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Optimal Lewenstein–Sanpera decomposition for some bipartite systems

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Abstract
It is shown that for a given bipartite density matrix and by choosing a suitable separable set (instead of a product set) on the separable–entangled boundary, the optimal Lewenstein–Sanpera (LS) decomposition (with respect to an arbitrary separable set) can be obtained via a direct optimization procedure for a generic entangled density matrix. On the basis of this, we obtain the optimal LS decomposition for some bipartite systems such as $2 \otimes 2$ and $2 \otimes 3$ Bell decomposable (BD) states, a generic two qubit state in Wootters basis, iso-concurrence decomposable states, states obtained from BD states via one-parameter and three-parameter local operations and classical communications (LOCC), $d \otimes d$ Werner and isotropic states and a one-parameter $3 \otimes 3$ state. We also obtain the optimal decomposition for multi-partite isotropic states. It is shown that in all $2 \otimes 2$ systems considered here the average concurrence of the decomposition is equal to the concurrence. We also show that for some $2 \otimes 3$ Bell decomposable states, the average concurrence of the decomposition is equal to the lower bound of the concurrence of the state presented recently in Lozinski *et al* (2003 *Preprint* quant-ph/0302144), so an exact expression for concurrence of these states is obtained. It is also shown that for a $d \otimes d$ isotropic state where decomposition leads to a separable and an entangled pure state, the average I-concurrence of the decomposition is equal to the I-concurrence of the state.

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1. Introduction

In the past decade quantum entanglement has attracted much attention in connection with the theory of quantum information and computation. This is because of the potential resource that entanglement provides for quantum communication and information processing [1–3]. By definition, a bipartite mixed state ρ is said to be entangled if it cannot be expressed as

$$\rho = \sum_i w_i \rho_i^{(1)} \otimes \rho_i^{(2)} \qquad w_i \geqslant 0 \quad \sum_i w_i = 1$$

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

The central tasks of quantum information theory are to characterize and quantify entangled states. A first attempt at characterization of entangled states has been made by Peres and Horodecki *et al* [4, 5]. Peres showed that a necessary condition for separability of a bipartite system is that its partial transpose be positive. Horodecki *et al* have shown that this condition is sufficient for separability of composite systems only for dimensions $2 \otimes 2$ and $2 \otimes 3$.

Having a well-justified measure to quantify entanglement, particularly for mixed states of a bipartite system, is indeed worthwhile, and a number of measures has been proposed [3, 6–8]. Among them the entanglement of formation has more importance, since it intends to quantify the resources needed for creating a given entangled state.

Another interesting description of entanglement is the Lewenstein–Sanpera (LS) decomposition [9, 10]. Lewenstein and Sanpera have shown that any bipartite 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 the pure state multiplied by the weight of the pure part in the decomposition. The strategy of [9, 10] is based on the fact that for a given density matrix ρ and any set $V = \{|e_\alpha, f_\alpha\rangle\}$ of product states belonging to the range of ρ, one can subtract a separable density matrix $\rho_s^* = \sum_\alpha \Lambda_\alpha P_\alpha$ (not necessary normalized) with $\Lambda_\alpha \geqslant 0$ such that $\delta\rho = \rho - \rho_s^* \geqslant 0$. The separable state ρ_s^* provides the optimal separable approximation (OSA) to ρ in the sense that $\Lambda(V) = \mathrm{Tr}(\rho_s^*(V))$ is maximum. There also exists the best separable approximation (BSA) ρ_s^* for which $\Lambda = \max_V \Lambda(V)$. Obviously $\Lambda(V) \leqslant \Lambda(V')$ when $V \subset V'$.

In [9], the BSA has been obtained numerically in the case of a two qubit Werner state by choosing a set of several hundred P_α-projectors. Some analytical results are also obtained for special states of two qubit states [11]. Further, in [12] the BSA of a two qubit state has been obtained algebraically. They have also shown that in some cases the weight of the entangled part in the decomposition is equal to the concurrence of the state. In [13] we have obtained the optimal LS decomposition for a generic two qubit density matrix by using Wootters basis. It is shown that the average concurrence of the decomposition is equal to the concurrence of the state.

In this paper, we obtain the optimal LS decomposition for some bipartite density matrices ρ by choosing a suitable separable set S in which $\rho_s \in S$ and trying to maximize $\mathrm{Tr}(\rho_s)$. The separable state ρ_s^* which realizes the optimization is a kind of OSA in which $\Lambda(S) = \mathrm{Tr}(\rho_s^*(S))$ is maximal. Accordingly, as the OSA (with respect to the product set V) depends on the product set V, the OSA (with respect to the separable set S) also depends on the separable set S. There also exists the BSA ρ_s^* for which the optimization is taken over all the set of separable states, i.e. $\Lambda = \max_S \Lambda(S)$. Obviously, $\Lambda(S) \leqslant \Lambda(S')$ when $S \subset S'$. This approach is different from the others in the sense that the optimal decomposition is obtained for a given separable set S instead of a product set V. Also this approach is geometrically intuitive as will be explained in section 4 by providing a bunch of interesting bipartite systems such as $2 \otimes 2$ and $2 \otimes 3$ Bell decomposable (BD) states, a generic two qubit state in Wootters basis, iso-concurrence decomposable states, the states differing from BD states via one-parameter and three-parameter local operations and classical communications (LOCC), $d \otimes d$ Werner and isotropic states and a one-parameter $3 \otimes 3$ state. We also provide the optimal decomposition for multi-partite isotropic systems. As a by-product, we show that in all $2 \otimes 2$ systems considered here the average concurrence of the decomposition is equal to the concurrence. We also show that for some $2 \otimes 3$ Bell decomposable states for which the entangled part of the decomposition is only a pure state, the average concurrence of the decomposition is equal to the lower bound of the concurrence of the state presented recently in [14]; consequently an exact expression for the concurrence of these states is given. In the case of $d \otimes d$ isotropic states, we show that the average I-concurrence of the decomposition is equal to the I-concurrence of the state.

The paper is organized as follows. In section 2 we, briefly, review concurrence as presented in [8]. In section 3 we first review Lewenstein–Sanpera decomposition for a bipartite density matrix, then a new prescription for finding the optimal decomposition is presented. Some important bipartite examples are considered in section 4. The paper ends with a brief conclusion in section 5.

2. Concurrence

In this section, we review the concurrence of two qubit mixed states as introduced in [8]. The generalized concurrence is also reviewed, briefly.

2.1. Wootters concurrence

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 for creating a given entangled state [3]. Wootters in [8] has shown that for a two qubit system the entanglement of formation of a mixed state ρ can be defined as

$$E_f(\rho) = H\left(\tfrac{1}{2} + \tfrac{1}{2}\sqrt{1 - C^2}\right) \tag{2.1}$$

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

$$C(\rho) = \max\{0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4\} \tag{2.2}$$

where the λ_i are the non-negative eigenvalues, in decreasing order, of the Hermitian matrix $R \equiv \sqrt{\sqrt{\rho}\tilde{\rho}\sqrt{\rho}}$ where the spin-flipped state $\tilde{\rho}$ is defined by

$$\tilde{\rho} = (\sigma_y \otimes \sigma_y)\rho^*(\sigma_y \otimes \sigma_y) \tag{2.3}$$

where ρ^* is the complex conjugate of ρ in a standard basis such as $\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$ and σ_y represent the Pauli matrix in the local basis $\{|0\rangle, |1\rangle\}$.

Consider a generic two qubit density matrix ρ with its subnormalized orthogonal eigenvectors $|v_i\rangle$, i.e. $\rho = \sum_i |v_i\rangle\langle v_i|$. There always exists a decomposition [8]

$$\rho = \sum_i |x_i\rangle\langle x_i| \tag{2.4}$$

where the Wootters bases $|x_i\rangle$ are defined by

$$|x_i\rangle = \sum_j^4 U_{ij}^*|v_j\rangle \qquad \text{for} \quad i = 1, 2, 3, 4 \tag{2.5}$$

such that

$$\langle x_i \mid \tilde{x}_j\rangle = (U\tau U^T)_{ij} = \lambda_i\delta_{ij} \tag{2.6}$$

where $\tau_{ij} = \langle v_i \mid \tilde{v}_j\rangle$ is a symmetric but not necessarily Hermitian matrix. The states $|x'_i\rangle$, which are going to be used in our notation, are defined as

$$|x'_i\rangle = \frac{|x_i\rangle}{\sqrt{\lambda_i}} \qquad \text{for} \quad i = 1, 2, 3, 4. \tag{2.7}$$

2.2. I-concurrence

Several attempts to generalize the notion of concurrence for arbitrary bipartite quantum systems have been made already [15–17]. Among them the so-called I-concurrence [17] is defined in terms of a universal-inverter superoperator which is a natural generalization to higher dimensions of the two qubit spin flip. I-concurrence of a joint pure state $|\psi\rangle$ of a $d_A \otimes d_B$ system is defined by Rungta *et al* [17] as

$$C(|\psi\rangle) = \sqrt{2\left(1 - \mathrm{tr}\left(\rho_A^2\right)\right)} = \sqrt{2\left(1 - \mathrm{tr}\left(\rho_B^2\right)\right)} \tag{2.8}$$

where $\rho_A = \mathrm{tr}_B(|\psi\rangle\langle\psi|)$ and ρ_B is defined similarly.

3. Lewenstein–Sanpera decomposition

According to the Lewenstein–Sanpera decomposition [9], any bipartite density matrix ρ can be written as

$$\rho = \lambda\rho_s + (1-\lambda)\rho_e \qquad \lambda \in [0, 1] \tag{3.9}$$

where ρ_s is a separable density matrix and ρ_e is an entangled state. The LS decomposition of a given density matrix ρ is not unique and, in general, there is a continuum set of LS decompositions to choose from. However, Lewenstein and Sanpera in [9, 10] have shown that the optimal decomposition is unique for which λ is maximal. Furthermore, they have demonstrated that in the case of a two qubit system ρ_e reduces to a single pure state.

The idea of [9, 10] is based on the method of subtracting projections on product vectors from a given state, that is, for a given density matrix ρ and any set $V = \{|e_\alpha, f_\alpha\rangle\}$ of product states belonging to the range of ρ, one can subtract a separable density matrix $\rho_s^* = \sum_\alpha \Lambda_\alpha P_\alpha$ (not necessary normalized) with all $\Lambda_\alpha \geqslant 0$ such that $\delta\rho = \rho - \rho_s^* \geqslant 0$. The separable state ρ_s^* provides the OSA in the sense that trace $\Lambda(V) = \mathrm{Tr}(\rho_s^*) \leqslant 1$ is maximal and the entangled part ρ_e is called an edge state, a state with no product vectors in the range [18]. Lewenstein and Sanpera provide the conditions that trace $\mathrm{Tr}(\rho_s^*)$ is maximal. They have also demonstrated that there exists the best separable approximation ρ_s^* for which $\Lambda = \max_V \Lambda(V)$, obviously, $\Lambda(V) \leqslant \Lambda(V')$ when $V \subset V'$.

In this paper we will deal with LS decomposition from a different point of view. Our approach is based on the fact that the set of separable density matrices is convex and compact [19, 20]. This follows from the fact that any separable density matrix $\rho_s \in \mathcal{S}$ can be written as a finite convex combination of pure product states. The density operators on $\mathcal{H}_1 \otimes \mathcal{H}_2$ form a compact and convex subset $\mathcal{D}$ of the Hilbert space of Hilbert–Schmidt class operators [20]. Let $\mathcal{P}$ denote the set of all pure product states. $\mathcal{P}$ is a tensor product of two spheres which are compact in the finite dimensional case. So $\mathcal{P}$ is also compact [19]. The set of all finite convex combinations of product states $\mathcal{P}$ is defined as the convex hull of $\mathcal{P}$, i.e. $\mathcal{S} = \mathrm{conv}\,\mathcal{P}$, and the convex hull of a compact set $\mathcal{P}$ is also compact, so the set of separable density matrices is compact [19].

Based on the above fact we obtain the optimal LS decomposition for some bipartite systems. For a given density matrix ρ, we choose a suitable separable set $S \subset \mathcal{S}$ on the separable–entangled boundary, and express ρ as a convex combination of a separable state $\rho_s \in S$ and an arbitrary entangled state ρ_e, i.e. $\rho = \lambda\rho_s + (1-\lambda)\rho_e$. Then we evaluate λ and provide the conditions that λ is maximal under the restrictions that ρ_s is in the separable set S and maintaining the positivity of the difference $\rho - \lambda\rho_s$, i.e. ρ_e remains non-negative. With this aim we allow ρ_s to move on the surface defined by S, and simultaneously search for the ρ_e with corresponding maximal λ. This restricts ρ_e to some entangled states and gives ρ_s as a function of ρ and restricted ρ_e. The only matter that should be noted in choosing the set S for which $\rho_s \in S$ is that all states on the line segment connecting ρ_s and ρ, i.e. $\rho_\epsilon = \epsilon\rho_s + (1-\epsilon)\rho$ for $0 \leqslant \epsilon \leqslant 1$, must be entangled. This guarantees that the obtained decomposition is indeed maximal. Obviously, the decomposition depends on the separable set S, therefore the maximality of λ depends on the size of the separable set S, i.e. the better the choice of the set S (the larger in size), the greater the λ achieved. In the case that S involves all separable states then $\lambda = \max_S \lambda(S)$ and the corresponding ρ_s^* is the BSA. In all examples considered in this paper we will see that the rank of ρ_e is less than the rank of ρ. This means that ρ_e is an edge state with no product vectors in its range as pointed out in [18]. Moreover, in the case of a two qubit system it is shown that ρ_e reduces to a pure entangled state as we expect from the results of [9, 10]. For these systems ρ_s is defined as a function of ρ and the concurrence of an entangled pure state. To make our consideration clearer, we provide some examples in the next section.

4. Some important examples

In this section we obtain the optimal decomposition for some categories of states, namely, $2 \otimes 2$ Bell decomposable states, a generic two qubit state in Wootters basis, iso-concurrence decomposable states, some $2\otimes 2$ states obtaining from BD states via one-parameter and three-parameter LOCC operations, $2 \otimes 3$ Bell decomposable states, $d \otimes d$ Werner and isotropic states, a one-parameter $3 \otimes 3$ state and finally multi-partite isotropic states.

4.1. $2 \otimes 2$ *Bell decomposable states*

We begin by considering a $2\otimes 2$ Bell decomposable state. A BD state acting on $H^4 \cong H^2 \otimes H^2$ Hilbert space is defined by

$$\rho = \sum_{i=1}^{4} p_i |\psi_i\rangle\langle\psi_i| \qquad 0 \leqslant p_i \leqslant 1 \qquad \sum_{i=1}^{4} p_i = 1 \tag{4.10}$$

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

$$|\psi_1\rangle = |\phi^+\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle) \qquad |\psi_2\rangle = |\phi^-\rangle = \frac{1}{\sqrt{2}}(|00\rangle - |11\rangle) \tag{4.11}$$

$$|\psi_3\rangle = |\psi^+\rangle = \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle) \qquad |\psi_4\rangle = |\psi^-\rangle = \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle). \tag{4.12}$$

A BD state is separable iff $p_i \leqslant \frac{1}{2}$ for all $i = 1, 2, 3, 4$ [21]. In the following we consider the case that ρ is entangled for which $p_1 > \frac{1}{2}$. To obtain the optimal LS decomposition we choose $\rho_s = \sum_{i=1}^4 p_i' |\psi_i\rangle\langle\psi_i|$ with $p_1' = \frac{1}{2}$ as a boundary separable state and $\rho_e = \sum_{i=1}^4 p_i'' |\psi_i\rangle\langle\psi_i|$. Inserting these equations into the decomposition given in equation (3.9) we get

$$p_i = \lambda p_i' + (1-\lambda) p_i'' \qquad \text{for} \quad i = 1, 2, 3, 4. \tag{4.13}$$

From equation (4.13) we get $\lambda = \frac{C''-C}{C''}$ and $\frac{\mathrm{d}\lambda}{\mathrm{d}C''} = \frac{C}{C''^2} \geqslant 0$ where $C = 2p_1 - 1$ and $C'' = 2p_1'' - 1$ are the concurrence of ρ and ρ_e, respectively. This means that in order to obtain the optimal decomposition, i.e. having maximal λ, we require that C'' takes its maximal value, where this happens as long as $p''_2 = p''_3 = p''_4 = 0$, i.e. ρ_e is a pure entangled state. Considering the above arguments we get the following results for λ, ρ_s and ρ_e:

$$\begin{aligned} &\lambda = 1 - C && \rho_e = |\psi_1\rangle\langle\psi_1| \\ &p'_1 = \frac{1}{2} && p'_j = \frac{p_j}{\lambda} \qquad \text{for} \quad j = 2, 3, 4. \end{aligned} \tag{4.14}$$

Equation (4.14) simply shows that the average concurrence of the decomposition is equal to the concurrence of state, i.e. $(1-\lambda)C(|\psi\rangle) = C$.

4.2. A generic two qubit state in Wootters's basis

In this subsection we obtain the optimal LS decomposition for a generic two qubit density matrix by using Wootters basis. As we mentioned already in section 2.1 a generic two qubit density matrix can be written in terms of its Wootters basis as $\rho = \sum_i \lambda_i |x'_i\rangle\langle x'_i|$. Now in order to obtain the optimal LS decomposition we choose $\rho_s = \sum_i \lambda'_i |x'_i\rangle\langle x'_i|$ with $\lambda'_1 - \lambda'_2 - \lambda'_3 - \lambda'_4 = 0$ as a boundary separable state and $\rho_e = \sum_i \lambda''_i |x'_i\rangle\langle x'_i|$. Inserting these equations into the decomposition given in equation (3.9) we get

$$\lambda_i = \lambda\lambda'_i + (1-\lambda)\lambda''_i \qquad \text{for} \quad i = 1, 2, 3, 4. \tag{4.15}$$

From equation (4.15) we get $\lambda = \frac{C''-C}{C''}$ and $\frac{\mathrm{d}\lambda}{\mathrm{d}C''} = \frac{C}{C''^2} \geqslant 0$ where $C = \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4$ and $C'' = \lambda''_1 - \lambda''_2 - \lambda''_3 - \lambda''_4$ are the concurrence of ρ and ρ_e, respectively. This means that in order to obtain the optimal decomposition, i.e. having maximal λ, we require that C'' takes its maximal value, which happens as long as $\lambda''_2 = \lambda''_3 = \lambda''_4 = 0$, i.e. ρ_e is a pure entangled state with concurrence λ''_1. Considering the above arguments we get the following results for λ, ρ_s and ρ_e:

$$\begin{aligned} &\lambda = 1 - \frac{C}{\lambda''_1} && \rho_e = \lambda''_1 |x'_1\rangle\langle x'_1| \\ &\lambda'_1 = \frac{\lambda_2 + \lambda_3 + \lambda_4}{\lambda} && \lambda'_j = \frac{\lambda_j}{\lambda} \quad \text{for} \quad j = 2, 3, 4. \end{aligned} \tag{4.16}$$

Equation (4.16) simply shows that the average concurrence of the decomposition is equal to the concurrence of state, i.e. $(1-\lambda)C(|\psi\rangle) = C$. The decomposition (4.16) is in agreement with the results obtained in [13].

4.3. Iso-concurrence decomposable states

In this section we define the so-called iso-concurrence decomposable (ICD) states, then we give their separability condition and evaluate the optimal decomposition. The iso-concurrence states are defined by

$$|\phi_1\rangle = \cos\theta|00\rangle + \sin\theta|11\rangle) \qquad |\phi_2\rangle = \sin\theta|00\rangle - \cos\theta|11\rangle) \tag{4.17}$$

$$|\phi_3\rangle = \cos\theta|01\rangle + \sin\theta|10\rangle) \qquad |\phi_4\rangle = \sin\theta|01\rangle - \cos\theta|10\rangle). \tag{4.18}$$

It is quite easy to see that the above states are orthogonal and thus span the Hilbert space of $2 \otimes 2$ systems. Also by choosing $\theta = \frac{\pi}{4}$ the above states reduce to Bell states. Now we can define a ICD state as

$$\rho = \sum_{i=1}^{4} p_i |\phi_i\rangle\langle\phi_i| \qquad 0 \leqslant p_i \leqslant 1 \qquad \sum_{i=1}^{4} p_i = 1. \tag{4.19}$$

These states form a four simplex (tetrahedral) with its vertices defined by $p_1 = 1$, $p_2 = 1$, $p_3 = 1$ and $p_4 = 1$, respectively.

Peres–Horodecki's criterion [4, 5] for separability implies that the state given in equation (4.19) is separable if and only if the following inequalities are satisfied:

$$(p_1 - p_2)\sin 2\theta \leqslant \sqrt{4p_3p_4 + (p_3 - p_4)^2\sin^2 2\theta} \tag{4.20}$$

$$(p_2 - p_1)\sin 2\theta \leqslant \sqrt{4p_3p_4 + (p_3 - p_4)^2\sin^2 2\theta} \tag{4.21}$$

$$(p_3 - p_4)\sin 2\theta \leqslant \sqrt{4p_1p_2 + (p_1 - p_2)^2\sin^2 2\theta} \tag{4.22}$$

$$(p_4 - p_3)\sin 2\theta \leqslant \sqrt{4p_1p_2 + (p_1 - p_2)^2\sin^2 2\theta}. \tag{4.23}$$

Inequalities (4.20)–(4.23) divide the tetrahedral density matrices into five regions. The central region, defined by the above inequalities, forms a deformed octahedron and are separable states. In the other four regions one of the above inequalities will not hold, therefore they represent entangled states. Below we consider the entangled states corresponding to the violation of inequality (4.20), i.e. the states which satisfy the following inequality:

$$(p_1 - p_2)\sin 2\theta > \sqrt{4p_3p_4 + (p_3 - p_4)^2\sin^2 2\theta}. \tag{4.24}$$

All other ICD states can be obtained via local unitary transformations. Now we will obtain the concurrence of ICD states. Following the Wootters protocol given in subsection 2.1 we get for the state ρ given in equation (4.19)

$$\tau = \begin{pmatrix} -p_1\sin 2\theta & \sqrt{p_1p_2}\cos 2\theta & 0 & 0 \\ \sqrt{p_1p_2}\cos 2\theta & p_2\sin 2\theta & 0 & 0 \\ 0 & 0 & p_3\sin 2\theta & -\sqrt{p_3p_4}\cos 2\theta \\ 0 & 0 & -\sqrt{p_3p_4}\cos 2\theta & -p_4\sin 2\theta \end{pmatrix}. \tag{4.25}$$

Now it is easy to evaluate λ_i which yields

$$\begin{aligned} \lambda_{1,2} &= \tfrac{1}{2}\big(\pm(p_1 - p_2)\sin 2\theta + \sqrt{4p_1p_2 + (p_1 - p_2)^2\sin^2 2\theta}\big) \\ \lambda_{3,4} &= \tfrac{1}{2}\big(\pm(p_3 - p_4)\sin 2\theta + \sqrt{4p_3p_4 + (p_3 - p_4)^2\sin^2 2\theta}\big). \end{aligned} \tag{4.26}$$

Thus, one can evaluate the concurrence of ICD states as

$$C = (p_1 - p_2)\sin 2\theta - \sqrt{4p_3p_4 + (p_3 - p_4)^2\sin^2 2\theta}. \tag{4.27}$$

It is worth noting that this obtained concurrence is equal to the amount of violation of inequality (4.24). Note that the concurrence of an ICD state can be written as

$$A_{11} - A_{22} - \sqrt{(A_{33} + A_{44})^2 - 4A_{34}^2} \tag{4.28}$$

where A_{ij} denote matrix representation of the ICD states in Bell basis, that is

$$A_{11} = \tfrac{1}{2}(p_1 + p_2 + (p_1 - p_2)\sin 2\theta) \qquad A_{22} = \tfrac{1}{2}(p_1 + p_2 - (p_1 - p_2)\sin 2\theta) \tag{4.29}$$

$$A_{33} = \tfrac{1}{2}(p_3 + p_4 + (p_3 - p_4)\sin 2\theta) \qquad A_{44} = \tfrac{1}{2}(p_3 + p_4 - (p_3 - p_4)\sin 2\theta) \tag{4.30}$$

$$A_{12} = \tfrac{1}{2}(p_1 - p_2)\cos 2\theta \qquad A_{34} = \tfrac{1}{2}(p_3 - p_4)\cos 2\theta. \tag{4.31}$$

Now in order to obtain the optimal LS decomposition we parametrize ρ_s like the ICD state with matrix elements A'_{ij} (in the Bell basis) which are defined like A_{ij} except for p_i and θ which are replaced with p'_i and θ', respectively. We also choose ρ_e similar to ρ with matrix elements A''_{ij}

parametrized with p_i'' and θ''. For simplicity the rank of ρ_e is considered to be 2, namely $p_3'' = p_4'' = 0$. Using these considerations together with equation (3.9) we get

$$A_{ij} = \lambda A_{ij}' + (1-\lambda) A_{ij}''. \tag{4.32}$$

Taking into account the fact that ρ_s is a boundary separable state with zero concurrence and using equation (4.28), we get $\lambda = \frac{C''-C}{C''}$ and $\frac{\mathrm{d}\lambda}{\mathrm{d}C''} = \frac{C}{C''^2} \geqslant 0$, where C and C'' are the concurrence of ρ and ρ_e, respectively. Obviously we observe that λ becomes maximal when ρ_e is a pure entangled state. Considering this fact and setting $p_2'' = 0$ we arrive at

$$p_1 + p_2 + (p_1 - p_2)\sin 2\theta = \lambda(p_1' + p_2' + (p_1' - p_2')\sin 2\theta') + (1-\lambda)(1 + \sin 2\theta'') \tag{4.33}$$

$$p_1 + p_2 - (p_1 - p_2)\sin 2\theta = \lambda(p_1' + p_2' - (p_1' - p_2')\sin 2\theta') + (1-\lambda)(1 - \sin 2\theta'') \tag{4.34}$$

$$p_3 + p_4 + (p_3 - p_4)\sin 2\theta = \lambda(p_3' + p_4' + (p_3' - p_4')\sin 2\theta') \tag{4.35}$$

$$p_3 + p_4 - (p_3 - p_4)\sin 2\theta = \lambda(p_3' + p_4' - (p_3' - p_4')\sin 2\theta') \tag{4.36}$$

$$(p_1 - p_2)\cos 2\theta = \lambda(p_1' - p_2')\cos 2\theta' + (1-\lambda)\cos 2\theta'' \tag{4.37}$$

$$(p_3 - p_4)\cos 2\theta = \lambda(p_3' - p_4')\cos 2\theta'. \tag{4.38}$$

In order to solve the above equations we consider two cases separately.

(i) *Case 1*. First let us consider the case that $\theta, \theta' \neq \frac{\pi}{4}$. In this case equations (4.33)–(4.38) yield

$$\begin{aligned} &\theta = \theta' = \theta'' \\ &\lambda = 1 - (p_1 - p_2) + \sqrt{\frac{4p_3p_4}{\sin 2\theta^2} + (p_3 - p_4)^2} \\ &p_1' = \frac{p_1 - (1-\lambda)}{\lambda} \qquad p_j' = \frac{p_j}{\lambda} \qquad \text{for} \quad j = 2, 3, 4. \end{aligned} \tag{4.39}$$

This case corresponds to the results of [22].

(ii) *Case 2*. Now let us consider the case that $\theta = \frac{\pi}{4}$, i.e. ρ is a Bell decomposable state. The only non-trivial solution of equation (4.38) is $p_3' = p_4'$. Equations (4.35) and (4.36) show that this restricts the density matrix to $p_3 = p_4$. Combining all, we arrive at the following ρ_s for decomposition:

$$\tan 2\theta' = \frac{p_1 + p_2 - 1}{C}\tan 2\theta'' \qquad \lambda = 1 - \frac{C}{\sin 2\theta''} \tag{4.40}$$

$$p_{1,2}' = \frac{1}{2\lambda}\left(p_1 + p_2 - \frac{C}{\sin 2\theta''} \pm \frac{1 - p_1 - p_2}{\sin 2\theta'}\right) \tag{4.41}$$

$$p_3' = p_4' = \frac{p_3}{\lambda}. \tag{4.42}$$

where $C = 2p_1 - 1$ is the concurrence of ρ. The separability of density matrix ρ_s implies that $p_i' \geqslant 0$ for all i (recall that the separability condition has already been imposed over ρ_s by putting its concurrence equal to zero). So p_i' should satisfy the following condition:

$$\sin 2\theta'' \geqslant \frac{(p_1 + p_2)C}{p_1 C + p_2} \tag{4.43}$$

where the above inequality turns to equality whenever the rank of ρ_s is 3. This condition also guarantees positivity of λ. It is worth emphasizing that this case involves the result of [23] as a special case. There authors have obtained the optimal decomposition for a special kind of BD state, namely a specific Werner state with $p_1 = \frac{5}{8}$ (of course, in their treatment they take singlet state $|\psi_4\rangle$ as the dominant pure state in the Werner state, i.e. $p_4 = \frac{5}{8}$).

4.4. One-parameter LOCC operations

In this subsection we will obtain the optimal decomposition for some two qubit states which can be obtained from BD states by using LOOC operations. In [13] we have shown that a generic two qubit density matrix $\rho = \sum_i \lambda_i |x_i'\rangle\langle x_i'|$ with corresponding set of positive numbers λ_i and Wootters basis $|x_i'\rangle$ can be obtained from a Bell decomposable state with the same set of positive numbers λ_i but with different Wootters basis via $SO(4,c)$ transformation. It is also shown that local unitary transformations correspond to $SO(4,r)$ transformations, hence, ρ can be represented as the coset space $SO(4,c)/SO(4,r)$ together with the positive numbers λ_i. Therefore, a generic two qubit density matrix ρ can be represented in the Bell basis as $\rho = Y\Lambda Y^\dagger$ where $Y \in SO(4,c)/SO(4,r)$ and $\Lambda = \mathrm{diag}(\lambda_1,\lambda_2,\lambda_3,\lambda_4)$ [13]. It is also demonstrated in [13] that the above representation of a two qubit density matrix is equivalent to the LOCC operations on Bell decomposable states. In the following we consider the case that Y is a one-parameter matrix:

$$Y = \begin{pmatrix} \cosh\theta & \mathrm{i}\sinh\theta & 0 & 0 \\ -\mathrm{i}\sinh\theta & \cosh\theta & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \tag{4.44}$$

thus

$$\rho = Y\Lambda Y^\dagger = \begin{pmatrix} \lambda_1\cosh^2\theta + \lambda_2\sinh^2\theta & \mathrm{i}(\lambda_1+\lambda_2)\sinh\theta\cosh\theta & 0 & 0 \\ -\mathrm{i}(\lambda_1+\lambda_2)\sinh\theta\cosh\theta & \lambda_1\sinh^2\theta + \lambda_2\cosh^2\theta & 0 & 0 \\ 0 & 0 & \lambda_3 & 0 \\ 0 & 0 & 0 & \lambda_4 \end{pmatrix}. \tag{4.45}$$

Obviously, the normalization condition leads to $(\lambda_1+\lambda_2)\cosh 2\theta + \lambda_3 + \lambda_4 = 1$. We choose ρ_s in the same form as ρ, i.e. $\rho_s = Y'\Lambda' Y'^\dagger$ where $\Lambda' = \mathrm{diag}(\lambda_1',\lambda_2',\lambda_3',\lambda_4')$ and Y' is defined as Y but here θ is replaced with θ'. Now in order to obtain the optimal LS decomposition we have to get a generic density matrix for ρ_e. After doing so, it can be easily seen that equation (3.9) requires that ρ_e also has the same form as ρ and ρ_s, i.e. $\rho_e = Y''\Lambda'' Y''^\dagger$ where $\Lambda'' = \mathrm{diag}(\lambda_1'',\lambda_2'',\lambda_3'',\lambda_4'')$ and Y'' is defined as Y but with θ'' instead of θ. Inserting the above equations in equation (3.9) we get

$$Y\Lambda Y^\dagger = \lambda(Y'\Lambda' Y'^\dagger) + (1-\lambda)(Y''\Lambda'' Y''^\dagger). \tag{4.46}$$

Now multiplying equation (4.46) by Y''^T and Y''^*, respectively from the left and right and using the orthogonality of Y'' we get

$$(Y''^T Y)\Lambda(Y^\dagger Y''^*) = \lambda(Y''^T Y')\Lambda'(Y'^\dagger Y''^*) + (1-\lambda)\Lambda'' \tag{4.47}$$

where it can be written as

$$\begin{aligned}(\lambda_1\cosh^2(\theta-\theta'') &+ \lambda_2\sinh^2(\theta-\theta''))\\ &= \lambda(\lambda_1'\cosh^2(\theta'-\theta'') + \lambda_2'\sinh^2(\theta'-\theta'')) + (1-\lambda)\lambda_1''\end{aligned} \tag{4.48}$$

$$\begin{aligned}(\lambda_1\sinh^2(\theta-\theta'') &+ \lambda_2\cosh^2(\theta-\theta''))\\ &= \lambda(\lambda_1'\sinh^2(\theta'-\theta'') + \lambda_2'\cosh^2(\theta'-\theta'')) + (1-\lambda)\lambda_2''\end{aligned} \tag{4.49}$$

$$\lambda_3 = \lambda\lambda_3'' + (1-\lambda)\lambda_3'' \tag{4.50}$$

$$\lambda_4 = \lambda\lambda_4'' + (1-\lambda)\lambda_4'' \tag{4.51}$$

$$(\lambda_1+\lambda_2)\sinh 2(\theta-\theta'') + \lambda(\lambda_1'+\lambda_2')\sinh 2(\theta'-\theta'') = 0. \tag{4.52}$$

Subtracting equations (4.49), (4.50) and (4.51) from equation (4.48) and using the fact that ρ_s is a boundary separable state, hence having zero concurrence, i.e. $\lambda_1' - \lambda_2' - \lambda_3' - \lambda_4' = 0$, we get $\lambda = \frac{C''-C}{C''}$, $\frac{d\lambda}{dC''} = \frac{C}{C''^2} \geqslant 0$ where $C = \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4$ and $C'' = \lambda_1'' - \lambda_2'' - \lambda_3'' - \lambda_4''$ are the concurrence of ρ and ρ_e, respectively. This shows that maximal λ is achieved when $\lambda_2'' = \lambda_3'' = \lambda_4'' = 0$, i.e. ρ_e is a pure entangled state with concurrence λ_1''. Implying the above results we can solve equations (4.48)–(4.52) for λ and ρ_s where we get

$$\lambda = 1 - C\cosh 2\theta'' \tag{4.53}$$

$$\tanh 2(\theta' - \theta'') = \frac{(\lambda_1 + \lambda_2)\sinh 2(\theta - \theta'')}{(\lambda_1 + \lambda_2)\cosh 2(\theta - \theta'') - C} \tag{4.54}$$

$$\lambda_{1,2}' = \frac{1}{2\lambda}\left(\frac{(\lambda_1 + \lambda_2)\cosh 2(\theta - \theta'') - C}{\cosh 2(\theta' - \theta'')} \pm (\lambda_3 + \lambda_4)\right) \tag{4.55}$$

$$\lambda_j' = \frac{\lambda_j}{\lambda} \qquad \text{for} \quad j = 3, 4 \tag{4.56}$$

where in equation (4.53) we have used $\lambda_1'' = \frac{1}{\cosh 2\theta''}$ which follows from the normalization condition of ρ_e. Finally from the positivity conditions for λ and λ_i we see that the following inequalities should hold:

$$\cosh 2\theta'' \leqslant \frac{1}{C} \qquad \cosh 2(\theta - \theta'') \leqslant \frac{\lambda_1 - \lambda_2}{\lambda_1 + \lambda_2} + \frac{2\lambda_1\lambda_2}{(\lambda_1 + \lambda_2)C}. \tag{4.57}$$

In the case that the second inequality is saturated, the rank of ρ_s reduces to 3. It is worth noting that the generalized Werner state of the second kind which is defined as a mixture of an arbitrary pure state $|\chi\rangle$ and the totally mixed state $\rho_0 = I/4$, i.e. $\rho = x|\chi\rangle\langle\chi| + (1-x)\rho_0$, can be obtained from the above example by setting $\lambda_2 \cosh 2\theta = \lambda_3 = \lambda_4$ and $x = (4\lambda_1\cosh 2\theta - 1)/3$ also, where Englert *et al* obtained the optimal decomposition of this state in [11]. Since the separable set S is a subset of the one considered in [11], the optimal decomposition obtained here is different from the one obtained in [11]. Note that the above decomposition is not a special case of the decomposition considered in subsection 4.2. There we considered the case that all ρ, ρ_s and ρ_e were expressed in the same Wootters basis. Here their Wootters bases are parametrized differently, namely θ, θ' and θ'', respectively. The optimal decomposition given by equations (4.53)–(4.56) involves some interesting special cases as follows:

case (i) $\theta = \theta'$. In this case from equations (4.53)–(4.56) we get $\theta'' = \theta$, which yields the results of subsection 4.2 for a one-parameter Wootters basis.

case (ii) $\theta = 0, \theta'' \neq 0$. This case leads to the optimal decomposition of a BD state in terms of the non-maximal entangled pure state. This case can also be considered as a generalization of the result of [23].

case (iii) $\theta \neq 0, \theta'' = 0$. This case leads to the optimal decomposition of a one-parameter LOCC transformed BD state in terms of a maximal entangled pure state.

4.5. Three-parameter LOCC transformed BD states

Following the previous subsection we consider here the case that ρ can be obtained from BD states via three-parameter LOCC transformation as $\rho = Y\Lambda Y^\dagger$ with [13]

$$Y = \begin{pmatrix} \cosh\theta\cosh\xi\cosh\phi + \sinh\theta\sinh\phi & \mathrm{i}(\cosh\theta\cosh\xi\sinh\phi + \sinh\theta\cosh\phi) & \mathrm{i}\cosh\theta\sinh\xi & 0 \\ -\mathrm{i}(\sinh\theta\cosh\xi\cosh\phi + \cosh\theta\sinh\phi) & \sinh\theta\cosh\xi\sinh\phi + \cosh\theta\cosh\phi & \sinh\theta\sinh\xi & 0 \\ -\mathrm{i}\sinh\xi\cosh\phi & \sinh\xi\sinh\phi & \cosh\xi & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \tag{4.58}$$

where normalization condition leads to

$$\begin{aligned} \mathrm{Tr}(\rho) = {} & ((\lambda_1\cosh^2\phi + \lambda_2\sinh^2\phi)\cosh^2\xi + \lambda_3\sinh^2\xi + (\lambda_1\sinh^2\phi + \lambda_2\cosh^2\phi))\cosh 2\theta \\ & + (\lambda_1\cosh^2\phi + \lambda_2\sinh\phi)\sinh^2\xi + \lambda_3\cosh^2\xi \\ & + (\lambda_1 + \lambda_2)\cosh\xi\sinh 2\theta\sinh 2\phi + \lambda_4 = 1. \end{aligned} \tag{4.59}$$

We choose ρ_s below in the same form as ρ, i.e. $\rho_s = Y'\Lambda'Y'^{\dagger}$ where $\Lambda' = \mathrm{diag}(\lambda'_1, \lambda'_2, \lambda'_3, \lambda'_4)$ and Y' are defined as Y but here θ, ξ and ϕ are replaced with θ', ξ' and ϕ'. Now to obtain the optimal LS decomposition we should take a generic density matrix for ρ_e. It can be easily seen that equation (3.9) requires that ρ_e also has the same form as ρ and ρ_s. So we get $\rho_e = Y''\Lambda''Y''^{\dagger}$ where $\Lambda'' = \mathrm{diag}(\lambda''_1, \lambda''_2, \lambda''_3, \lambda''_4)$ and Y'' is defined as Y but here θ, ξ and ϕ are replaced with θ'', ξ'' and ϕ''. By using the above considerations and equation (3.9) we get

$$Y\Lambda Y^{\dagger} = \lambda(Y'\Lambda'Y'^{\dagger}) + (1-\lambda)(Y''\Lambda''Y''^{\dagger}). \tag{4.60}$$

Now multiplying equation (4.60) by Y''^{T} and Y''^{*}, respectively from the left and right and using the orthogonality of Y'' we get

$$(Y''^{T}Y)\Lambda(Y^{\dagger}Y''^{*}) = \lambda(Y''^{T}Y')\Lambda'(Y'^{\dagger}Y''^{*}) + (1-\lambda)\lambda''. \tag{4.61}$$

Subtracting the last three diagonal elements of matrix equation (4.61) from the first one and using the fact that ρ_s has zero concurrence, i.e. $\lambda'_1 - \lambda'_2 - \lambda'_3 - \lambda'_4 = 0$, we get after some algebraic calculations $\lambda = \frac{C''-C}{C''}$ and $\frac{\mathrm{d}\lambda}{\mathrm{d}C''} = \frac{C}{C''^2} \geqslant 0$ where $C = \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4$ and $C'' = \lambda''_1 - \lambda''_2 - \lambda''_3 - \lambda''_4$ are the concurrence of ρ and ρ_e, respectively. This shows that maximal λ is achieved when $\lambda''_2 = \lambda''_3 = \lambda''_4 = 0$, i.e. ρ_e is a pure entangled state with concurrence λ''_1. Considering the above results we can write equation (4.60) as

$$\rho_{11} = \lambda\rho'_{11} + (1-\lambda)\lambda''_1(\cosh\theta\cosh\xi\cosh\phi + \sinh\theta\sinh\phi)^2 \tag{4.62}$$

$$\rho_{22} = \lambda\rho'_{22} + (1-\lambda)\lambda''_1(\sinh\theta\cosh\xi\cosh\phi + \cosh\theta\sinh\phi)^2 \tag{4.63}$$

$$\rho_{33} = \lambda\rho'_{33} + (1-\lambda)\lambda''_1\sinh^2\xi\cosh^2\phi \tag{4.64}$$

$$\rho_{44} = \lambda\rho'_{44} \tag{4.65}$$

$$\rho_{12} = \lambda\rho'_{12} + (1-\lambda)\lambda''_1((\cosh^2\xi\cosh^2\phi + \sinh^2\phi)\sinh 2\theta + \cosh\xi\cosh 2\theta\sinh 2\phi) \tag{4.66}$$

$$\rho_{13} = \lambda\rho'_{13} + (1-\lambda)\lambda''_1(\cosh\theta\cosh^2\phi\sinh 2\xi + \sinh\theta\sinh\xi\sinh 2\phi) \tag{4.67}$$

$$\rho_{23} = \lambda\rho'_{23} + (1-\lambda)\lambda''_1(\sinh\theta\cosh^2\phi\sinh 2\xi + \cosh\theta\sinh\xi\sinh 2\phi) \tag{4.68}$$

where

$$\begin{aligned} \rho_{11} = {} & (\lambda_1(\cosh\theta\cosh\xi\cosh\phi + \sinh\theta\sinh\phi)^2 \\ & + \lambda_2(\cosh\theta\cosh\xi\sinh\phi + \sinh\theta\cosh\phi)^2 + \lambda_3(\cosh\theta\sinh\xi)^2) \end{aligned} \tag{4.69}$$

$$\begin{aligned} \rho_{22} = {} & (\lambda_1(\sinh\theta\cosh\xi\cosh\phi + \cosh\theta\sinh\phi)^2 \\ & + \lambda_2(\sinh\theta\cosh\xi\sinh\phi + \cosh\theta\cosh\phi)^2 + \lambda_3(\sinh\theta\sinh\xi)^2) \end{aligned} \tag{4.70}$$

$$\rho_{33} = (\lambda_1\sinh^2\xi\cosh^2\phi + \lambda_2\sinh^2\xi\sinh^2\phi + \lambda_3\cosh^2\xi) \tag{4.71}$$

$$\rho_{44} = \lambda_4 \tag{4.72}$$

$$\rho_{12} = ((\lambda_1(\cosh^2\xi\cosh^2\phi + \sinh^2\phi) + \lambda_2(\cosh^2\xi\sinh^2\phi + \cosh^2\phi) + \lambda_3\sinh^2\xi)\sinh 2\theta \\ + (\lambda_1 + \lambda_2)\cosh\xi\sinh 2\phi\cosh 2\theta) \tag{4.73}$$

$$\rho_{13} = ((\lambda_1\cosh^2\phi + \lambda_2\sinh^2\phi + \lambda_3)\cosh\theta\sinh 2\xi + (\lambda_1 + \lambda_2)\sinh\theta\sinh\xi\sinh 2\phi) \tag{4.74}$$

$$\rho_{23} = ((\lambda_1\cosh^2\phi + \lambda_2\sinh^2\phi + \lambda_3)\sinh\theta\sinh 2\xi + (\lambda_1 + \lambda_2)\cosh\theta\sinh\xi\sinh 2\phi') \tag{4.75}$$

and ρ'_{ij} are defined in the same form as ρ_{ij} but here all parameters are expressed in terms of the prime parameters. After tedious but straightforward calculations we arrive at the following results for ρ_s:

$$\tanh\xi' = \frac{-F\sinh\theta' + G\cosh\theta'}{(p_1 + p_2 - A)\sinh 2\theta' + E\cosh 2\theta'} \tag{4.76}$$

$$\tanh 2\xi' = \frac{-F\cosh\theta' + G\sinh\theta'}{p_1\cosh^2\theta' + p_2\sinh^2\theta' + p_3 - \frac{1}{2}(A\cosh 2\theta' - E\sinh 2\theta' + B + 2D)} \tag{4.77}$$

$$\tanh 2\phi' = \frac{F\sinh\theta' - G\cosh\theta'}{\sinh\xi'(\Lambda\lambda'_3 + (p_1 + p_2 - A)\cosh 2\theta' - p_3 + E\sinh 2\theta' + D)} \tag{4.78}$$

$$\lambda'_3 = \frac{1}{2\lambda}\left(\frac{-F\cosh\theta' + G\sinh\theta'}{\sinh 2\xi'} - p_1\cosh^2\theta' - p_2\sinh^2\theta' + P_3 \right. \\ \left. + \frac{1}{2}(A\cosh 2\theta' - E\sinh 2\theta' + B - 2D)\right) \tag{4.79}$$

$$\lambda'_1 = \frac{1}{2\lambda}\left(\frac{1}{\cosh 2\phi'}(\Lambda\lambda'_3 + (p_1 + p_2 - A)\cosh 2\theta' - P_3 + E\sinh 2\theta' + D) \right. \\ \left. + \Lambda\lambda'_3 + p_1 - p_2 - p_3 - B + D\right) \tag{4.80}$$

$$\lambda'_2 = \frac{1}{2\lambda}\left(\frac{1}{\cosh 2\phi'}(\Lambda\lambda'_3 + (p_1 + p_2 - A)\cosh 2\theta' - P_3 + E\sinh 2\theta' + D) \right. \\ \left. - \Lambda\lambda'_3 - p_1 + p_2 + p_3 + B - D\right) \tag{4.81}$$

$$\lambda'_4 = \frac{p_4}{\lambda} \tag{4.82}$$

where

$$A = (1-\lambda)\lambda''_1((\cosh^2\xi\cosh^2\phi + \sinh^2\phi)\cosh 2\theta + \cosh\xi\sinh 2\theta\sinh 2\phi) \tag{4.83}$$

$$B = (1-\lambda)\lambda''_1(\cosh^2\xi\cosh^2\phi - \sinh^2\phi) \tag{4.84}$$

$$D = (1-\lambda)\lambda''_1\sinh^2\xi\cosh^2\phi \tag{4.85}$$

$$E = (1-\lambda)\lambda''_1((\cosh^2\xi\cosh^2\phi + \sinh^2\phi)\sinh 2\theta + \cosh\xi\cosh 2\theta\sinh 2\phi) - \rho_{12} \tag{4.86}$$

$$F = (1-\lambda)\lambda''_1(\cosh\theta\cosh^2\phi\sinh 2\xi + \sinh\theta\sinh\xi\sinh 2\phi) - \rho_{13} \tag{4.87}$$

$$G = (1-\lambda)\lambda''_1(\sinh\theta\cosh^2\phi\sinh 2\xi + \cosh\theta\sinh\xi\sinh 2\phi) - \rho_{23}. \tag{4.88}$$

The parameters θ' and ξ' are obtained by solving equations (4.76) and (4.77); using the remaining equations we can determine the parameters of ρ_s in terms of parameters of ρ

and ρ_e. Note that the one-parameter density matrix which was considered in the previous subsection can be obtained from the three-parameter density matrix by setting $\phi = \phi' = \phi'' = \xi = \xi' = \xi'' = 0$. One can see that the equations in the one-parameter case are solvable and we can express the parameters of the separable and entangled parts in the LS decomposition in terms of the parameters of the density matrix ρ which is the reason for its separate consideration in the previous subsection.

4.6. $2 \otimes 3$ *Bell decomposable state*

In this subsection we obtain the optimal LS decomposition for the Bell decomposable states of $2 \otimes 3$ quantum systems. A Bell decomposable density matrix acting on $2 \otimes 3$ Hilbert space can be defined by

$$\rho = \sum_{i=1}^{6} p_i |\psi_i\rangle\langle\psi_i| \qquad 0 \leqslant p_i \leqslant 1 \qquad \sum_{i=1}^{6} p_i = 1 \tag{4.89}$$

where $|\psi_i\rangle$ are Bell states in $H^6 \cong H^2 \otimes H^3$ Hilbert space, defined by

$$\begin{aligned} |\psi_1\rangle &= \tfrac{1}{\sqrt{2}}(|11\rangle + |22\rangle) \qquad & |\psi_2\rangle &= \tfrac{1}{\sqrt{2}}(|11\rangle - |22\rangle) \\ |\psi_3\rangle &= \tfrac{1}{\sqrt{2}}(|12\rangle + |23\rangle) \qquad & |\psi_4\rangle &= \tfrac{1}{\sqrt{2}}(|12\rangle - |23\rangle) \\ |\psi_5\rangle &= \tfrac{1}{\sqrt{2}}(|13\rangle + |21\rangle) \qquad & |\psi_6\rangle &= \tfrac{1}{\sqrt{2}}(|13\rangle - |21\rangle). \end{aligned} \tag{4.90}$$

It is quite easy to see that the above states are orthogonal and hence they can span the Hilbert space of $2 \otimes 3$ systems. From the Peres–Horodecki [4, 5] criterion for separability we deduce that the state given in equation (4.89) is separable if and only if the following inequalities are satisfied:

$$(p_1 - p_2)^2 \leqslant (p_3 + p_4)(p_5 + p_6) \tag{4.91}$$

$$(p_3 - p_4)^2 \leqslant (p_5 + p_6)(p_1 + p_2) \tag{4.92}$$

$$(p_5 - p_6)^2 \leqslant (p_1 + p_2)(p_3 + p_4). \tag{4.93}$$

In what follows we always assume without loss of generality that $p_1 \geqslant p_2$, $p_3 \geqslant p_4$ and $p_5 \geqslant p_6$. Recently in [14], an analytical lower bound of the concurrence of any $2 \otimes K$ mixed state is derived as

$$C(\rho) \geqslant \sqrt{\sum_{i>j} C^2(\rho^{(ij)})} \tag{4.94}$$

where $\rho^{(ij)}$ are unnormalized states restricted to $2 \otimes 2$ subsystems under projection operators $P^{(ij)}$ as

$$\rho^{(ij)} = P^{(ij)} \rho P^{(ij)} \qquad P^{(ij)} = I_2 \otimes (|i\rangle\langle i| + |j\rangle\langle j|) \tag{4.95}$$

and $C(\rho^{(ij)})$ are the Wootters concurrence of the corresponding restricted $2 \otimes 2$ density matrices. For our $2 \otimes 3$ Bell decomposable state we get

$$C(\rho^{(12)}) = \max\{0, p_1 - p_2 - \sqrt{(p_3 + p_4)(p_5 + p_6)}\} \tag{4.96}$$

$$C(\rho^{(23)}) = \max\{0, p_3 - p_4 - \sqrt{(p_1 + p_2)(p_5 + p_6)}\} \tag{4.97}$$

$$C(\rho^{(13)}) = \max\{0, p_5 - p_6 - \sqrt{(p_1 + p_2)(p_3 + p_4)}\}. \tag{4.98}$$

It is interesting to note that each Wootters concurrence given in equations (4.96)–(4.98) corresponds to the separability conditions given in equations (4.91)–(4.93), respectively. Now in order to obtain the optimal LS decomposition for BD state given in equation (4.89) we choose $\rho_s = \sum_i p_i'|\psi_i\rangle\langle\psi_i|$ and $\rho_e = \sum_i p_i''|\psi_i\rangle\langle\psi_i|$. We also assume without loss of generality that ρ_s lies on the separable–entangled boundary defined by (all other cases where ρ_s lies on the other surfaces can be treated similarly)

$$p_1' - p_2' = \sqrt{(p_3' + p_4')(p_5' + p_6')}. \tag{4.99}$$

Moreover, ρ_s must satisfy the two other separability conditions (4.92) and (4.93). This means that the entangled state ρ violates separability condition (4.91), i.e. we have

$$p_1 \geqslant p_2 + \sqrt{(p_3 + p_4)(p_5 + p_6)}. \tag{4.100}$$

However, two other inequalities (4.92) and (4.93) may be violated simultaneously. Taking into account the above considerations and equation (3.9) we get after some elementary calculations the following equation:

$$\begin{aligned}(1-\lambda)^2((p_1''-p_2'')^2 &- (p_3''+p_4'')(p_5''+p_6'')) - (1-\lambda)(2(p_1-p_2)(p_1''-p_2'')\\ &- (p_3+p_4)(p_5''+p_6'') - (p_5+p_6)(p_3''+p_4''))\\ &+ ((p_1-p_2)^2 - (p_3+p_4)(p_5+p_6)) = 0.\end{aligned} \tag{4.101}$$

In the rest of this subsection we will use equation (4.101) to calculate λ for some possible values of p_i'', $i = 1, 2, \ldots, 6$, which are as follows:

(i) $p'' = 1$. In this case equation (4.101) gives the following results:

$$\lambda = 1 - p_1 - p_2 + \sqrt{(p_3 + p_4)(p_5 + p_6)} \qquad \rho_e = |\psi_1\rangle\langle\psi_1| \tag{4.102}$$

$$p_1' = \frac{p_1 - (1-\lambda)}{\lambda} \qquad p_j' = \frac{p_j}{\lambda} \qquad \text{for} \quad j = 2, \ldots, 6. \tag{4.103}$$

Furthermore, ρ_s must satisfy the separability conditions (4.92) and (4.93) which leads to the following restrictions for ρ:

$$\begin{aligned}(p_3 - p_4)^2 &\leqslant (p_5 + p_6)\big(2p_2 + \sqrt{(p_3 + p_4)(p_5 + p_6)}\big)\\ (p_5 - p_6)^2 &\leqslant (p_3 + p_4)\big(2p_2 + \sqrt{(p_3 + p_4)(p_5 + p_6)}\big).\end{aligned} \tag{4.104}$$

By using equation (4.100) one can see that conditions (4.104) are stronger than the separability conditions (4.92) and (4.93), that is in this case only separability condition (4.91) is violated by ρ. It is worth mentioning that for these states we are able to give an exact expression for concurrence. As concurrence $C(\rho)$ is defined as the infimum over all possible pure state decompositions, no decomposition can have average concurrence smaller than $C(\rho)$. Since the decomposition given by equations (4.102) and (4.103) constitutes a maximal entangled pure state $|\psi_1\rangle$ and a separable state ρ_s, it follows that its average concurrence is equal to the weight of the entangled part, namely $(1-\lambda)$. On the other hand, for the entangled states restricted by equations (4.100) and (4.104) we get $C(\rho^{(12)}) \geqslant 0$ and $C(\rho^{(13)}) = C(\rho^{(13)}) = 0$. This means that the lower bound is equal to $(1-\lambda)$, i.e.

$$C(\rho) = (1-\lambda) = p_1 - p_2 - \sqrt{(p_3 + p_4)(p_5 + p_6)}. \tag{4.105}$$

(ii) $p_1'' + p_2'' = 1$. In this case by performing optimization procedure $\frac{\partial\lambda}{\partial p_1''} = \frac{\partial\lambda}{\partial p_2''} = 0$ in equation (4.101) (under constraint $p_1'' + p_2'' = 1$), we can see that the equations obtained from the optimization procedure restrict the density matrix ρ to rank 4, namely $p_3 = p_4 = 0$ or $p_5 = p_6 = 0$. Under these circumstances we get $\lambda = \frac{C''-C}{C''}$ and $\frac{\mathrm{d}\lambda}{\mathrm{d}C''}$, where C and C''

are the concurrence of ρ and ρ_e, respectively. This means that maximum λ happens when $p''_2 = 0$ which reduces to the results of the previous case.

(iii) $p''_1 + p''_3 = 1$. After the optimization procedure with the constraint $p''_1 + p''_3 = 1$ we get

$$\lambda = 1 - (p_1 - p_2) - (p_3 + p_4) - \tfrac{1}{4}(p_5 + p_6)$$
$$p'_1 = \frac{2p_2 - p_5 - p_6}{2\lambda} \qquad p'_3 = \frac{p_5 + p_6 - 4p_4}{4\lambda} \qquad p'_j = \frac{p_j}{\lambda} \qquad \text{for} \quad j = 2, 4, 5, 6 \tag{4.106}$$

where the following inequalities should be imposed in order that ρ_s be a separable state:

$$\begin{aligned} &2\big(p_4 - \tfrac{1}{8}(p_5 + p_6)\big)^2 \leqslant (p_5 + p_6)\big(p_2 - \tfrac{1}{4}(p_5 + p_6)\big) \\ &2(p_5 - p_6)^2 \leqslant (p_5 + p_6)\big(p_2 - \tfrac{1}{4}(p_5 + p_6)\big) \\ &4p_4 \leqslant p_5 + p_6 \leqslant 2p_2. \end{aligned} \tag{4.107}$$

(iv) $p''_1 + p''_5 = 1$. Analogous to the case $p''_1 + p''_3 = 1$ we get

$$\lambda = 1 - (p_1 - p_2) - \tfrac{1}{4}(p_3 + p_4) - (p_5 + p_6)$$
$$p'_1 = \frac{2p_2 - p_3 - p_4}{2\lambda} \qquad p'_3 = \frac{p_3 + p_4 - 4p_6}{4\lambda} \qquad p'_j = \frac{p_j}{\lambda} \qquad \text{for} \quad j = 2, 3, 4, 6 \tag{4.108}$$

with restrictions

$$\begin{aligned} &2(p_3 - p_4)^2 \leqslant (p_3 + p_4)\big(p_2 - \tfrac{1}{4}(p_3 + p_4)\big) \\ &2\big(p_6 - \tfrac{1}{8}(p_3 + p_4)\big)^2 \leqslant (p_3 + p_4)\big(p_2 - \tfrac{1}{4}(p_3 + p_4)\big) \\ &4p_6 \leqslant p_3 + p_4 \leqslant 2p_2. \end{aligned} \tag{4.109}$$

(v) $p''_1 + p''_3 + P''_5 = 1$. In this case it follows from optimization that rank ρ should be 4, namely $p_4 = p_6 = 0$. Under this condition we get

$$\lambda = 2p_2 \qquad p'_1 = p'_2 = \tfrac{1}{2} \qquad p'_3 = p'_4 = p'_5 = p'_6 = 0. \tag{4.110}$$

4.7. Werner states

The Werner states are the only states that are invariant under $U \otimes U$ operations. For $d \otimes d$ systems the Werner states are defined by [24]

$$\rho_f = \frac{1}{d^3 - d}((d - f)I + (df - 1)F) \qquad -1 \leqslant f \leqslant 1 \tag{4.111}$$

where I stands for the identity operator and $F = \sum_{i,j} |ij\rangle\langle ji|$. It is shown that a Werner state is separable iff $0 \leqslant f \leqslant 1$. Now to obtain the optimal LS decomposition for Werner states we choose $\rho_{f=0}$ as the separable part and $\rho_{f'}$ as the entangled state, i.e. $\rho_f = \lambda\rho_{f=0} + (1-\lambda)\rho_{f'}$. Then from equation (3.9) we get $\lambda = \frac{f'-f}{f'}$ and $\frac{\mathrm{d}\lambda}{\mathrm{d}f'} = \frac{f}{f'^2} \leqslant 0$, that is λ is maximum when $f' = -1$. Using the above results we get

$$\lambda = f + 1 \qquad \rho_e = \frac{1}{d(d-1)}(I - F). \tag{4.112}$$

4.8. Isotropic states

The isotropic states are the only ones that are invariant under $U \otimes U^*$ operations, where * denotes complex conjugation. The isotropic states of $d \otimes d$ systems are defined by [25]

$$\rho_F = \frac{1-F}{d^2-1}(I - |\psi^+\rangle\langle\psi^+|) + F|\psi^+\rangle\langle\psi^+| \qquad 0 \leqslant F \leqslant 1 \tag{4.113}$$

where $|\psi^+\rangle = \frac{1}{\sqrt{d}}\sum_i |ii\rangle$ is the maximally entangled state. It is shown that an isotropic state is separable when $0 \leqslant F \leqslant \frac{1}{d}$ [25]. Now in order to obtain the optimal LS decomposition we choose a boundary isotropic separable state with $F = 1/d$ as the separable part and $\rho_{F'}$ as the entangled state where we get $\lambda = \frac{d(F'-F)}{dF'-1}$ and $\frac{d\lambda}{dF'} = \frac{d^2(F-1/d)}{(dF'-1)^2} \geqslant 0$, that is, λ is maximum when $F' = 1$. Using the above results we get

$$\lambda = \frac{d(1-F)}{d-1} \qquad \rho_e = |\psi^+\rangle\langle\psi^+|. \tag{4.114}$$

It is interesting to stress that the average I-concurrence of the decomposition (4.114) is equal to the I-concurrence of the state obtained in [26]. By using equation (2.8) one can easily see that $C(|\psi^+\rangle) = \sqrt{2(1-1/d)}$, which can be used to evaluate the average I-concurrence of the decomposition

$$(1-\lambda)C(|\psi^+\rangle) = \sqrt{\frac{2d}{d-1}}\left(F - \frac{1}{d}\right) \qquad \text{for} \quad \frac{1}{d} \leqslant F \leqslant 1 \tag{4.115}$$

which is equal to the I-concurrence of isotropic states which has been obtained in [26].

4.9. One-parameter $3 \otimes 3$ *state*

Finally, let us consider a one-parameter state acting on $H^9 \cong H^3 \otimes H^3$ Hilbert space as [27]

$$\rho_\alpha = \frac{2}{7}|\psi^+\rangle\langle\psi^+| + \frac{\alpha}{7}\sigma_+ + \frac{5-\alpha}{7}\sigma_- \qquad 2 \leqslant \alpha \leqslant 5 \tag{4.116}$$

where

$$\begin{aligned} |\psi^+\rangle &= \tfrac{1}{\sqrt{3}}(|11\rangle + |22\rangle + |33\rangle) \\ \sigma_+ &= \tfrac{1}{3}(|12\rangle\langle 12| + |23\rangle\langle 23| + |31\rangle\langle 31|) \\ \sigma_- &= \tfrac{1}{3}(|21\rangle\langle 21| + |32\rangle\langle 32| + |13\rangle\langle 13|). \end{aligned} \tag{4.117}$$

ρ_α is separable iff $2 \leqslant \alpha \leqslant 3$, it is bound entangled iff $3 \leqslant \alpha \leqslant 4$ and it is distillable entangled state iff $4 \leqslant \alpha \leqslant 5$ [27]. To obtain LS decomposition for ρ_α we choose the boundary separable state with $\alpha = 3$ as ρ_s and $\rho_e = \rho_{\alpha'}$. After some calculations we get $\lambda = \frac{\alpha-\alpha'}{3-\alpha'}$ and $\frac{d\lambda}{d\alpha'} = \frac{\alpha-3}{(3-\alpha')^2} \geqslant 0$. So the optimal LS decomposition is achieved by choosing $\alpha' = 5$ and we get

$$\lambda = \frac{5-\alpha}{2} \qquad \rho_e = \frac{2}{7}|\psi^+\rangle\langle\psi^+| + \frac{5}{7}\sigma_+. \tag{4.118}$$

4.10. Multi-partite isotropic states

In this subsection we obtain the optimal LS decomposition for a n-partite d-level system. Let us consider the following mixture of the completely random state $\rho_0 = I/d^n$ and the maximally entangled state $|\psi^+\rangle$:

$$\rho(s) = (1-s)\frac{I}{d^n} + s|\psi^+\rangle\langle\psi^+| \qquad 0 \leqslant s \leqslant 1 \tag{4.119}$$

where I denotes the identity operator in d^n-dimensional Hilbert space and $|\psi^+\rangle = \frac{1}{\sqrt{d}}\sum_{i=1}^{d}|ii\cdots i\rangle$. The separability properties of the state (4.119) are considered in [28]. It is shown that the above state is separable iff $s = s_0 = (1+d^{n-1})^{-1}$.

Now to obtain the optimal LS decomposition we choose $\rho(s_0)$ as the separable part and $\rho(s')$ as the entangled part. By using equation (3.9) we get $\lambda = \frac{s'-s}{s'-(1+d^{n-1})^{-1}}$ and $\frac{\mathrm{d}\lambda}{\mathrm{d}s'} = \frac{s-(1+d^{n-1})^{-1}}{(s'-(1+d^{n-1})^{-1})^2}$. This means that the maximum λ is achieved when $s' = 1$, so we get

$$\lambda = \frac{(1-s)(1+d^{n-1})}{d^{n-1}} \qquad \rho_e = |\psi^+\rangle\langle\psi^+|. \tag{4.120}$$

5. Conclusion

We have shown that for a given bipartite density matrix and by choosing a suitable separable set on the separable–entangled boundary, the optimal Lewenstein–Sanpera decomposition can be obtained via optimization over a generic entangled density matrix. Based on this, the optimal LS decomposition is obtained for some bipartite systems. We have obtained the optimal decomposition for some bipartite states such as $2\otimes 2$ and $2\otimes 3$ Bell decomposable states, a generic two qubit state in Wootters basis, iso-concurrence decomposable states, the states obtained from BD states via one-parameter and three-parameter LOCC operations, $d\otimes d$ Werner and isotropic states, a one-parameter $3\otimes 3$ state and the multi-partite isotropic state. It is shown that in all $2\otimes 2$ systems considered here the average concurrence of the decomposition is equal to the concurrence. We also obtain an exact expression for the concurrence of some $2\otimes 3$ Bell decomposable states. In the case of $d\otimes d$ isotropic states it is shown that the average I-concurrence of the decomposition is equal to the I-concurrence of the states. We conjecture that for all optimal decompositions that the entangled part is only a pure state, the average I-concurrence of the decomposition is equal to the I-concurrence of the state.

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