density matrix is only obtained by using Wootters's basis. It is shown that the average concurrence of the decomposition is equal to the concurrence of the state. It is also shown that all the entanglement content of the state is concentrated in the Wootters's state  $|x_1\rangle$  associated with the largest eigenvalue  $\lambda_1$  of the Hermitian matrix  $\sqrt{\sqrt{\rho}\tilde{\rho}\sqrt{\rho}}$ . It is shown that a given density matrix  $\rho$  with corresponding set of positive numbers  $\lambda_i$  and Wootters's basis can transforms under SO(4,c) into a generic  $2\times 2$  matrix with the same set of positive numbers but with new Wootters's basis, where the local unitary transformations correspond to SO(4,r) transformations, hence,  $\rho$  can be represented as coset space SO(4,c)/SO(4,r) together with positive numbers  $\lambda_i$ .

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#### 1 Introduction

Perhaps, quantum entanglement is the most non-classical features of quantum mechanics [1, 2] which has recently been attracted much attention although it was discovered many decades ago by Einstein and Schrödinger [1, 2]. It plays a central role in quantum information theory and provides potential resource for quantum communication and information processing [3, 4, 5]. Entanglement is usually arise from quantum correlations between separated subsystems which can not be created by local actions on each subsystems. By definition, a bipartite mixed state  $\rho$  is said to be separable if it can be expressed as

$$ho = \sum_i w_i \, 
ho_i^{(1)} \otimes 
ho_i^{(2)}, \qquad w_i \geq 0, \quad \sum_i w_i = 1,$$

where  $\rho_i^{(1)}$  and  $\rho_i^{(2)}$  denote density matrices of subsystems 1 and 2, respectively. Otherwise the state is entangled.

The central tasks of quantum information theory is to characterize and quantify entangled states. A first attempt in characterization of entangled states has been made by Peres and Horodecki et al. [6, 7]. Peres showed that a necessary condition for separability of a two partite system is that its partial transposition be positive. Horodecki et al. have shown that this condition is sufficient for separability of composite systems only for dimensions  $2 \otimes 2$  and  $2 \otimes 3$ .

There is also an increasing attention in quantifying entanglement, particularly for mixed states of a bipartite system, and a number of measures have been proposed [5, 8, 9, 10]. Among them the entanglement of formation has more importance, since it intends to quantify the resources needed to create a given entangled state.

An interesting description of entanglement is Lewenstein-Sanpera decomposition which intends to construct best separable approximation (BSA) of an entangled density matrix [11]. Lewenstein and Sanpera in [11] have shown that any two partite density matrix can be represented optimally as a sum of a separable state and an entangled state. They have also shown that for two qubit systems the decomposition reduces to a mixture of a mixed separable state and an entangled pure state, thus all entanglement content of the state is concentrated in the pure entangled state. This leads to an unambiguous measure of entanglement for any two qubit state as entanglement of pure state multiplied by the weight of pure part in the decomposition.

The numerical method for finding the BSA has been reported in Ref. [11]. Also in two qubit systems some analytical results for special states were found in [12]. An attempt to generalize the results of Ref. [11] is made in [13]. In [14] an algebraic approach to find BSA of a two qubit state is attempted. They have also shown that the weight of the entangled part in the decomposition is equal to the concurrence of the state.

In this paper we give an analytical expression for optimal Lewenstein-Sanpera (L-S) decomposition of a generic two qubit density matrix. We first obtain L-S decomposition for a generic Bell decomposable (BD) state. We provide two product ensemble for BSA to prove that the obtained decomposition is optimal, the one which has a geometric interpretation and the other in terms of Wootters's product states. It is shown that both product ensemble verify the optimality of the decomposition, that is, although the BSA is unique, the product ensemble, in general, is not unique. As a byproduct we show that separable state optimizing L-S decomposition, minimizes the von Neumann relative entropy introduced in [8, 9] as a measure of entanglement. We also obtain optimal decomposition for arbitrary full rank two qubit density matrix via local quantum operation and classical communications (LQCC). It is shown that although Wootters's product states can be used to prove optimality of the decomposition in the case of BD states, their LQCC transformed states are not enable to prove the optimality of the decomposition for a generic state obtained from BD states via LQCC operation. This shows that even though the separable part of density matrix can be written in different form of products, the products in Wootters's basis are the best one to work.

Considering the above motivation, by using Wootters's basis, an analytical expression for optimal Lewenstein-Sanpera decomposition for a generic two qubit density matrix has been obtained. Wootters in [10] has shown that for any two qubit density matrix  $\rho$  there

always exist a decomposition  $\rho = \sum_i |x_i\rangle \langle x_i|$  such that  $\langle x_i|\tilde{x}_j\rangle = \lambda_i\delta_{ij}$ , where  $\lambda_i$  are square roots of eigenvalues, in decreasing order, of the non-Hermitian matrix  $\rho\tilde{\rho}$ . Based on this the concurrence of the mixed state  $\rho$  is defined by  $\max(0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4)$  [10]. We show that all entanglement content of the state is concentrated in the Wootters's state  $|x_1\rangle$  associated with the largest eigenvalue  $\lambda_1$ . It is also shown that the average concurrence of the decomposition is equal to the concurrence of the state.

Finally we show that a given density matrix  $\rho$  with corresponding set of positive numbers  $\lambda_i$  and Wootters's basis can transforms under SO(4,c) into a generic two qubit density matrix with the same set of positive numbers but with new Wootters's basis, where the local unitary transformations correspond to SO(4,r) transformations, hence,  $\rho$  can be represented as coset space SO(4,c)/SO(4,r) together with positive numbers  $\lambda_i$ . By giving an explicit parameterization we characterize a generic orbit of group of local unitary transformations.

The paper is organized as follows. In section 2 we review concurrence and Wootters's basis as presented in [10]. In section 3 Lewenstein-Sanpera decomposition for two qubit density matrix is reviewed. Some theorems of Ref. [11] where we are going to use in whole paper to prove the optimality of the presented decomposition is also reviewed in section 3. In section 4 we first introduce Bell decomposable states and evaluate their concurrence via the method presented by Wootters. We obtain L-S decomposition of these states and prove the optimality of the decomposition by introducing two distinct product ensemble for separable part. Relation between L-S decomposition and relative entropy is also discussed in section 4. In section 5 optimal decomposition of arbitrary full rank two qubit density matrix is obtained via LQCC operation. In section 6 we give an analytical expression for L-S decomposition of a generic two qubit density matrix. Characterization of the density matrix in terms of orthogonal group is presented in Appendix B. This Appendix is devoted to explicit parameterization of a generic density matrix up to a local unitary transformation. The paper is ended with a brief conclusion in section 7.

#### $\mathbf{2}$ Concurrence and Wootters's Basis

In this section we review concurrence and Wootters's basis of two qubit mixed states as introduced in [10]. From the various measures proposed to quantify entanglement, the entanglement of formation has a special position which in fact intends to quantify the resources needed to create a given entangled state [5]. In the case of pure state if the density matrix obtained from partial trace over other subsystems is not pure the state is entangled. For the pure state  $|\psi\rangle$  of a bipartite system, entropy of the density matrix associated with either of the two subsystems is a good measure of entanglement

$$E(\psi) = -Tr(\rho_A \log_2 \rho_A) = -Tr(\rho_B \log_2 \rho_B),$$

where  $\rho_A = Tr_B(|\psi\rangle\langle\psi|)$  and  $\rho_B$  is defined similarly. Due to classical correlations where exist in the mixed state each subsystem can have non-zero entropy even if there is no entanglement, therefore von Neumann entropy of a subsystem is no longer a good measure of entanglement. For a mixed state entanglement of formation is defined as the minimum of average entropy of the state over all pure state decompositions of the state [5]

$$E_f(\rho) = \min \sum_i p_i E(\psi_i). \tag{1}$$

Wootters in [10] has shown that for a two qubit system entanglement of formation of a mixed state  $\rho$  can be defined as

$$E_f(\rho) = H\left(\frac{1}{2} + \frac{1}{2}\sqrt{1 - C^2}\right),$$
 (2)

where  $H(x) = -x \ln x - (1-x) \ln (1-x)$  is binary entropy and concurrence  $C(\rho)$  is defined by

$$C(\rho) = \max\{0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4\},\tag{3}$$

where the  $\lambda_i$  are the non-negative eigenvalues, in decreasing order, of the Hermitian matrix  $R \equiv \sqrt{\sqrt{\rho}\tilde{\rho}\sqrt{\rho}}$  and

$$\tilde{\rho} = (\sigma_y \otimes \sigma_y) \rho^* (\sigma_y \otimes \sigma_y), \tag{4}$$

where  $\rho^*$  is the complex conjugate of  $\rho$  when it is expressed in a standard basis such as  $\{|\uparrow\uparrow\rangle\,,|\uparrow\downarrow\rangle\},\{|\downarrow\uparrow\rangle\,,|\downarrow\downarrow\rangle\}$  and  $\sigma_y$  represent Pauli matrix in local basis  $\{|\uparrow\rangle\,,|\downarrow\downarrow\rangle\}$ .

Consider a generic two qubit density matrix  $\rho$  with its subnormalized orthogonal eigenvectors  $|v_i\rangle$ , i.e.  $\rho = \sum_i |v_i\rangle \langle v_i|$ . There always exist a decomposition [10]

$$\rho = \sum_{i} |x_{i}\rangle \langle x_{i}| \tag{5}$$

where Wootters's basis  $|x_i\rangle$  are defined by

$$|x_{i}\rangle = \sum_{j=1}^{4} U_{ij}^{*} |v_{i}\rangle, \quad \text{for} \quad i = 1, 2, 3, 4,$$
 (6)

such that

$$\langle x_i \mid \tilde{x}_j \rangle = (U\tau U^T)_{ij} = \lambda_i \delta_{ij}, \tag{7}$$

where  $\tau_{ij} = \langle v_i \mid \tilde{v}_j \rangle$  is a symmetric but not necessarily Hermitian matrix. To construct  $|x_i\rangle$  we use the fact that for any symmetric matrix  $\tau$  one can always find a unitary matrix U in such a way that  $\lambda_i$  are real and non-negative, that is, they are the square roots of eigenvalues of  $\tau\tau^*$  which are the same as eigenvalues of R. Moreover one can always find U such that  $\lambda_i$  appear in decreasing order.

Wootters in [10] has also shown that in the case that  $\rho$  is separable ,i.e.,  $\lambda_1 - \lambda_2 - \lambda_3 - \lambda_4 \leq 0$ , the density matrix with decomposition given in Eq. (5) can be expanded as

$$\rho = \sum_{i} |z_{i}\rangle \langle z_{i}| \tag{8}$$

where product states  $|z_i\rangle$  are defined as

$$|z_1\rangle = \frac{1}{2} \left( e^{i\theta_1} |x_1\rangle + e^{i\theta_2} |x_2\rangle + e^{i\theta_3} |x_3\rangle + e^{i\theta_4} |x_4\rangle \right),$$
 (9)

$$|z_2\rangle = \frac{1}{2} \left( e^{i\theta_1} |x_1\rangle + e^{i\theta_2} |x_2\rangle - e^{i\theta_3} |x_3\rangle - e^{i\theta_4} |x_4\rangle \right),$$
 (10)

$$|z_3\rangle = \frac{1}{2} \left( e^{i\theta_1} |x_1\rangle - e^{i\theta_2} |x_2\rangle + e^{i\theta_3} |x_3\rangle - e^{i\theta_4} |x_4\rangle \right),$$
 (11)

$$|z_4\rangle = \frac{1}{2} \left( e^{i\theta_1} |x_1\rangle - e^{i\theta_2} |x_2\rangle - e^{i\theta_3} |x_3\rangle + e^{i\theta_4} |x_4\rangle \right),$$
 (12)

where zero concurrence is guaranteed with  $\sum_{j=1} e^{2i\theta_j} \lambda_j = 0$ . In the next sections we are going to use the above product state as product ensemble of BSA.

# Lewenstein-Sanpera Decomposition

According to Lewenstein-Sanpera decomposition [11], any two qubit density matrix  $\rho$  can be written as

$$\rho = \lambda \rho_{sep} + (1 - \lambda) |\psi\rangle \langle\psi|, \qquad \lambda \in [0, 1], \tag{13}$$

where  $\rho_{sep}$  is a separable density matrix and  $|\psi\rangle$  is a pure entangled state. The Lewenstein-Sanpera (L-S) decomposition of a given density matrix  $\rho$  is not unique and, in general, there is a continuum set of L-S decomposition to choose from. The optimal decomposition is, however, unique for which  $\lambda$  is maximal and

$$\rho = \lambda^{(opt)} \rho_{sep}^{(opt)} + (1 - \lambda^{(opt)}) |\psi^{(opt)}\rangle \langle \psi^{(opt)}|, \qquad \lambda^{(opt)} \in [0, 1].$$

$$(14)$$

Lewenstein and Sanpera in [11] have shown that any other decomposition of the form  $\rho =$  $\tilde{\lambda}\tilde{\rho}_{sep} + (1-\tilde{\lambda})|\tilde{\psi}\rangle\langle\tilde{\psi}|$  with  $\tilde{\rho} \neq \rho^{(opt)}$  necessarily implies that  $\tilde{\lambda} < \lambda^{(opt)}$  [11]. They have also shown that a given decomposition is optimal if the separable part of the decomposition can be expanded in terms of product states  $|e_{\alpha}, f_{\alpha}\rangle$ , i.e.

$$\lambda \rho_{sep} = \sum_{\alpha} \Lambda_{\alpha} |e_{\alpha}, f_{\alpha}\rangle \langle e_{\alpha}, f_{\alpha}|, \qquad (15)$$

such that the following conditions are satisfied [11]:

- i) All  $\Lambda_{\alpha}$  are maximal with respect to  $\rho_{\alpha} = \Lambda_{\alpha} |e_{\alpha}, f_{\alpha}\rangle \langle e_{\alpha}, f_{\alpha}| + (1-\lambda) |\psi\rangle \langle \psi|$  and projector  $P_{\alpha} = |e_{\alpha}, f_{\alpha}\rangle \langle e_{\alpha}, f_{\alpha}|.$
- ii) All pairs  $(\Lambda_{\alpha}, \Lambda_{\beta})$  are maximal with respect to  $\rho_{\alpha\beta} = \Lambda_{\alpha} |e_{\alpha}, f_{\alpha}\rangle \langle e_{\alpha}, f_{\alpha}| + \Lambda_{\beta} |e_{\beta}, f_{\beta}\rangle \langle e_{\beta}, f_{\beta}| + \Lambda_{\beta} |e_{\beta}\rangle \langle e_{\beta}, f_{\beta}| + \Lambda_{\beta} |e_{\beta}\rangle \langle e_{\beta}, f_{\beta}| + \Lambda$  $(1-\lambda) |\psi\rangle \langle \psi|$  and the pairs of projector  $(P_{\alpha}, P_{\beta})$ .

Lewenstein and Sanpera in [11] have shown that  $\Lambda_{\alpha}$  is maximal with respect to  $\rho_{\alpha}$  and  $P_{\alpha} = |e_{\alpha}, f_{\alpha}\rangle \langle e_{\alpha}, f_{\alpha}| \text{ iff: a) if } |e_{\alpha}, f_{\alpha}\rangle \notin \mathcal{R}(\rho_{\alpha}) \text{ then } \Lambda_{\alpha} = 0, \text{ and b) if } |e_{\alpha}, f_{\alpha}\rangle \in \mathcal{R}(\rho_{\alpha}) \text{ then } \Lambda_{\alpha} = \langle e_{\alpha}, f_{\alpha}| \rho_{\alpha}^{-1} |e_{\alpha}, f_{\alpha}\rangle^{-1} > 0.$ 

They have also shown that a pair  $(\Lambda_1, \Lambda_2)$  is maximal with respect to  $\rho_{12}$  and a pair of projectors  $(P_1, P_2)$  iff: a) if  $|e_1, f_1\rangle$ ,  $|e_2, f_2\rangle$  do not belong to  $\mathcal{R}(\rho_{12})$  then  $\Lambda_1 = \Lambda_2 = 0$ ; b) if  $|e_1, f_1\rangle$  does not belong, while  $|e_2, f_2\rangle \in \mathcal{R}(\rho_{12})$  then  $\Lambda_1 = 0, \ \Lambda_2 = \langle e_2, f_2 | \rho_{12}^{-1} | e_2, f_2 \rangle^{-1}$ ; c) if  $|e_1, f_1\rangle, |e_2, f_2\rangle \in \mathcal{R}(\rho_{12}) \text{ and } \langle e_1, f_1| \rho_{12}^{-1} |e_2, f_2\rangle = 0 \text{ then } \Lambda_i = \langle e_i, f_i| \rho_{12}^{-1} |e_i, f_i\rangle^{-1}, \ i = 1, 2;$ d) finally, if  $|e_1, f_1\rangle$ ,  $|e_2, f_2\rangle \in \mathcal{R}(\rho_{12})$  and  $\langle e_1, f_1| \rho_{12}^{-1} |e_2, f_2\rangle \neq 0$  then

$$\Lambda_{1} = (\langle e_{2}, f_{2} | \rho_{12}^{-1} | e_{2}, f_{2} \rangle - | \langle e_{1}, f_{1} | \rho_{12}^{-1} | e_{2}, f_{2} \rangle |)/D, 
\Lambda_{2} = (\langle e_{1}, f_{1} | \rho_{12}^{-1} | e_{1}, f_{1} \rangle - | \langle e_{1}, f_{1} | \rho_{12}^{-1} | e_{2}, f_{2} \rangle |)/D,$$
(16)

where  $D = \langle e_1, f_1 | \rho_{12}^{-1} | e_1, f_1 \rangle \langle e_2, f_2 | \rho_{12}^{-1} | e_2, f_2 \rangle - | \langle e_1, f_1 | \rho_{12}^{-1} | e_2, f_2 \rangle |^2$ . In the next sections we are going to use the above algorithm to prove the optimality of the L-S decomposition.

#### 4 Lewenstein-Sanpera Decomposition for Bell Decomposable States

Here in this section we obtain L-S decomposition for Bell decomposable (BD) states. A two qubit BD state is defined by

$$\rho = \sum_{i=1}^{4} p_i |\psi_i\rangle \langle \psi_i|, \qquad 0 \le p_i \le 1, \quad \sum_{i=1}^{4} p_i = 1.$$
 (17)

where  $|\psi_i\rangle$  are Bell states given by

$$|\psi_1\rangle = \frac{1}{\sqrt{2}}(|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle),\tag{18}$$

$$|\psi_2\rangle = \frac{1}{\sqrt{2}}(|\uparrow\uparrow\rangle - |\downarrow\downarrow\rangle),$$
 (19)

$$|\psi_3\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle),$$
 (20)

$$|\psi_4\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle). \tag{21}$$

BD states form a four simplex (tetrahedral) with its vertices defined by  $p_1 = 1$ ,  $p_2 = 1$ ,  $p_3 = 1$  and  $p_4 = 1$  [15]. A necessary condition for separability of composite quantum systems is presented by Peres [6]. He showed that if a state is separable then the matrix obtained from partial transposition must be positive. Horodecki et al. in [7] have shown that Peres criterion provides sufficient condition only for separability of mixed quantum states of dimensions  $2 \otimes 2$  and  $2 \otimes 3$ . This implies that the state given in Eq. (17) is separable if and only if the following inequalities are satisfying

$$p_i \le \frac{1}{2}, \quad \text{for} \quad i = 1, 2, 3, 4.$$
 (22)

In the rest of the paper we consider entangled states for which  $p_1 \geq \frac{1}{2}$ .

Before going to evaluate L-S decomposition for BD states let us evaluate concurrence and Wootters's basis of these states which are to be used latter. Starting from the spectral decomposition for BD states, given in (17), we define subnormalized orthogonal eigenvectors  $|v_i\rangle$  as

$$|v_i\rangle = \sqrt{p_i} |\psi_i\rangle, \qquad \langle v_i | v_j\rangle = p_i \delta_{ij}.$$
 (23)

Following the method given in section 2 we get for the state of  $\rho$  given in Eq. (17)

$$\tau = \operatorname{diag}(-p_1, p_2, p_3, -p_4), \qquad U = \operatorname{diag}(i, 1, 1, i). \tag{24}$$

Now it is easy to evaluate  $\lambda_i$  which yields

$$\lambda_1 = p_1, \quad \lambda_2 = p_2, \quad \lambda_3 = p_3, \quad \lambda_4 = p_4.$$
 (25)

where we use the fact  $p_1 \ge 1/2$  and we assume without loss of generality that  $p_2 \ge p_3 \ge p_4$ . One can now easily evaluate the concurrence and Wootters's basis of BD states as

$$C = p_1 - p_2 - p_3 - p_4 = 2p_1 - 1, (26)$$

and

$$|x_{1}\rangle = -i\sqrt{p_{1}} |\psi_{1}\rangle, \qquad |x_{2}\rangle = \sqrt{p_{2}} |\psi_{2}\rangle, |x_{3}\rangle = \sqrt{p_{3}} |\psi_{3}\rangle, \qquad |x_{4}\rangle = -i\sqrt{p_{4}} |\psi_{4}\rangle$$
(27)

respectively, where  $|\psi_i\rangle$  are Bell states given in Eq. (18) to (21).

Now we are in position to evaluate L-S decomposition for BD states. To this aim we write  $\rho$  as a convex sum of pure state  $|\psi_1\rangle$  and separable state  $\rho_s$  as

$$\rho = \lambda \rho_s + (1 - \lambda) |\psi_1\rangle \langle \psi_1|, \qquad (28)$$

where  $\rho_s$  is a boundary separable BD state for which  $p_1 = \frac{1}{2}$ . Expanding  $\rho_s$  as  $\rho_s = \sum_{i=1}^4 p_i' |\psi_i\rangle \langle \psi_i|$  and using Eq. (17) for  $\rho$  we arrive at the following results

$$p'_1 = \frac{1}{2}, p'_i = \frac{p_i}{2(1-p_1)} \text{for} i = 2, 3, 4,$$
 (29)

and

$$\lambda = 2(1 - p_1). \tag{30}$$

It is worth to note that average concurrence of the decomposition is equal to the concurrence of the state, i.e.

$$(1 - \lambda)C(|\psi_1\rangle) = 2p_1 - 1. \tag{31}$$

In the rest of this section we show that thus obtained decomposition is optimal. To do so we provide two product ensemble for  $\rho_s$  and show that  $\rho_s$  can be expanded in terms of each ensemble such that corresponding coefficients are maximal.

#### 4.1 Canonical product states

In this subsection we show that the decomposition given in Eq. (28) is optimal. We begin by using the fact that  $\rho_s$  given in Eq. (29) can be written as the following convex sum of product states [15]

$$\rho_s = 2(p_3'\sigma_1 + p_4'\sigma_2 + p_2'\sigma_3),\tag{32}$$

where  $p'_i$  are given in Eq. (29) and  $\sigma_i$  are defined by

$$\sigma_{1} = \frac{1}{2}(|\psi_{1}\rangle\langle\psi_{1}| + |\psi_{3}\rangle\langle\psi_{3}|) = \frac{1}{2}(|x_{+}\rangle\langle x_{+}| \otimes |x_{+}\rangle\langle x_{+}| + |x_{-}\rangle\langle x_{-}| \otimes |x_{-}\rangle\langle x_{-}|), 
\sigma_{2} = \frac{1}{2}(|\psi_{1}\rangle\langle\psi_{1}| + |\psi_{4}\rangle\langle\psi_{4}|) = \frac{1}{2}(|y_{+}\rangle\langle y_{+}| \otimes |y_{-}\rangle\langle y_{-}| + |y_{-}\rangle\langle y_{-}| \otimes |y_{+}\rangle\langle y_{+}|), 
\sigma_{3} = \frac{1}{2}(|\psi_{1}\rangle\langle\psi_{1}| + |\psi_{2}\rangle\langle\psi_{2}|) = \frac{1}{2}(|z_{+}\rangle\langle z_{+}| \otimes |z_{+}\rangle\langle z_{+}| + |z_{-}\rangle\langle z_{-}| \otimes |z_{-}\rangle\langle z_{-}|),$$
(33)

and  $|x_{\pm}\rangle$ ,  $|y_{\pm}\rangle$  and  $|z_{\pm}\rangle$  are eigenstates corresponding to eigenvalues  $\pm 1$  of  $\sigma_x$ ,  $\sigma_y$  and  $\sigma_z$ , respectively. Using the above results we rewrite  $\rho$  given in Eq. (28) in terms of product states and pure entangled state

$$\rho = \sum_{\alpha=1}^{6} \Lambda_{\alpha} |e_{\alpha}, f_{\alpha}\rangle \langle e_{\alpha}, f_{\alpha}| + (1 - \lambda) |\psi_{1}\rangle \langle \psi_{1}|, \qquad (34)$$

where  $|e_{\alpha}, f_{\alpha}\rangle$ ,  $\alpha = 1, 2, ..., 6$  are product states defined by

$$|e_{1}, f_{1}\rangle = |x_{+}\rangle \otimes |x_{+}\rangle , \qquad |e_{2}, f_{2}\rangle = |x_{-}\rangle \otimes |x_{-}\rangle , |e_{3}, f_{3}\rangle = |y_{+}\rangle \otimes |y_{-}\rangle , \qquad |e_{4}, f_{4}\rangle = |y_{-}\rangle \otimes |y_{+}\rangle , |e_{5}, f_{5}\rangle = |z_{+}\rangle \otimes |z_{+}\rangle , \qquad |e_{6}, f_{6}\rangle = |z_{-}\rangle \otimes |z_{-}\rangle ,$$

$$(35)$$

and  $\Lambda_{\alpha}$ ,  $\alpha = 1, 2, ...6$  are given by

$$\Lambda_1 = \Lambda_2 = p_3', \qquad \Lambda_3 = \Lambda_4 = p_4', \qquad \Lambda_5 = \Lambda_6 = p_2'.$$
 (36)

Now, in order to show that decomposition (28) with  $\lambda$  given in (30) is optimal we have to show that all coefficients  $\Lambda_{\alpha}$  in Eq. (34) are maximal. To do so we first need to show that  $\Lambda_{\alpha}$ s are maximal with respect to  $\rho_{\alpha}$  and  $P_{\alpha}$ .

Matrices  $\rho_{\alpha} = \rho - \sum_{\alpha' \neq \alpha}^{6} \Lambda_{\alpha'} P_{\alpha'} = \Lambda_{\alpha} P_{\alpha} + (1 - \lambda) |\psi_{1}\rangle \langle \psi_{1}|$  with  $P_{\alpha} = |e_{\alpha}, f_{\alpha}\rangle \langle e_{\alpha}, f_{\alpha}|$  for  $(\alpha = 1, 2, ..., 6)$  have two zero eigenvalues and two non zero eigenvalues. In Bell basis its kernel and range are separated. After restriction to its range, it is straightforward to evaluate  $\rho_{\alpha}^{-1}$  and we find that  $\langle e_{\alpha}, f_{\alpha}| \rho_{\alpha}^{-1} |e_{\alpha}, f_{\alpha}\rangle = 1/\Lambda_{\alpha}$ .

In order to prove that the pair  $(\Lambda_{\alpha}, \Lambda_{\beta})$  are maximal with respect to  $\rho_{\alpha\beta}$  and the pair of projectors  $(P_{\alpha}, P_{\beta})$ , we proceed as follows:

- a) Matrices  $\rho_{i,i+1} = \Lambda_i P_i + \Lambda_{i+1} P_{i+1} + (1-\lambda) |\psi_1\rangle \langle \psi_1|$  for (i=1,3,5) have a two dimensional range. In Bell basis its range and kernel are separated and one can obtain  $\langle e_i, f_i | \rho_{i,i+1}^{-1} | e_i, f_i \rangle = (\Lambda_{i+1} + (1-\lambda))/\Gamma_i$ ,  $\langle e_{i+1}, f_{i+1} | \rho_{i,i+1}^{-1} | e_{i+1}, f_{i+1} \rangle = (\Lambda_i + (1-\lambda))/\Gamma_i$  and  $\langle e_i, f_i | \rho_{i,i+1}^{-1} | e_{i+1}, f_{i+1} \rangle = (1-\lambda)/(2\Gamma_i)$ , where  $\Gamma_i = \Lambda_i \Lambda_{i+1} + \frac{1}{2}(1-\lambda)$ . Using the above results together with Eqs. (16) we obtain the maximality of pair  $(\Lambda_i, \Lambda_{i+1})$  with respect to  $\rho_{i,i+1}$  and the pair of projectors  $(P_i, P_{i+1})$  for i=1,3 and 5.
- b) For other possibility of  $\alpha$  and  $\beta$ , matrices  $\rho_{\alpha\beta} = \Lambda_{\alpha} P_{\alpha} + \Lambda_{\beta} P_{\beta} + (1 \lambda) |\psi_{1}\rangle \langle \psi_{1}|$  have rank 3. Using the Bell basis we can evaluate  $\rho_{\alpha\beta}^{-1}$  and we find that  $\langle e_{\alpha}, f_{\alpha}|\rho_{\alpha\beta}^{-1}|e_{\beta}, f_{\beta}\rangle = 0$  for  $\alpha \neq \beta$ ,  $\langle e_{\alpha}, f_{\alpha}|\rho_{\alpha\beta}^{-1}|e_{\alpha}, f_{\alpha}\rangle = 1/\Lambda_{\alpha}$ . This completes the proof that all coefficients  $\Lambda_{\alpha}$  are maximal and decomposition (28) is optimal.

#### 4.2 Wootters's product states

We now provide another product ensemble to show that the decomposition given in Eq. (28) is optimal. To this aim by using the fact that for marginal states  $\rho_s$  (located at the boundary of separable region) the eigenvalues  $\lambda_i$  satisfy constraint  $\lambda_1 - \lambda_2 - \lambda_3 - \lambda_4 = 0$ , we can choose the phase factors  $\theta_i$  in Eqs. (9) to (12) as  $\theta_2 = \theta_3 = \theta_4 = \theta_1 - \frac{\pi}{2}$ . Choosing  $\theta_1 = 0$  we arrive at the following product ensemble for  $\rho_s$ 

$$|z_{1}\rangle = \frac{1}{2}(-i\sqrt{p'_{1}}|\psi_{1}\rangle - i\sqrt{p'_{2}}|\psi_{2}\rangle - i\sqrt{p'_{3}}|\psi_{3}\rangle - \sqrt{p'_{4}}|\psi_{4}\rangle), |z_{2}\rangle = \frac{1}{2}(-i\sqrt{p'_{1}}|\psi_{1}\rangle - i\sqrt{p'_{2}}|\psi_{2}\rangle + i\sqrt{p'_{3}}|\psi_{3}\rangle + \sqrt{p'_{4}}|\psi_{4}\rangle), |z_{3}\rangle = \frac{1}{2}(-i\sqrt{p'_{1}}|\psi_{1}\rangle + i\sqrt{p'_{2}}|\psi_{2}\rangle - i\sqrt{p'_{3}}|\psi_{3}\rangle + \sqrt{p'_{4}}|\psi_{4}\rangle), |z_{4}\rangle = \frac{1}{2}(-i\sqrt{p'_{1}}|\psi_{1}\rangle + i\sqrt{p'_{2}}|\psi_{2}\rangle + i\sqrt{p'_{3}}|\psi_{3}\rangle - \sqrt{p'_{4}}|\psi_{4}\rangle),$$
(37)

where  $p_i'$  are defined in Eq. (29). Let us consider the set of four product vectors  $\{|z_{\alpha}\rangle\}$  and one entangled state  $|\psi_1\rangle$ . In Ref. [10] it is shown that the ensemble  $\{|z_{\alpha}\rangle\}$  are linearly independent. Evaluating Wronskian determinant of vectors  $|\psi_1\rangle$  and  $|z_{\alpha}\rangle$  we get  $W_{\alpha}=\frac{1}{8}$ . This implies that vector  $|\psi_1\rangle$  is linearly independent with respect to all vectors  $|z_{\alpha}\rangle$ . Also evaluating the Wronskian  $W_{\alpha\beta}$  for three vectors  $|\psi_1\rangle$ ,  $|z_{\alpha}\rangle$  and  $|z_{\beta}\rangle$  we get

$$W_{12} = W_{34} = \frac{1}{8}p_2'(1-2p_2'), \quad W_{13} = W_{24} = \frac{1}{8}p_3'(1-2p_3'), \quad W_{14} = W_{23} = \frac{1}{8}p_4'(1-2p_4').$$
 (38)

Equations (38) shows that in the cases that  $\rho$  has full rank three vectors  $|z_{\alpha}\rangle$ ,  $|z_{\beta}\rangle$  and  $|\psi_{1}\rangle$  are linearly independent. Now consider matrices  $\rho_{\alpha} = \Lambda_{\alpha} |z_{\alpha}\rangle \langle z_{\alpha}| + (1-\lambda) |\psi_{1}\rangle \langle \psi_{1}|$ . Due to independence of  $|z_{\alpha}\rangle$  and  $|\psi_{1}\rangle$  we can deduce that the range of  $\rho_{\alpha}$  is two dimensional. Thus after restriction to its range and defining their dual basis  $|\hat{z}_{\alpha}\rangle$  and  $|\hat{\psi}_{1}\rangle$ , we can expand restricted inverse  $\rho_{\alpha}^{-1}$  as  $\rho_{\alpha}^{-1} = \Lambda_{\alpha}^{-1} |\hat{z}_{\alpha}\rangle \langle \hat{z}_{\alpha}| + (1-\lambda)^{-1} |\hat{\psi}_{1}\rangle \langle \hat{\psi}_{1}|$  (see Appendix A). Using Eq. (76) it is easy to see that  $\langle z_{\alpha}|\rho_{\alpha}^{-1}|z_{\alpha}\rangle = \Lambda_{\alpha}^{-1}$ . This shows that  $\Lambda_{\alpha}$  are maximal with respect to  $\rho_{\alpha}$  and the projector  $P_{\alpha}$ .

Similarly by considering matrices  $\rho_{\alpha\beta} = \Lambda_{\alpha} |z_{\alpha}\rangle \langle z_{\alpha}| + \Lambda_{\beta} |z_{\beta}\rangle \langle z_{\beta}| + (1-\lambda) |\psi_{1}\rangle \langle \psi_{1}|$  and taking into account the independency of three vectors  $|z_{\alpha}\rangle$ ,  $|z_{\beta}\rangle$  and  $|\psi_{1}\rangle$  we see that rang

of  $\rho_{\alpha\beta}$  is three dimensional, where after restricting to its range and defining dual basis  $|\hat{z}_{\alpha}\rangle$ ,  $|\hat{z}_{eta}\rangle$  and  $|\hat{\psi}_{1}\rangle$  we can write restricted inverse  $\rho_{\alpha\beta}^{-1}$  as  $\rho_{\alpha\beta}^{-1} = \Lambda_{\alpha}^{-1}|\hat{z}_{\alpha}\rangle\langle\,\hat{z}_{\alpha}| + \Lambda_{\beta}^{-1}|\hat{z}_{\beta}\rangle\langle\,\hat{z}_{\beta}| + (1-\epsilon)^{-1}$  $\lambda$ )<sup>-1</sup>| $\hat{\psi}_1$ \langle\langle\hat{\psi}\_1|. Then it is straightforward to get  $\langle z_{\alpha}|
ho_{\alpha\beta}^{-1}|z_{\alpha}\rangle=\Lambda_{\alpha}^{-1}$ ,  $\langle z_{\beta}|
ho_{\alpha\beta}^{-1}|z_{\beta}\rangle=\Lambda_{\beta}^{-1}$  and  $\langle z_{\alpha} | \rho_{\alpha\beta}^{-1} | z_{\beta} \rangle = 0$ . This implies that the pairs  $(\Lambda_{\alpha}, \Lambda_{\beta})$  are maximal with respect to  $\rho_{\alpha\beta}$  and the pairs of projectors  $(P_{\alpha}, P_{\beta})$ , thus complete the proof that the decomposition given in Eq. (28) is optimal.

We now consider cases that  $\rho$  has not full rank. Let  $p_{\alpha} = 0$  for  $\alpha \neq 1$ . In this case Eq. (38) shows that the pairs  $\{|z_1\rangle, |z_{\alpha}\rangle\}$  and also  $\{|z_{\beta}\rangle, |z_{\gamma}\rangle\}$  for  $\beta, \gamma \neq 1, \alpha$  are no longer independent with respect to  $|\psi_1\rangle$ . In former case we express  $|\psi_1\rangle$  in terms of  $|z_1\rangle$ ,  $|z_\alpha\rangle$  then matrix  $\rho_{1\alpha}$  can be written in terms of two basis  $|z_1\rangle$ ,  $|z_{\alpha}\rangle$  and after some calculations we get  $\langle z_1|\rho_{1\alpha}^{-1}|z_1\rangle=\frac{\Lambda_{\alpha}+2(1-\lambda)}{\Gamma_{1\alpha}}$ ,  $\langle z_{\alpha}|\rho_{1\alpha}^{-1}|z_{\alpha}\rangle=\frac{\Lambda_{1}+2(1-\lambda)}{\Gamma_{1\alpha}}$  and  $\langle z_1|\rho_{1\alpha}^{-1}|z_{\alpha}\rangle=\frac{-2(1-\lambda)}{\Gamma_{1\alpha}}$  where  $\Gamma_{1\alpha}=\Lambda_1\Lambda_{\alpha}+2(1-\lambda)(\Lambda_1+\Lambda_{\alpha})$ . By using the above results together with Eqs. (16) we obtain the maximality of pair  $(\Lambda_1, \Lambda_{\alpha})$  with respect to  $\rho_{1\alpha}$  and the pair of projectors  $(P_1, P_{\alpha})$ .

Similarly in latter case we express  $|\psi_1\rangle$  in terms of  $|z_{\beta}\rangle$ ,  $|z_{\gamma}\rangle$  then matrix  $\rho_{\beta\gamma}$  can be written in terms of two basis  $|z_{\beta}\rangle$ ,  $|z_{\gamma}\rangle$  and we get  $\left\langle z_{\beta}|\rho_{\beta\gamma}^{-1}|z_{\beta}\right\rangle = \frac{\Lambda_{\gamma}+2(1-\lambda)}{\Gamma_{\beta\gamma}}$ ,  $\left\langle z_{\gamma}|\rho_{\beta\gamma}^{-1}|z_{\gamma}\right\rangle = \frac{\Lambda_{\beta}+2(1-\lambda)}{\Gamma_{\beta\gamma}}$ and  $\left\langle z_{\beta} | \rho_{\beta\gamma}^{-1} | z_{\gamma} \right\rangle = \frac{-2(1-\lambda)}{\Gamma_{\beta\gamma}}$  where  $\Gamma_{\beta\gamma} = \Lambda_{\beta}\Lambda_{\gamma} + 2(1-\lambda)(\Lambda_{\beta} + \Lambda_{\gamma})$ . Again using the above results together with Eqs. (16) we obtain the maximality of pairs  $(\Lambda_{\beta}, \Lambda_{\gamma})$  with respect to  $\rho_{\beta\gamma}$  and the pairs of projectors  $(P_{\beta}, P_{\gamma})$ .

Finally let us consider the cases that rank  $\rho$  is 2. Let  $p_{\alpha} = p_{\beta} = 0$  for  $\alpha, \beta \neq 1$ . In these cases we have  $|z_{\alpha}\rangle = |z_{\beta}\rangle$  and  $|z_{1}\rangle = |z_{\gamma}\rangle$  for  $\gamma \neq 1, \alpha, \beta$ . It is now sufficient to take  $|z_{1}\rangle$  and  $|z_{\alpha}\rangle$  as product ensemble. But Eq. (38) shows that these vectors are not independent with respect to  $|\psi_1\rangle$ . We express  $|\psi_1\rangle$  in terms of  $|z_1\rangle$  and  $|z_\alpha\rangle$  then matrix  $\rho_{1\alpha}$  can be written in terms of two vectors  $|z_1\rangle$  and  $|z_{\alpha}\rangle$  and after some calculations we get  $\langle z_1|\rho_{1\alpha}^{-1}|z_1\rangle=\frac{\Lambda_{\alpha}+2(1-\lambda)}{\Gamma_{1\alpha}}$ ,  $\langle z_{\alpha}|\rho_{1\alpha}^{-1}|z_{\alpha}\rangle = \frac{\Lambda_1+2(1-\lambda)}{\Gamma_{1\alpha}}$  and  $\langle z_1|\rho_{1\alpha}^{-1}|z_{\alpha}\rangle = \frac{-2(1-\lambda)}{\Gamma_{1\alpha}}$  where  $\Gamma_{1\alpha} = \Lambda_1\Lambda_{\alpha} + 2(1-\lambda)(\Lambda_1 + \Lambda_{\alpha})$ . Using the above results together with Eqs. (16) we obtain the maximality of pairs  $(\Lambda_1, \Lambda_{\alpha})$ with respect to  $\rho_{1\alpha}$  and the pairs of projectors  $(P_1, P_{\alpha})$ .

Also it is worth to note that the decomposition (28) satisfies conditions for BSA of Ref. [14]. According to theorem 1 of Ref. [14], decomposition given in (28) is the optimal decomposition if and only if: rank $(\rho_s^{T_B}) = 3$ , i.e.  $\exists_{|\phi\rangle} \rho_s^{T_B} |\phi\rangle = 0$ , and either

(i) 
$$\exists_{\alpha>0} (|\phi\rangle \langle \phi|)^{T_B} |\psi\rangle = -\alpha |\psi\rangle$$
, or  
(ii)  $\operatorname{rank}(\rho_s) = 3$ ,  $i.e. \exists_{|\tilde{\phi}\rangle} \rho_s |\tilde{\phi}\rangle = 0$ , and  $\exists_{\alpha,\nu\geq 0} \left(\nu |\tilde{\phi}\rangle \langle \tilde{\phi}| + (|\phi\rangle \langle \phi|)^{T_B}\right) |\psi\rangle = -\alpha |\psi\rangle$ .  
(39)

It is now straightforward to see that  $\rho_s^{T_B}$  has three non vanishing eigenvalues, that is, its rank is 3. Its one dimensional kernel is along the Bell state  $|\psi_4\rangle$  given in Eq. (21). Actually the density matrices corresponding to the interior of tetrahedral satisfy condition (i) while those at its boundary satisfy condition (ii), respectively.

#### Relative entropy of entanglement and L-S decomposition

Vedral et al. in [8, 9] introduced a class of distance measures suitable for entanglement measures. According to their methods, entanglement measure for a given state  $\rho$  is defined as

$$E(\rho) = \min_{\sigma \in \mathcal{D}} D(\rho \parallel \sigma), \tag{40}$$

where D is any measure of distance (not necessarily a metric) between two density matrix  $\rho$  and  $\sigma$ , and  $\mathcal{D}$  is the set of all separable states. They have also shown that von Neumann relative entropy defined by

 $S(\rho \parallel \sigma) = Tr\{\rho \ln \frac{\rho}{\sigma}\},\tag{41}$ 

satisfies three conditions that a good measure of entanglement must satisfy [8]. Here, we would like to emphasis that  $\rho_s$  given in Eq. (29) minimizes von Neumann relative entropy given in (41). Authors in [8] have shown that for BD states given in Eq. (17), separable state  $\sigma$  that minimize relative entropy is

$$p'_1 = \frac{1}{2}$$
, and  $p'_i = \frac{p_i}{2(1-p_1)}$  for  $i = 2, 3, 4$ . (42)

It is worth to note that the above equation is the same as Eq. (29), that is, separable state optimizing L-S decomposition minimizes von Neumann relative entropy, too.

# 5 L-S Decomposition under LQCC

In this section we study the behavior of L-S decomposition under local quantum operations and classical communications (LQCC). A general LQCC is defined by [16, 17]

$$\rho' = \frac{(A \otimes B)\rho(A \otimes B)^{\dagger}}{Tr((A \otimes B)\rho(A \otimes B)^{\dagger})},\tag{43}$$

where operators A and B can be written as

$$A \otimes B = U_A f^{\mu,a,\mathbf{m}} \otimes U_B f^{\nu,b,\mathbf{n}}, \tag{44}$$

where  $U_A$  and  $U_B$  are unitary operators acting on subsystems A and B, respectively and the filtration f defined by

$$f^{\mu,a,\mathbf{m}} = \mu(I_2 + a\,\mathbf{m}.\sigma),$$
  

$$f^{\nu,b,\mathbf{n}} = \nu(I_2 + b\,\mathbf{n}.\sigma).$$
(45)

As it is shown in Refs. [16, 17], the concurrence of the state  $\rho$  transforms under LQCC of the form given in Eq. (43) as

$$C(\rho') = \frac{\mu^2 \nu^2 (1 - a^2)(1 - b^2)}{Tr((A \otimes B)\rho(A \otimes B)^{\dagger})} C(\rho).$$
 (46)

Performing LQCC on L-S decomposition of BD states we get

$$\rho' = \frac{(A \otimes B)\rho(A \otimes B)^{\dagger}}{Tr((A \otimes B)\rho(A \otimes B)^{\dagger})} = \lambda'\rho'_s + (1 - \lambda')|\psi'_1\rangle\langle\psi'_1|, \tag{47}$$

with  $\rho_s'$  and  $|\psi_1'\rangle$  defined as

$$\rho_s' = \frac{(A \otimes B)\rho_s(A \otimes B)^{\dagger}}{Tr((A \otimes B)\rho_s(A \otimes B)^{\dagger})},\tag{48}$$

$$|\psi_1'\rangle = \frac{(A \otimes B) |\psi_1\rangle}{\sqrt{\langle \psi_1| (A^{\dagger} A \otimes B^{\dagger} B) |\psi_1\rangle}},\tag{49}$$

$$\lambda' = \frac{Tr((A \otimes B)\rho_s(A \otimes B)^{\dagger})}{Tr((A \otimes B)\rho(A \otimes B)^{\dagger})} \lambda. \tag{50}$$

Using Eq. (50), we get for the weight of entangled part in the decomposition (47)

$$(1 - \lambda') = \frac{\langle \psi_1 | (A^{\dagger} A \otimes B^{\dagger} B) | \psi_1 \rangle}{Tr((A \otimes B)\rho(A \otimes B)^{\dagger})} (1 - \lambda). \tag{51}$$

Now we can easily evaluate the average concurrence of  $\rho'$  in the L-S decomposition given in (47)

$$(1 - \lambda')C(|\psi_1'\rangle) = \frac{\mu^2 \nu^2 (1 - a^2)(1 - b^2)}{Tr((A \otimes B)\rho(A \otimes B)^{\dagger})} (1 - \lambda)C(|\psi_1\rangle), \tag{52}$$

where, by comparing the above equation with Eq. (46) we see that  $(1-\lambda)C(|\psi\rangle)$  (the average concurrence in the L-S decomposition) transforms like concurrence under LQCC. Now we would like to show that the decomposition given in Eq. (47) is optimal. To this aim, we perform LQCC action on matrices  $\rho_{\alpha} = \Lambda_{\alpha} |z_{\alpha}\rangle \langle z_{\alpha}| + (1-\lambda) |\psi_{1}\rangle \langle \psi_{1}|$  and get

$$\rho_{\alpha}' = \frac{(A \otimes B)\rho_{\alpha}(A \otimes B)^{\dagger}}{Tr((A \otimes B)\rho_{\alpha}(A \otimes B)^{\dagger})} = \Lambda_{\alpha}' |z_{\alpha}'\rangle \langle z_{\alpha}'| + (1 - \lambda') |\psi_{1}'\rangle \langle \psi_{1}'|$$
(53)

where

$$|z'_{\alpha}\rangle = \frac{(A \otimes B)|z_{\alpha}\rangle}{\sqrt{\langle z_{\alpha}|(A^{\dagger}A \otimes B^{\dagger}B)|z_{\alpha}\rangle}},\tag{54}$$

and

$$\Lambda_{\alpha}' = \frac{\langle z_{\alpha} | A^{\dagger} A \otimes B^{\dagger} B) | z_{\alpha} \rangle}{Tr((A \otimes B)\rho_{\alpha}(A \otimes B)^{\dagger})} \Lambda_{\alpha}. \tag{55}$$

Using the fact that LQCC transformations are invertible [17, 18, 19], we can evaluate  $\rho_{\alpha}^{\prime^{-1}}$  as

$$\rho_{\alpha}^{\prime^{-1}} = Tr((A \otimes B)\rho_{\alpha}(A \otimes B)^{\dagger}) (A^{\dagger} \otimes B^{\dagger})^{-1}\rho_{\alpha}^{-1}(A \otimes B)^{-1}.$$
 (56)

Using the above equation and Eq. (54) we get

$$\langle z_{\alpha}' | \rho_{\alpha}^{\prime^{-1}} | z_{\alpha}' \rangle = \frac{Tr((A \otimes B)\rho_{\alpha}(A \otimes B)^{\dagger})}{\langle z_{\alpha} | (A^{\dagger}A \otimes B^{\dagger}B) | z_{\alpha} \rangle} \langle z_{\alpha} | \rho_{\alpha}^{-1} | z_{\alpha} \rangle = \Lambda_{\alpha}^{\prime^{-1}}.$$
 (57)

Equation (57) shows that  $\Lambda'_{\alpha}$  are maximal with respect to  $\rho'_{\alpha}$  and the projector  $P'_{\alpha}$ .

Matrices  $\rho_{\alpha\beta} = \Lambda_{\alpha} \left| z_{\alpha} \right\rangle \left\langle z_{\alpha} \right| + \Lambda_{\beta} \left| z_{\beta} \right\rangle \left\langle z_{\beta} \right| + (1 - \lambda) \left| \psi_{1} \right\rangle \left\langle \psi_{1} \right|$  transform under LQCC as

$$\rho'_{\alpha\beta} = \frac{(A \otimes B)\rho_{\alpha,\beta}(A \otimes B)^{\dagger}}{Tr((A \otimes B)\rho_{\alpha\beta}(A \otimes B)^{\dagger})} = \Lambda'_{\alpha} |z'_{\alpha}\rangle \langle z'_{\alpha}| + \Lambda'_{\beta} |z'_{\beta}\rangle \langle z'_{\beta}| + (1 - \lambda') |\psi'_{1}\rangle \langle \psi'_{1}| \qquad (58)$$

where

$$|z'_{\alpha,\beta}\rangle = \frac{(A \otimes B)|z_{\alpha,\beta}\rangle}{\sqrt{\langle z_{\alpha,\beta}| (A^{\dagger} A \otimes B^{\dagger} B)|z_{\alpha,\beta}\rangle}},\tag{59}$$

and

$$\Lambda'_{\alpha,\beta} = \frac{\langle z_{\alpha,\beta} | (A^{\dagger} A \otimes B^{\dagger} B) | z_{\alpha,\beta} \rangle}{Tr((A \otimes B)\rho_{\alpha\beta}(A \otimes B)^{\dagger})} \Lambda_{\alpha,\beta}.$$
 (60)

We now consider cases that  $\rho$  is full rank. For these cases we could show in subsection (4-2) that all vectors  $|z_{\alpha}\rangle$ ,  $|z_{\beta}\rangle$  and  $|\psi_1\rangle$  are linearly independent. Using the above results and invertibility of LQCC actions we arrive at the following results

$$\langle z'_{\alpha} | \rho'_{\alpha\beta}^{-1} | z'_{\alpha} \rangle = \frac{Tr((A \otimes B)\rho_{\alpha\beta}(A \otimes B)^{\dagger})}{\langle z_{\alpha} | (A^{\dagger}A \otimes B^{\dagger}B) | z_{\alpha} \rangle} \langle z_{\alpha} | \rho_{\alpha\beta}^{-1} | z_{\alpha} \rangle = \Lambda'_{\alpha},$$

$$\langle z'_{\beta} | \rho'_{\alpha\beta}^{-1} | z'_{\beta} \rangle = \frac{Tr((A \otimes B)\rho_{\alpha\beta}(A \otimes B)^{\dagger})}{\langle z_{\beta} | (A^{\dagger}A \otimes B^{\dagger}B) | z_{\beta} \rangle} \langle z_{\beta} | \rho_{\alpha\beta}^{-1} | z_{\beta} \rangle = \Lambda'_{\beta},$$

$$\langle z'_{\alpha} | \rho'_{\alpha\beta}^{-1} | z'_{\beta} \rangle = \frac{Tr((A \otimes B)\rho_{\alpha\beta}(A \otimes B)^{\dagger})}{\sqrt{\langle z_{\alpha} | (A^{\dagger}A \otimes B^{\dagger}B) | z_{\alpha} \rangle \langle z_{\beta} | (A^{\dagger}A \otimes B^{\dagger}B) | z_{\beta} \rangle}} \langle z_{\alpha} | \rho_{\alpha\beta}^{-1} | z_{\beta} \rangle = 0.$$
(61)

Equations. (61) show that the pair  $(\Lambda'_{\alpha}, \Lambda'_{\beta})$  are maximal with respect to  $\rho'_{\alpha,\beta}$  and the pair of projectors  $(P'_{\alpha}, P'_{\beta})$ . For other cases that  $\rho$  is not full rank we saw that there is some dependency between three vectors  $|z_{\alpha}\rangle$ ,  $|z_{\beta}\rangle$  and  $|\psi_{1}\rangle$  such that  $\langle z_{\alpha}|\rho_{\alpha\beta}^{-1}\rangle|z_{\beta}\rangle\neq 0$ . This implies that in general  $\langle z'_{\alpha}|\rho'_{\alpha\beta}^{-1}|z'_{\beta}\rangle\neq 0$ . In the next section we are going to evaluate, directly, L-S decomposition for arbitrary two qubit density matrix and by using associated Wootters's product states we will prove the optimality in general.

As Verstraete et al. have been shown in Refs. [18, 19] the LQCC operation correspond to left and right multiplication of the density matrix by Lorentz transformations. In Appendix B we will show that a given density matrix with corresponding set of positive numbers  $\lambda_i$  and Wootters's basis can transforms under SO(4,c) into a generic two qubit density matrix, with the same set of positive numbers but with new Wootters's basis. We will also show that the local unitary transformations correspond to SO(4,r) transformations, hence,  $\rho$  can be represented as coset space SO(4,c)/SO(4,r) together with positive numbers  $\lambda_i$ . Since Lorentz group is isomorphic to Sl(2,c) and considering the fact that sl(2,c) and so(4,c) are the complexification of su(2,c) and so(3,1,r), respectively, so both approach are identical.

# 6 Lewenstein-Sanpera Decomposition for a Generic Two Qubit State

Here in this section we obtain L-S decomposition for a generic two qubit density matrix by using Wootters's basis. First we define states  $|x_i'\rangle$  in terms of Wootters's basis as

$$|x_i'\rangle = \frac{|x_i\rangle}{\sqrt{\lambda_i}}, \quad \text{for } i = 1, 2, 3, 4.$$
 (62)

Thus the decomposition given in Eq. (5) becomes

$$\rho = \sum_{i} \lambda_{i} \left| x_{i}^{\prime} \right\rangle \left\langle x_{i}^{\prime} \right|, \tag{63}$$

which can be rewritten in the following form

$$\rho = \sum_{i=1}^{4} \lambda_{i} |x'_{i}\rangle \langle x'_{i}| 
= (\lambda_{1} - \lambda_{2} - \lambda_{3} - \lambda_{4}) |x'_{1}\rangle \langle x'_{1}| + (\lambda_{2} + \lambda_{3} + \lambda_{4}) |x'_{1}\rangle \langle x'_{1}| + \sum_{j=2}^{4} \lambda_{j} |x'_{j}\rangle \langle x'_{j}| 
= (1 - \lambda) |\psi\rangle \langle \psi| + \lambda \rho_{sep},$$
(64)

where separable density matrix  $\rho_{sep}$  and entangled pure state  $|\psi\rangle$  are given by

$$\rho_{sep} = \left(\frac{\lambda_2 + \lambda_3 + \lambda_4}{\lambda \lambda_1}\right) |x_1\rangle \langle x_1| + \frac{1}{\lambda} \sum_{j=2}^4 |x_j\rangle \langle x_j|, \qquad (65)$$

and

$$|\psi\rangle = \frac{|x_1\rangle}{\sqrt{\langle x_1|x_1\rangle}},\tag{66}$$

respectively, and parameter  $\lambda$  is equal to

$$\lambda = 1 - \left(\frac{\lambda_1 - \lambda_2 - \lambda_3 - \lambda_4}{\lambda_1}\right) \langle x_1 | x_1 \rangle. \tag{67}$$

Equation (66) shows that all entanglement content of the state is concentrated in the Wootters's state  $|x_1\rangle$  associated with the largest eigenvalue  $\lambda_1$ . It is also worth to note that average concurrence of the decomposition is

$$(1 - \lambda) \left\langle \psi | \tilde{\psi} \right\rangle = (\lambda_1 - \lambda_2 - \lambda_3 - \lambda_4), \tag{68}$$

that is, it is equal to the concurrence of the state.

In order to show that the decomposition given in (64) is optimal we first note that  $\rho_{sep}$ can be written as

$$\rho_{sep} = \sum_{i=1}^{4} |x_i''\rangle \langle x_i''|, \qquad (69)$$

where  $|x_i''\rangle$  are defined by

$$|x_1''\rangle = \sqrt{\frac{\lambda_2 + \lambda_3 + \lambda_4}{\lambda \lambda_1}} |x_1\rangle, \qquad |x_j''\rangle = \frac{1}{\sqrt{\lambda}} |x_j\rangle, \quad \text{for } j = 2, 3, 4.$$
 (70)

Obviously, the basis  $|x_i''\rangle$  (i=1,2,3,4) satisfy the following relations

$$\left\langle x_i^{\prime\prime}| ilde{x_j^{\prime\prime}}
ight
angle =\lambda_i^{\prime\prime}\delta_{ij},$$

where  $|\tilde{x}_i''|$  are corresponding dual basis. Now using the fact that the eigenvalues  $\lambda_i''$  of boundary separable state  $\rho_{sep}$  satisfy the constraint  $\lambda_1'' - \lambda_2'' - \lambda_3'' - \lambda_4'' = 0$ , and by choosing phase factors  $\theta_i$  of Eqs. (9) to (12) as  $\theta_2 = \theta_3 = \theta_4 = -\frac{\pi}{2}$  and  $\theta_1 = 0$  we arrive at the following product ensemble for  $\rho_{sep}$ 

$$|z_1
angle = rac{1}{2\sqrt{\lambda}}\left(\sqrt{rac{\lambda_2+\lambda_3+\lambda_4}{\lambda_1}}\ket{x_1}-i\ket{x_2}-i\ket{x_3}-i\ket{x_4}
ight),$$
 (71)

$$|z_2\rangle = rac{1}{2\sqrt{\lambda}}\left(\sqrt{rac{\lambda_2 + \lambda_3 + \lambda_4}{\lambda_1}} \ket{x_1} - i\ket{x_2} + i\ket{x_3} + i\ket{x_4}\right),$$
 (72)

$$|z_3\rangle = \frac{1}{2\sqrt{\lambda}} \left( \sqrt{\frac{\lambda_2 + \lambda_3 + \lambda_4}{\lambda_1}} |x_1\rangle + i |x_2\rangle - i |x_3\rangle + i |x_4\rangle \right),\tag{73}$$

$$|z_4
angle = rac{1}{2\sqrt{\lambda}}\left(\sqrt{rac{\lambda_2+\lambda_3+\lambda_4}{\lambda_1}}\,|x_1
angle+i\,|x_2
angle+i\,|x_3
angle-i\,|x_4
angle
ight).$$
 (74)

It can be easily seen that all  $|z_i\rangle$  have zero concurrence and also  $\rho_{sep}$  can be expanded as

$$\rho_{sep} = \sum_{i=1}^{4} |z_i\rangle \langle z_i|. \tag{75}$$

Now we have to show that the decomposition given in (64) is optimal. We first consider the cases that  $\rho$  has full rank. Let us consider the set of four product vectors  $\{|z_i\rangle\}$  and one entangled state  $|x_1\rangle$ . In Ref. [10] it is shown that the ensemble  $\{|z_i\rangle\}$  are linearly independent, also it is straightforward to see that three vectors  $|z_{\alpha}\rangle$ ,  $|z_{\beta}\rangle$  and  $|x_1\rangle$  are linearly independent. Now let us consider matrices  $\rho_{\alpha} = \Lambda_{\alpha} |z_{\alpha}\rangle \langle z_{\alpha}| + (1-\lambda) |x_1\rangle \langle x_1|$ . Due to independency of  $|z_{\alpha}\rangle$  and  $|x_1\rangle$  we can deduce that the range of  $\rho_{\alpha}$  is two dimensional, thus after restriction to its range and defining dual basis  $|\hat{z}_{\alpha}\rangle$  and  $|\hat{x}_1\rangle$  we can expand restricted inverse  $\rho_{\alpha}^{-1}$  as  $\rho_{\alpha}^{-1} = \Lambda_{\alpha}^{-1} |\hat{z}_{\alpha}\rangle \langle \hat{z}_{\alpha}| + (1-\lambda)^{-1} |\hat{x}_1\rangle \langle \hat{x}_1|$  (see Appendix A). Using Eq. (76) it is easy to see that  $\langle z_{\alpha}|\rho_{\alpha}^{-1}|z_{\alpha}\rangle = \Lambda_{\alpha}^{-1}$ . This shows that  $\Lambda_{\alpha}$  are maximal with respect to  $\rho_{\alpha}$  and the projector  $P_{\alpha} = |z_{\alpha}\rangle \langle z_{\alpha}|$ .

Similarly considering matrices  $\rho_{\alpha\beta}=\Lambda_{\alpha}\,|z_{\alpha}\rangle\,\langle z_{\alpha}|+\Lambda_{\beta}\,|z_{\beta}\rangle\,\langle z_{\beta}|+(1-\lambda)\,|x_{1}\rangle\,\langle x_{1}|$  and taking into account the independency of vectors  $|z_{\alpha}\rangle,\,|z_{\beta}\rangle$  and  $|x_{1}\rangle$  we see that the rang of  $\rho_{\alpha\beta}$  is three dimensional where after restriction to its range and defining their dual basis  $|\hat{z}_{\alpha}\rangle,\,|\hat{z}_{\beta}\rangle$  and  $|\hat{x}_{1}\rangle$  we can write restricted inverse  $\rho_{\alpha\beta}^{-1}$  as  $\rho_{\alpha\beta}^{-1}=\Lambda_{\alpha}^{-1}|\hat{z}_{\alpha}\rangle\langle\,\hat{z}_{\alpha}|+\Lambda_{\beta}^{-1}|\hat{z}_{\beta}\rangle\langle\,\hat{z}_{\beta}|+(1-\lambda)^{-1}|\hat{x}_{1}\rangle\langle\,\hat{x}_{1}|.$  Then it is straightforward to get  $\langle z_{\alpha}|\,\rho_{\alpha\beta}^{-1}\,|z_{\alpha}\rangle=\Lambda_{\alpha}^{-1},\,\langle z_{\beta}|\,\rho_{\alpha\beta}^{-1}\,|z_{\beta}\rangle=\Lambda_{\beta}^{-1}$  and  $\langle z_{\alpha}|\,\rho_{\alpha\beta}^{-1}\,|z_{\beta}\rangle=0$ . This implies that the pair  $(\Lambda_{\alpha},\Lambda_{\beta})$  are maximal with respect to  $\rho_{\alpha\beta}$  and the pair of projectors  $(P_{\alpha},P_{\beta})$ , thus complete the proof that the decomposition given in Eq. (64) is optimal.

We now consider the cases that  $\rho$  has rank three, that is  $\lambda_4=0$ . In this case the pairs  $\{|z_1\rangle,|z_4\rangle\}$  and also  $\{|z_2\rangle,|z_3\rangle\}$  are no longer independent with respect to  $|x_1\rangle$ . In former case we can evaluate  $|x_1\rangle$  in terms of  $|z_1\rangle$  and  $|z_4\rangle$  then matrix  $\rho_{14}$  can be written in terms of two basis  $|z_1\rangle$  and  $|z_4\rangle$  which yields after some calculations,  $\langle z_1|\rho_{14}^{-1}|z_1\rangle=\frac{1}{\Gamma_{14}}\left(\Lambda_4+(1-\lambda)\left(\frac{\lambda_1}{\lambda_2+\lambda_3}\right)\right),\ \langle z_4|\rho_{14}^{-1}|z_4\rangle=\frac{1}{\Gamma_{14}}\left(\Lambda_1+(1-\lambda)\left(\frac{\lambda_1}{\lambda_2+\lambda_3}\right)\right)$  and  $\langle z_1|\rho_{14}^{-1}|z_4\rangle=\frac{1}{\Gamma_{14}}\left((1-\lambda)\left(\frac{\lambda_1}{\lambda_2+\lambda_3}\right)\right)$  where  $\Gamma_{14}=\left(\Lambda_1\Lambda_4+(\Lambda_1+\Lambda_4)(1-\lambda)\left(\frac{\lambda_1}{\lambda_2+\lambda_3}\right)\right)$ . Using the above results together with Eqs. (16) we obtain the maximality of pair  $(\Lambda_1,\Lambda_4)$  with respect to  $\rho_{14}$  and the pair of projectors  $(P_1,P_4)$ . Similarly in the second case one can express  $|x_1\rangle$  in terms of  $|z_2\rangle$  and  $|z_3\rangle$  and evaluate  $\rho_{23}^{-1}$ , which get  $\langle z_2|\rho_{23}^{-1}|z_2\rangle=\frac{1}{\Gamma_{23}}\left(\Lambda_3+(1-\lambda)\left(\frac{\lambda_1}{\lambda_2+\lambda_3}\right)\right),$   $\langle z_3|\rho_{23}^{-1}|z_3\rangle=\frac{1}{\Gamma_{23}}\left(\Lambda_2+(1-\lambda)\left(\frac{\lambda_1}{\lambda_2+\lambda_3}\right)\right)$  and  $\langle z_2|\rho_{23}^{-1}|z_3\rangle=\frac{1}{\Gamma_{23}}\left((1-\lambda)\left(\frac{\lambda_1}{\lambda_2+\lambda_3}\right)\right)$  with  $\Gamma_{23}=\left(\Lambda_2\Lambda_3+(\Lambda_2+\Lambda_3)(1-\lambda)\left(\frac{\lambda_1}{\lambda_2+\lambda_3}\right)\right)$ , together with Eqs. (16) we obtain the maximality of pair  $(\Lambda_2,\Lambda_3)$  with respect to  $\rho_{23}$  and the pair of projectors  $(P_2,P_3)$ . For other choices of  $\alpha$  and  $\beta$  three vectors  $|z_\alpha\rangle$ ,  $|z_\beta\rangle$  and  $|x_1\rangle$  remain linearly independent thus we can prove maximality of pairs  $(\Lambda_\alpha,\Lambda_\beta)$  in the same way it is proved in full rank case.

Finally let us consider cases that  $\rho$  has rank two, that is  $\lambda_3 = \lambda_4 = 0$ . In this case we have  $|z_1\rangle = |z_2\rangle$  and  $|z_3\rangle = |z_4\rangle$ . It is now sufficient to take  $|z_1\rangle$  and  $|z_3\rangle$  as product ensemble. But in this case vectors  $|z_1\rangle$  and  $|z_3\rangle$  are not independent with respect to  $|x_1\rangle$ . We

express  $|x_1\rangle$  in terms of  $|z_1\rangle$  and  $|z_3\rangle$  then matrix  $\rho_{13}$  can be written in terms of two vectors  $|z_1
angle$  and  $|z_3
angle$  and after some calculations we get  $\langle z_1|
ho_{13}^{-1}|z_1
angle = rac{1}{\Gamma_{13}}\left(\Lambda_3 + (1-\lambda)\left(rac{\lambda_1}{\lambda_2}
ight)\right)$ ,  $\langle z_3 | \rho_{13}^{-1} | z_3 \rangle = \frac{1}{\Gamma_{13}} \left( \Lambda_1 + (1 - \lambda) \left( \frac{\lambda_1}{\lambda_2} \right) \right) \text{ and } \langle z_1 | \rho_{13}^{-1} | z_3 \rangle = \frac{-1}{\Gamma_{13}} \left( (1 - \lambda) \left( \frac{\lambda_1}{\lambda_2} \right) \right) \text{ where } \Gamma_{13} = \frac{1}{\Gamma_{13}} \left( (1 - \lambda) \left( \frac{\lambda_1}{\lambda_2} \right) \right)$  $\left(\Lambda_1\Lambda_3+(\Lambda_1+\Lambda_3)(1-\lambda)\left(\frac{\lambda_1}{\lambda_2}\right)\right)$ . Using the above results together with Eqs. (16) we obtain the maximality of pairs  $(\Lambda_1, \Lambda_3)$  with respect to  $\rho_{13}$  and the pairs of projectors  $(P_1, P_3)$ .

### Conclusion

We have obtained the Lewenstein-Sanpera decomposition for BD states and full rank two qubit density matrices obtained from them via some LQCC action. We have also obtained Lewenstein-Sanpera decomposition for a generic two qubit density matrix by using Wootters's basis. It is shown that the average concurrence of the decomposition is equal to the concurrence of the state. It is also shown that all entanglement content of the state is concentrated in the Wootters's state  $|x_1\rangle$  associated with the largest eigenvalue  $\lambda_1$ . In summary, the importance of Wootters's basis in construction of product set of  $2 \otimes 2$  system has been shown and further progress in L-S decomposition of bipartite systems may depend on the existence of the Wootters's like basis for these systems.

On the other hand, for BD states it is also shown that separable state optimizing L-S decomposition, minimizes the von Neumann relative entropy as a measure of entanglement. So it would be important to find a type of relative entropy such that corresponding separable state giving separable part of the L-S decomposition minimizes the distance between density matrix and the set of separable states, too.

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# Appendix A

Let us consider the set of linearly independent vectors  $\{|\phi_i\rangle\}$ , then one can define their dual vectors  $\{|\hat{\phi}_i\rangle\}$  such that the following relations

$$\left\langle \hat{\phi}_i \mid \phi_j \right\rangle = \delta_{ij} \tag{76}$$

hold. It is straightforward to show that the  $\{|\phi_i\rangle\}$  and their dual  $\{|\hat{\phi}_i\rangle\}$  posses the following completeness relation

$$\sum_{i} |\hat{\phi}_{i}\rangle\langle\phi_{i}| = I, \qquad \sum_{i} |\phi_{i}\rangle\langle\hat{\phi}_{i}| = I. \tag{77}$$

Consider an invertible operator M which is expanded in terms of states  $|\phi_i\rangle$  as

$$M = \sum_{i} a_{ij} |\phi_i\rangle \langle \phi_j| \tag{78}$$

Then the inverse of M denoted by  $M^{-1}$  can be expanded in terms of dual bases as

$$M^{-1} = \sum_{i} b_{ij} |\hat{\phi}_i\rangle\langle\hat{\phi}_j| \tag{79}$$

where  $b_{ij} = (A^{-1})_{ij}$  and  $(A)_{ij} = a_{ij}$ .

## Appendix B: Coset structure for a generic $2 \otimes 2$ density matrix in Wootters's basis

In this Appendix we obtain an explicit parameterization for a generic two qubit density matrix in Wootters's basis. To this aim for any density matrix  $\rho$  with decomposition given in Eq. (63) we define matrix X as

$$X = (|x_1'\rangle, |x_2'\rangle, |x_3'\rangle, |x_4'\rangle). \tag{80}$$

$$\widetilde{X} = \left( \left| \widetilde{x'}_1 \right\rangle, \left| \widetilde{x'}_2 \right\rangle, \left| \widetilde{x'}_3 \right\rangle, \left| \widetilde{x'}_4 \right\rangle \right), \tag{81}$$

Eq. (7) takes the following form

$$\widetilde{X}^{\dagger}X = X^{T}\sigma_{y} \otimes \sigma_{y}X = I. \tag{82}$$

Since matrix  $\sigma_y \otimes \sigma_y$  is symmetric it can be diagonalized as

$$\sigma_y \otimes \sigma_y = O^T \eta^2 O, \tag{83}$$

where O is an orthogonal matrix defined by

$$O = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 0 & 1\\ 0 & 1 & 1 & 0\\ 0 & 1 & -1 & 0\\ 1 & 0 & 0 & -1 \end{pmatrix}, \tag{84}$$

and  $\eta$  is the diagonal matrix

$$\eta = \begin{pmatrix}
i & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & i & 0 \\
0 & 0 & 0 & 1
\end{pmatrix}.$$
(85)

Using Eq. (83) we can rewrite Eq. (82) as

$$Y^T Y = I, (86)$$

where

$$Y = \eta \, OX. \tag{87}$$

Equation (86) shows that Y is a complex 4-dimensional orthogonal matrix. This means that a given density matrix  $\rho$  with corresponding set of positive numbers  $\lambda_i$  and Wootters's basis can transforms under SO(4,c) into a generic  $2 \times 2$  density matrix with the same set of positive numbers but with new Wootters's basis. This implies that the space of two qubit density matrices can be characterize with 12-dimensional (as real manifold) space of complex orthogonal group SO(4,c) together with four positive numbers  $\lambda_i$ . Of course the normalization condition reduces number of parameters to 15.

As far as entanglement is concerned the states  $\rho$  and  $\rho'$  are equivalent if they are on the same orbit of the group of local transformation, that is, if there exist local unitary transformation  $U_1 \otimes U_2$  such that  $\rho' = (U_1 \otimes U_2) \rho (U_1 \otimes U_2)^{\dagger}$ , where  $U_1$  and  $U_2$  are unitary transformations acting on Hilbert spaces of particles A and B, respectively.

It can be easily seen that under above mentioned local unitary transformations of density matrix  $\rho$ , the matrix X transforms as

$$X \to X' = (U_1 \otimes U_2)X. \tag{88}$$

It is worth to mention that X' also satisfy Eq. (82). To show that this is indeed the case, we need to note that  $X'^T \sigma_y \otimes \sigma_y X' = X^T (U_1^T \sigma_y U_1) \otimes (U_2^T \sigma_y U_2) X$ . By using  $(\sigma_y)_{ij} = -i\epsilon_{ij}$  we

get  $(U^T \sigma_y U)_{ij} = -i\epsilon_{kl} U_{ki} U_{lj} = -i \det(U)\epsilon_{ij} = (\sigma_y)_{ij}$ , where we have used the fact that  $U_i$  has unit determinant, since it belongs to SU(2) group. This implies that

$$X'^{T}\sigma_{y}\otimes\sigma_{y}X'=I. \tag{89}$$

By defining Y' as

$$Y' = \eta \, OX', \tag{90}$$

one can easily show that Y' satisfies the orthogonality condition

$$Y^{\prime T}Y^{\prime} = I, \tag{91}$$

too. Now by using Eq. (90) and inverting Eq. (88), we can express Y' in terms of Y

$$Y' = (\eta O)(U_1 \otimes U_2)(\eta O)^{-1}Y. \tag{92}$$

Now by using the fact that  $(\eta O) \exp(\mathcal{U}_1 \otimes \mathcal{U}_2)(\eta O)^{-1} = \exp((\eta O)(\mathcal{U}_1 \otimes \mathcal{U}_2)(\eta O)^{-1})$  and using the explicit form for generators  $(\mathcal{U}_1 \otimes \mathcal{U}_2)$  of local group, one can (after some algebraic calculations) see that  $(\eta O)(\mathcal{U}_1 \otimes \mathcal{U}_2)(\eta O)^{-1}$  is real antisymmetric matrix. This means that under local unitary transformations matrix Y transforms with SO(4,r) group. So we can parameterize the space of two qubit density matrices as 6-dimensional coset space SO(4,c)/SO(4,r) together with 4 positive numbers  $\lambda_i$ , which again normalization condition reduces the number of parameters to 9.

In the following we will obtain an explicit parameterization for a generic two qubit density matrix. First note that we can decompose coset SO(4,c)/SO(4,r) as [20]

$$\frac{SO(4,c)}{SO(4,r)} = \frac{SO(4,c)/SO(4,r)}{SO(2,c)/SO(2,r) \otimes SO(2,c)/SO(2,r)} \bigotimes \left(\frac{SO(2,c)}{SO(2,r)} \otimes \frac{SO(2,c)}{SO(2,r)}\right), \tag{93}$$

that is, coset representative Y can be decomposed as  $Y = Y_1Y_2$ . One can easily show that coset representative of SO(2,c)/SO(2,r) has the following form

$$\exp\begin{pmatrix} 0 & i\phi \\ -i\phi & 0 \end{pmatrix} = \begin{pmatrix} \cosh\phi & i\sinh\phi \\ -i\sinh\phi & \cosh\phi \end{pmatrix}. \tag{94}$$

Thus  $Y_2$  can be written as

$$Y_2 = \begin{pmatrix} \frac{\cosh \phi_1 & i \sinh \phi_1}{-i \sinh \phi_1 & \cosh \phi_1} & 0 \\ 0 & \frac{\cosh \phi_2 & i \sinh \phi_2}{-i \sinh \phi_2 & \cosh \phi_2} \end{pmatrix}. \tag{95}$$

On the other hand  $Y_1$  can be evaluated as

$$Y_{1} = \exp\left(\frac{0 | iB}{-iB^{T} | 0}\right)$$

$$= \left(\frac{\cosh\sqrt{BB^{T}} | iB\frac{\sinh\sqrt{B^{T}B}}{\sqrt{B^{T}B}}}{-i\frac{\sinh\sqrt{B^{T}B}}{\sqrt{B^{T}B}}}B^{T} | \cosh\sqrt{B^{T}B}\right) = \left(\frac{\sqrt{I+CC^{T}} | iC}{-iC^{T} | \sqrt{I+C^{T}C}}\right), \quad (96)$$

where B is a 2 × 2 matrix and in the last step we used  $C = B \frac{\sinh \sqrt{B^T B}}{\sqrt{B^T B}}$ . Now using the singular value decomposition  $C = O_1 D O_2^T$ , Eq. (96) becomes

$$Y_{1} = \left( \begin{array}{c|c} O_{1}\sqrt{I+D^{2}}O_{1}^{T} & iO_{1}DO_{2}^{T} \\ \hline -iO_{2}DO_{1}^{T} & O_{2}\sqrt{I+D^{2}}O_{2}^{T} \end{array} \right), \tag{97}$$

where D is a non-negative diagonal matrix. It can be easily seen that Eq. (97) can be decomposed as

$$Y_1 = \begin{pmatrix} \begin{array}{c|c} O_1 & 0 \\ \hline 0 & O_2 \end{array} \end{pmatrix} \begin{pmatrix} \begin{array}{c|c} \sqrt{I+D^2} & iD \\ \hline -iD & \sqrt{I+D^2} \end{array} \end{pmatrix} \begin{pmatrix} \begin{array}{c|c} O_1^T & 0 \\ \hline 0 & O_2^T \end{array} \end{pmatrix}.$$
(98)

By combining Eqs. (95) and (98) we get

$$Y = \begin{pmatrix} O_1 & 0 \\ \hline 0 & O_2 \end{pmatrix} \begin{pmatrix} \sqrt{I + D^2} & iD \\ \hline -iD & \sqrt{I + D^2} \end{pmatrix} \begin{pmatrix} O_1' & 0 \\ \hline 0 & O_2' \end{pmatrix}. \tag{99}$$

Finally using parameterization given in Eq. (95) we get

$$Y = \begin{pmatrix} \frac{\cosh \theta_{1} & i \sinh \theta_{1} & 0}{-i \sinh \theta_{1} & \cosh \theta_{1}} & 0 \\ 0 & \frac{\cosh \theta_{2} & i \sinh \theta_{2}}{-i \sinh \theta_{2} & \cosh \theta_{2}} \end{pmatrix} \times \begin{pmatrix} \frac{\cosh \xi_{1} & 0 & i \sinh \xi_{1} & 0}{0 & \cosh \xi_{2} & 0 & i \sinh \xi_{2}} \\ \frac{0 & \cosh \xi_{2} & 0 & i \sinh \xi_{2}}{-i \sinh \xi_{1} & 0} & \cosh \xi_{1} & 0 \\ 0 & -i \sin \xi_{2} & 0 & \cosh \xi_{2} \end{pmatrix} \times \begin{pmatrix} \frac{\cosh \phi_{1} & i \sinh \phi_{1}}{-i \sinh \phi_{1} & \cosh \phi_{1}} & 0 \\ \frac{-i \sinh \phi_{1} & \cosh \phi_{1}}{0} & \frac{\cosh \phi_{2} & i \sinh \phi_{2}}{-i \sinh \phi_{2} & \cosh \phi_{2}} \end{pmatrix}, \quad (100)$$

where  $\sinh \xi_i$  (for i=1,2) are diagonal elements of D with the conditions  $\xi_i \geq 0$ . Using above results and Eq. (80) and (87) we can evaluate the states  $|x_i\rangle$  as

$$|x_{1}\rangle = \sqrt{\frac{\lambda_{1}}{2}} \begin{pmatrix} a_{11} + ib_{11} \\ a_{12} + ib_{12} \\ a_{13} + ib_{13} \\ a_{14} + ib_{14} \end{pmatrix}, \qquad |x_{2}\rangle = \sqrt{\frac{\lambda_{2}}{2}} \begin{pmatrix} a_{21} + ib_{21} \\ a_{22} + ib_{22} \\ a_{23} + ib_{23} \\ a_{24} + ib_{24} \end{pmatrix}, \tag{101}$$

$$|x_{3}\rangle = \sqrt{\frac{\lambda_{3}}{2}} \begin{pmatrix} a_{31} + ib_{31} \\ a_{32} + ib_{32} \\ a_{33} + ib_{33} \\ a_{34} + ib_{34} \end{pmatrix}, \qquad |x_{4}\rangle = \sqrt{\frac{\lambda_{4}}{2}} \begin{pmatrix} a_{41} + ib_{41} \\ a_{42} + ib_{42} \\ a_{43} + ib_{43} \\ a_{44} + ib_{44} \end{pmatrix}, \tag{102}$$

where

and

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a_{11} = -(\sinh \xi_1 \sinh \theta_2 \cosh \phi_1 + \sinh \xi_2 \cosh \theta_2 \sinh \phi_1),
a_{12} = -(\sinh \xi_1 \cosh \theta_2 \cosh \phi_1 + \sinh \xi_2 \sinh \theta_2 \sinh \phi_1),
a_{13} = (\sinh \xi_1 \cosh \theta_2 \cosh \phi_1 + \sinh \xi_2 \sinh \theta_2 \sinh \phi_1),
a_{14} = (\sinh \xi_1 \sinh \theta_2 \cosh \phi_1 + \sinh \xi_2 \cosh \theta_2 \sinh \phi_1),
a_{21} = (\cosh \xi_1 \cosh \theta_1 \sinh \phi_1 + \cosh \xi_2 \sinh \theta_1 \cosh \phi_1),
a_{22} = (\cosh \xi_1 \sinh \theta_1 \sinh \phi_1 + \cosh \xi_2 \cosh \theta_1 \cosh \phi_1),
a_{23} = (\cosh \xi_1 \sinh \theta_1 \sinh \phi_1 + \cosh \xi_2 \cosh \theta_1 \cosh \phi_1),
a_{24} = (\cosh \xi_1 \cosh \theta_1 \sinh \phi_1 + \cosh \xi_2 \sinh \theta_1 \cosh \phi_1),
                                                                                                                       (103)
a_{31} = (\sinh \xi_1 \cosh \theta_1 \cosh \phi_2 + \sinh \xi_2 \sinh \theta_1 \sinh \phi_2),
a_{32} = (\sinh \xi_1 \sinh \theta_1 \cosh \phi_2 + \sinh \xi_2 \cosh \theta_1 \sinh \phi_2),
a_{33} = (\sinh \xi_1 \sinh \theta_1 \cosh \phi_2 + \sinh \xi_2 \cosh \theta_1 \sinh \phi_2),
a_{34} = (\sinh \xi_1 \cosh \theta_1 \cosh \phi_2 + \sinh \xi_2 \sinh \theta_1 \sinh \phi_2),
a_{41} = (\cosh \xi_1 \sinh \theta_2 \sinh \phi_2 + \cosh \xi_2 \cosh \theta_2 \cosh \phi_2),
a_{42} = (\cosh \xi_1 \cosh \theta_2 \sinh \phi_2 + \cosh \xi_2 \sinh \theta_2 \cosh \phi_2),
a_{43} = -(\cosh \xi_1 \cosh \theta_2 \sinh \phi_2 + \cosh \xi_2 \sinh \theta_2 \cosh \phi_2),
a_{44} = -(\cosh \xi_1 \sinh \theta_2 \sinh \phi_2 + \cosh \xi_2 \cosh \theta_2 \cosh \phi_2),
b_{11} = -(\cosh \xi_1 \cosh \theta_1 \cosh \phi_1 + \cosh \xi_2 \sinh \theta_1 \sinh \phi_1),
b_{12} = -(\cosh \xi_1 \sinh \theta_1 \cosh \phi_1 + \cosh \xi_2 \cosh \theta_1 \sinh \phi_1),
b_{13} = -(\cosh \xi_1 \sinh \theta_1 \cosh \phi_1 + \cosh \xi_2 \cosh \theta_1 \sinh \phi_1),
b_{14} = -(\cosh \xi_1 \cosh \theta_1 \cosh \phi_1 + \cosh \xi_2 \sinh \theta_1 \sinh \phi_1),
b_{21} = -(\sinh \xi_1 \sinh \theta_2 \sinh \phi_1 + \sinh \xi_2 \cosh \theta_2 \cosh \phi_1),
b_{22} = -(\sinh \xi_1 \cosh \theta_2 \sinh \phi_1 + \sinh \xi_2 \sinh \theta_2 \cosh \phi_1),
b_{23} = (\sinh \xi_1 \cosh \theta_2 \sinh \phi_1 + \sinh \xi_2 \sinh \theta_2 \cosh \phi_1),
b_{24} = (\sinh \xi_1 \sinh \theta_2 \sinh \phi_1 + \sinh \xi_2 \cosh \theta_2 \cosh \phi_1),
                                                                                                                       (104)
b_{31} = -(\cosh \xi_1 \sinh \theta_2 \cosh \phi_2 + \cosh \xi_2 \cosh \theta_2 \sinh \phi_2),
b_{32} = -(\cosh \xi_1 \cosh \theta_2 \cosh \phi_2 + \cosh \xi_2 \sinh \theta_2 \sinh \phi_2),
b_{33} = (\cosh \xi_1 \cosh \theta_2 \cosh \phi_2 + \cosh \xi_2 \sinh \theta_2 \sinh \phi_2),
b_{34} = (\cosh \xi_1 \sinh \theta_2 \cosh \phi_2 + \cosh \xi_2 \cosh \theta_2 \sinh \phi_2)
b_{41} = (\sinh \xi_1 \cosh \theta_1 \sinh \phi_2 + \sinh \xi_2 \sinh \theta_1 \cosh \phi_2),
b_{42} = (\sinh \xi_1 \sinh \theta_1 \sinh \phi_2 + \sinh \xi_2 \cosh \theta_1 \cosh \phi_2),
b_{43} = (\sinh \xi_1 \sinh \theta_1 \sinh \phi_2 + \sinh \xi_2 \cosh \theta_1 \cosh \phi_2),
b_{44} = (\sinh \xi_1 \cosh \theta_1 \sinh \phi_2 + \sinh \xi_2 \sinh \theta_1 \cosh \phi_2).
```

Equations (101) and (102) together with the normalization condition  $\sum_{i=1}^{4} \langle x_i | x_i \rangle = 1$  give a parameterization for a generic orbit of two qubit density matrix up to local unitary group. As an example let us consider Bell decomposable states given in Eq. (17). These states can be obtained by choosing  $\theta_1 = \theta_2 = \xi_1 = \xi_2 = \phi_1 = \phi_2 = 0$ , where we get  $\lambda_i = p_i$  and the states  $|x_i\rangle$  reduce to BD states given in Eqs. (27).