Detecting three-qubit bound MUB diagonal entangled states via Nonlinear optimal entanglement witnesses

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Abstract

One of the important approaches to detect quantum entanglement is using linear entanglement witnesses (EWs). In this paper, by determining the envelope of the boundary hyper-planes defined by a family of linear EWs, a set of powerful nonlinear optimal EWs is manipulated. These EWs enable us to detect some three qubits bound MUB (mutually unbiased bases) diagonal entangled states, i.e., the PPT (positive partial transpose) entangled states. Also, in some particular cases, the introduced nonlinear optimal EWs are powerful enough to separate the bound entangled regions from the separable ones. Finally, we present numerical examples to demonstrate the practical accessibility of this approach.

Keywords :nonlinear optimal entanglement witnesses, mutually unbiased bases, *MUB* diagonal states

1 Introduction

In the recent years it became clear that quantum entanglement [1] is one of the most important resources in the rapidly expanding field of quantum information processing, with remarkable applications such as quantum parallelism [2], quantum cryptography [3], quantum teleportation [4, 5], quantum dense coding [6, 7] and reduction of communication complexity [8]. The above ideas are based on the fact that quantum entanglement, in particular, the occasionally occurrence of entangled states produce nonclassical phenomena. Therefore, specifying that a particular quantum state is entangled or separable is important because if the quantum state be separable then its statistic properties can be explained entirely by classical statistics.

In this paper, we will deal with three qubit systems with 2^3-dimensional Hilbert space $\mathcal{H}_2 \otimes \mathcal{H}_2 \otimes \mathcal{H}_2$, ($\mathcal{H}_d$ denotes the Hilbert space with dimension d). A density matrix ρ on this Hilbert space, is called fully separable if it can be written as a convex combination of pure product states as follows

$$\rho = \sum_i p_i |\alpha_i^{(1)}\rangle\langle\alpha_i^{(1)}| \otimes |\alpha_i^{(2)}\rangle\langle\alpha_i^{(2)}| \otimes |\alpha_i^{(3)}\rangle\langle\alpha_i^{(3)}|, \tag{1.1}$$

where $|\alpha_i^{(j)}\rangle$ are arbitrary but normalized vectors lie in $\mathcal{H}_2$, and $p_i \geq 0$ satisfy $\sum_i p_i = 1$ (hereafter we will refer to fully separable states as separable ones). The first and most widely used related criterion for distinguishing entangled states from separable ones, is the Positive Partial Transpose (PPT) criterion, introduced by Peres [9]. Furthermore, the necessary and sufficient condition for separability in $\mathcal{H}_2 \otimes \mathcal{H}_2$ and $\mathcal{H}_2 \otimes \mathcal{H}_3$ was shown by Horodecki in Ref. [10], which was based on a previous work by Woronowicz [11]. Partial transpose means transposition with respect to one of the subsystems. For a quantum state ρ_{AB} with matrix entries $\rho_{ij}^{mn} = \langle ij|\rho_{AB}|mn\rangle$, the partial transposition with respect to the subsystem B, denoted by $\rho_{AB}^{T_B}$, is defined by

$$(\rho_{ij}^{mn})^{T_B} = \rho_{in}^{mj}.$$

However, as it was shown in Ref. [12], in higher dimensions, there are PPT states that are nonetheless entangled. These states are called *PPT* entangled states (*PPTES*) or bound entangled states because they possess the peculiar property that no entanglement can be distilled from them by local operations [13]. Another approach to distinguish separable states from entangled ones involves the so called entanglement witness (*EW*) [14]. An *EW* for a given entangled state ρ is an observable W whose expectation value over all separable states is nonnegative, but strictly negative on ρ. There is a correspondence between EWs and linear positive (but not completely positive) maps via Jamiolkowski isomorphism [15]. As an example the partial transposition is a positive map (PM).

In this work, we consider those density matrices which are written as a linear combination of maximally commuting observables taken from the set of tensor products $A^i \otimes B^j \otimes C^k$, where $A, B, C \in \{I_2, \sigma_x, \sigma_y, \sigma_z\}$ and $i, j, k \in \{0, 1\}$ (σ_x, σ_y and σ_z are usual Pauli matrices). We will see later on that common eigenvectros of these observables form mutually unbiased bases (*MUB*)[16] and so we will refer to a set of such observables as set of *MUB* observables, for instance by using the notation $\sigma_i\sigma_j\sigma_k \equiv \sigma_i \otimes \sigma_j \otimes \sigma_k$, the set $\{III, \sigma_z\sigma_z I, \sigma_z I \sigma_z, I\sigma_z\sigma_z, \sigma_x\sigma_x\sigma_x, \sigma_x\sigma_y\sigma_y, \sigma_y\sigma_x\sigma_y, \sigma_y\sigma_y\sigma_x\}$ is a set of *MUB* observables. In fact, we consider tripartite *MUB* diagonal density matrices which are written in terms of *MUB* observables in a diagonal form. Then, we impose the *PPT* conditions (positivity of partial transposition with respect to all subsystems) to these density matrices and refer to the region of those density matrices which satisfy all of the obtained *PPT* conditions as "feasible region" (see Fig.1 and Fig.2 for example). In this way, we see that partial transposition plays an important role because in this type of density matrices, conditions obtained from positivity of partial transpositions are linear and feasible regions are completely contained in polygons; this allows us to investigate the separability or entanglement of the density matrices. In order to distinguish PPT entangled states (*PPTES*) from separable ones we construct some linear and nonlinear *EW*s. Namely, we consider density matrices that their common eigenvectors are maximally entangled states (*GHZ*-states) and construct an *EW* that detects such density matrices. Finally, we consider three categories relevant to some special choices of the parameters of density matrices, and by using the linear EWs we distinguish the region of *PPTES* and separable states completely. In other words, for density matrices contained in one of these three categories, we show that if the introduced linear EWs can not detect their entanglement, then they are necessarily separable.

We have also provided some numerical evidence suggesting that *PPTES* of three qubits can be detected by using the nonlinear EWs.

The paper is organized as follows: In section 2, we introduce the *MUB*-$(zzz)_G$ diagonal density matrices and consider the corresponding *PPT* conditions and feasible region. Section 3 is devoted to definition of an *EW* and construction of optimal linear *EW*s. In section 4, we obtain an envelope of family of linear *EWs* and construct some nonlinear *EW*s. Section 5 is devoted to classification and detection of *PPTES* for *MUB* diagonal density matrices in three categories. In section 6, we discuss some numerical analysis for evaluating the feasible region and the region of *PPTES*. The paper is ended with a brief conclusion together with two appendices.

2 *MUB* diagonal density matrices

In this section we introduce the so called *MUB* diagonal density matrices. The basic notions and definitions of *MUB* states relevant to our study are given in the Appendix *I*.

2.1 *MUB*-$(zzz)_G$ diagonal density matrices

In this subsection we introduce the *MUB*-$(zzz)_G$ diagonal density matrices which are considered through the paper. A *MUB*-$(zzz)_G$ diagonal density matrix for three qubits is defined as

$$\rho = \sum_{i=1}^{8} p_i |\psi_i\rangle\langle\psi_i| \ , \ 0 \leq p_i \leq 1 \ , \ \sum_{i=1}^{8} p_i = 1, \tag{2.2}$$

where three qubit GHZ states $|\psi_i\rangle$ for $i = 1, 2, ..., 8$ are given by

$$|\psi_1\rangle = \frac{1}{\sqrt{2}}[|000\rangle + |111\rangle], \;\; |\psi_2\rangle = \frac{1}{\sqrt{2}}[|000\rangle - |111\rangle],$$
$$|\psi_3\rangle = \frac{1}{\sqrt{2}}[|001\rangle + |110\rangle], \;\; |\psi_4\rangle = \frac{1}{\sqrt{2}}[|001\rangle - |110\rangle],$$
$$|\psi_5\rangle = \frac{1}{\sqrt{2}}[|010\rangle + |101\rangle], \;\; |\psi_6\rangle = \frac{1}{\sqrt{2}}[|010\rangle - |101\rangle],$$
$$|\psi_7\rangle = \frac{1}{\sqrt{2}}[|011\rangle + |100\rangle], \;\; |\psi_8\rangle = \frac{1}{\sqrt{2}}[|011\rangle - |100\rangle]. \quad (2.3)$$

Then, by using the MUB states in line 6 of Table I given in Appendix A, the density matrix ρ can be rewritten as follows

$$\rho = \frac{1}{8}[III + r_1\sigma_z\sigma_z I + r_2\sigma_z I\sigma_z + r_3 I\sigma_z\sigma_z + r_4\sigma_x\sigma_x\sigma_x + r_5\sigma_x\sigma_y\sigma_y + r_6\sigma_y\sigma_x\sigma_y + r_7\sigma_y\sigma_y\sigma_x], \quad (2.4)$$

where

$$r_1 = +p_1 + p_2 + p_3 + p_4 - p_5 - p_6 - p_7 - p_8,$$
$$r_2 = +p_1 + p_2 - p_3 - p_4 + p_5 + p_6 - p_7 - p_8,$$
$$r_3 = +p_1 + p_2 - p_3 - p_4 - p_5 - p_6 + p_7 + p_8,$$
$$r_4 = +p_1 - p_2 + p_3 - p_4 + p_5 - p_6 + p_7 - p_8,$$
$$r_5 = -p_1 + p_2 + p_3 - p_4 + p_5 - p_6 - p_7 + p_8,$$
$$r_6 = -p_1 + p_2 + p_3 - p_4 - p_5 + p_6 + p_7 - p_8,$$
$$r_7 = -p_1 + p_2 - p_3 + p_4 + p_5 - p_6 + p_7 - p_8. \quad (2.5)$$

It should be noticed that the MUB states of any line of Table I except for the states in the first three lines which are associated with separable states, can define a MUB diagonal density matrix, similarly. In the next subsection we impose the PPT conditions to the density matrix (2.4) in order to obtain the corresponding feasible region (region of those MUB diagonal density matrices which satisfy all of the PPT conditions).

2.2 Feasible regions

Here we are concerned with *MUB* diagonal density matrices of type (2.4) and by imposing the conditions obtained from positivity of partial transpositions with respect to each qubit, we obtain the so called feasible region. For these particular density matrices, the positivity of partial transpositions gives linear constraints on the parameters p_i for $i = 1, 2, ..., 8$. In order to obtain the feasible region for density matrix (2.4), first we group the conditions obtained from positivity of partial transpositions with respect to each subsystem (each qubit) in six partitions (p_3, p_4, p_5, p_6), (p_1, p_2, p_7, p_8), (p_1, p_2, p_5, p_6), (p_3, p_4, p_7, p_8), (p_1, p_2, p_3, p_4) and (p_5, p_6, p_7, p_8) as follows:

The positivity of partial transposition with respect to the first qubit gives the following constraints:

$$(p_3, p_4, p_5, p_6) \equiv \begin{cases} p_3 + p_4 + p_5 - p_6 \geq 0 \\ p_3 + p_4 - p_5 + p_6 \geq 0 \\ p_3 - p_4 + p_5 + p_6 \geq 0 \\ -p_3 + p_4 + p_5 + p_6 \geq 0 \end{cases} \tag{2.6}$$

$$(p_1, p_2, p_7, p_8) \equiv \begin{cases} p_1 + p_2 + p_7 - p_8 \geq 0 \\ p_1 + p_2 - p_7 + p_8 \geq 0 \\ p_1 - p_2 + p_7 + p_8 \geq 0 \\ -p_1 + p_2 + p_7 + p_8 \geq 0 \end{cases} \tag{2.7}$$

The positivity of partial transposition with respect to the second qubit gives:

$$(p_1, p_2, p_5, p_6) \equiv \begin{cases} p_1 + p_2 + p_5 - p_6 \geq 0 \\ p_1 + p_2 - p_5 + p_6 \geq 0 \\ p_1 - p_2 + p_5 + p_6 \geq 0 \\ -p_1 + p_2 + p_5 + p_6 \geq 0 \end{cases} \tag{2.8}$$

$$(p_3,p_4,p_7,p_8)\equiv\begin{cases} p_3+p_4+p_7-p_8\geq 0\\ p_3+p_4-p_7+p_8\geq 0\\ p_3-p_4+p_7+p_8\geq 0\\ -p_3+p_4+p_7+p_8\geq 0\end{cases} \tag{2.9}$$

The positivity of partial transposition with respect to the third qubit gives:

$$(p_1,p_2,p_3,p_4)\equiv\begin{cases} p_1+p_2+p_3-p_4\geq 0\\ p_1+p_2-p_3+p_4\geq 0\\ p_1-p_2+p_3+p_4\geq 0\\ -p_1+p_2+p_3+p_4\geq 0\end{cases} \tag{2.10}$$

$$(p_5,p_6,p_7,p_8)\equiv\begin{cases} p_5+p_6+p_7-p_8\geq 0\\ p_5+p_6-p_7+p_8\geq 0\\ p_5-p_6+p_7+p_8\geq 0\\ -p_5+p_6+p_7+p_8\geq 0\end{cases} \tag{2.11}$$

The region of those density matrices of type (2.4) which satisfy the above 24 constraints, is the feasible region. In order to specify the new perspective from this feasible region, we consider the parameters p_i in four pairs (p_1,p_2), (p_3,p_4), (p_5,p_6) and (p_7,p_8).

Now if we choose one of the pairs, say (p_1,p_2), then we can specify the projection of the feasible region to (p_1,p_2) plane with the following three inequalities (the last inequalities of (2.7), (2.8) and (2.10), respectivelyPPT conditions)

$$\begin{cases} p_1\leq p_2+p_7+p_8\\ p_1\leq p_2+p_5+p_6\\ p_1\leq p_2+p_3+p_4\end{cases}$$

By adding right hand side and left hand side of the above inequalities and using the equality $\sum_{i=1}^{8}p_i=1$, we get the following inequality

$$4p_1-2p_2\leq 1. \tag{2.12}$$

Similarly, one can obtain the inequality

$$4p_2 - 2p_1 \leq 1, \tag{2.13}$$

by exchanging 1 and 2 in the above steps. For an illustration see Fig. 1. It should be noticed that if we chose any other pair from (p_3, p_4), (p_5, p_6) and (p_7, p_8) instead of the pair (p_1, p_2), we would obtain the similar inequalities as in (2.12) and (2.13) for each pair.
According to Fig. 1, since the vertex points $(\frac{1}{2}, \frac{1}{2})$, $(\frac{1}{4}, 0)$, $(0, \frac{1}{4})$ and (0,0) satisfy the criterion (2.12), all of the points inside the shape will fulfill the PPT conditions (this is due to the fact that the feasible region is a convex region).

We can find another new projection of the feasible region in the (p_1, p_3) plane, concerning the following inequalities

$$\begin{cases} p_1 \leq p_2 + p_5 + p_6 \\ p_3 \leq p_4 + p_7 + p_8 \end{cases} \Rightarrow p_1 + p_3 \leq \frac{1}{2}. \tag{2.14}$$

This region is illustrated in Fig. 2; therefore we have presented a projection of the spatial shape in a two-dimensional space.

2.3 A special case of feasible region

Here, we discuss a special case of feasible region which will be appeared in subsection 5.3 as a region of bound entangled MUB diagonal density matrices (PPT entangled states). To this aim, we consider the line $p_1 + p_3 = \frac{1}{2}$ of the feasible region (2.14) in the (p_1, p_3) plane (see Fig. 2).

First we take the feasible region for the (p_3, p_4) plane (see Fig.3). If, we consider the following parametric line equation

$$p_3 = \alpha p_4 + \frac{1}{4}, \tag{2.15}$$

then (according to equations similar to (2.12) and (2.13) for the pair (p_3, p_4)), we obtain

$$4p_4 - 2p_3 = 1 \Rightarrow p_4 = \frac{p_3}{2} + \frac{1}{4} \tag{2.16}$$

By substituting (2.16) in (2.15) and using the fact that $0 \leq p_3 \leq 1/2$ (see Eq. (2.14)), one can obtain

$$p_3 = \frac{\alpha p_3}{2} + \frac{\alpha+1}{4} \quad \Rightarrow \quad 0 \leq p_3 = \frac{\alpha+1}{4-2\alpha} \leq \frac{1}{2},$$

so we get $-1 \leq \alpha \leq \frac{1}{2}$. According to the boundary condition $p_1 + p_3 = \frac{1}{2}$ and (2.15) we obtain:

$$p_1 = -\alpha p_4 + \frac{1}{4}. \tag{2.17}$$

Now by considering the PPT conditions

$$\begin{cases} -p_3 + p_4 + p_5 + p_6 \geq 0 \\ -p_3 + p_4 + p_7 + p_8 \geq 0 \end{cases}, \tag{2.18}$$

from equations (2.6) and (2.9), and adding the sides of the them, we obtain

$$(1-2\alpha)p_4 - p_2 \geq 0. \tag{2.19}$$

Also from the PPT conditions

$$\begin{cases} -p_1 + p_2 + p_5 + p_6 \geq 0 \\ -p_1 + p_2 + p_7 + p_8 \geq 0 \end{cases}, \tag{2.20}$$

given in (2.7) and (2.8), we get

$$-(1-2\alpha)p_4 + p_2 \geq 0. \tag{2.21}$$

Then, from (2.19) and (2.21) we conclude that $p_2 = (1-2\alpha)p_4$. Then, by using (2.15) and (2.17) one can easily conclude the following equations

$$p_3 - p_4 = (\alpha - 1)p_4 + \frac{1}{4}$$
$$p_1 - p_2 = -\alpha p_4 + \frac{1}{4} - (1-2\alpha)p_4 = (\alpha-1)p_4 + \frac{1}{4},$$

which indicate that $p_3 - p_4 = p_1 - p_2$. On the other hand, from the inequalities (2.19) and (2.21), one can deduce that the left hand sides of the inequalities (2.18) and (2.20) must be equal to zero. Therefore, for PPT density matrices with positive p_i's, we obtain

$$p_5 + p_6 = p_7 + p_8 = p_3 - p_4 = (\alpha-1)p_4 + \frac{1}{4} \geq 0 \quad \Rightarrow \quad p_4 \leq \frac{1}{4(1-\alpha)}$$

furthermore we obtain $p_3 \geq p_4$. Clearly, the PPT conditions (2.10) and (2.11) are satisfied by using the relations $p_1 + p_4 = p_2 + p_3$ and $p_5 + p_6 = p_7 + p_8$. The bound entanglement or separability of density matrices belonging to this special case of feasible region will be discussed in subsection 5.3 (as third category). For an illustration see Fig.3.

2.4 MUB-$(zzz)_G$ diagonal density matrices for which PPT conditions are necessary and sufficient for separability

In this section we consider the family of MUB-$(zzz)_G$ diagonal density matrices where the PPT criterions are necessary and sufficient for their separability.

2.4.1 Case (1)

In this case, we will put one of the pairs $(p_1, p_2), (p_3, p_4), (p_5, p_6)$ and (p_7, p_8) equal to $(0, 0)$, then we will see that the PPT conditions given in (2.6)-(2.11) are necessary and sufficient for separability of MUB-$(zzz)_G$ diagonal density matrices. For example, if we choose

$$p_1 = p_2 = 0,$$

then, by using the PPT conditions, we obtain

$$p_3 = p_4, \quad p_5 = p_6, \quad p_7 = p_8.$$

Then, the density matrices satisfying these conditions can be written as

$$\rho = \frac{1}{8}[III + r_1\sigma_z\sigma_z I + r_2\sigma_z I\sigma_z + r_3 I\sigma_z\sigma_z]. \tag{2.22}$$

The density matrix ρ in (2.22) is separable, since by using (2.5) we can rewrite ρ as

$$\rho = \frac{1}{4}\{p_3(III + \sigma_z\sigma_z I - \sigma_z I\sigma_z - I\sigma_z\sigma_z)$$

$$+p_5(III + \sigma_z I\sigma_z - \sigma_z\sigma_z I - I\sigma_z\sigma_z) + p_7(III + I\sigma_z\sigma_z I - \sigma_z I\sigma_z - \sigma_z\sigma_z I)\} =$$

$$p_3(|\psi_3\rangle\langle\psi_3| + |\psi_4\rangle\langle\psi_4|) + p_5(|\psi_5\rangle\langle\psi_5| + |\psi_6\rangle\langle\psi_6|) + p_7(|\psi_7\rangle\langle\psi_7| + |\psi_8\rangle\langle\psi_8|),$$

which is clearly a separable state, since it is a convex combination of projection operators.

2.4.2 Case (2)

In this case, we choose p_i's in each pair except for one of them to be equal, then we show that the PPT conditions (2.6)-(2.11) are necessary and sufficient for separability of MUB-$(zzz)_G$ diagonal density matrices. For example, we consider

$$p_1 \neq p_2, \quad p_3 = p_4, \quad p_5 = p_6, \quad p_7 = p_8.$$

Then, we can write the density matrix (2.2) as follows

$$\rho = (\frac{p_1 + p_2}{2})(|\psi_1\rangle\langle\psi_1| + |\psi_2\rangle\langle\psi_2|) + (\frac{p_1 - p_2}{2})(|\psi_1\rangle\langle\psi_1| - |\psi_2\rangle\langle\psi_2|) + p_3(|\psi_3\rangle\langle\psi_3| + |\psi_4\rangle\langle\psi_4|)+ \\ p_5(|\psi_5\rangle\langle\psi_5| + |\psi_6\rangle\langle\psi_6|) + p_7(|\psi_7\rangle\langle\psi_7| + |\psi_8\rangle\langle\psi_8|). \quad (2.23)$$

We assume that $p_3 < p_5 < p_7$ and $p_2 < p_1$ (the other cases give the same results as those which is obtained by this assumption in the following).

By substituting $p_3 = p_4$ in PPT conditions (2.10), we obtain $p_1 \leq p_2 + 2p_3$, so that we can write $p_1 = p_2 + 2p_3 - 2\epsilon_1$ ($p_1 > p_2 \Rightarrow 0 \leq \epsilon_1 \leq p_3$). Also, from the assumptions $p_3 < p_5$ and $p_3 < p_7$, one can write $p_5 = p_3 + \epsilon_5$ and $p_7 = p_3 + \epsilon_7$, respectively. By substituting these values of p_i's in the density matrix (2.23) and using the resolution of identity $\sum_{i=1}^{8} |\psi_i\rangle\langle\psi_i| = III$, one can write

$$\rho = \epsilon_1 III + (p_2 - \epsilon_1)(|\psi_1\rangle\langle\psi_1| + |\psi_2\rangle\langle\psi_2|) + (p_3 - \epsilon_1)(III + |\psi_1\rangle\langle\psi_1| - |\psi_2\rangle\langle\psi_2|) \\ + \epsilon_5(|\psi_5\rangle\langle\psi_5| + |\psi_6\rangle\langle\psi_6|) + \epsilon_7(|\psi_7\rangle\langle\psi_7| + |\psi_8\rangle\langle\psi_8|). \quad (2.24)$$

Then, from the fact that $(III \pm |\psi_1\rangle\langle\psi_1| - |\psi_2\rangle\langle\psi_2|)$ are separable states, one can see that for $\epsilon_1 < p_2$ in (2.24), the density matrix ρ is separable (since it is written as a convex combination of product states). For $\epsilon_1 > p_2$, we can write ρ as follows

$$\rho = p_2 III + (\epsilon_1 - p_2)(III - |\psi_1\rangle\langle\psi_1| - |\psi_2\rangle\langle\psi_2|) + (p_3 - \epsilon_1)(III + |\psi_1\rangle\langle\psi_1| - |\psi_2\rangle\langle\psi_2|) \\ +\epsilon_5(|\psi_5\rangle\langle\psi_5| + |\psi_6\rangle\langle\psi_6|) + \epsilon_7(|\psi_7\rangle\langle\psi_7| + |\psi_8\rangle\langle\psi_8|),$$

which is again a separable state. So in the second case, the PPT conditions are necessary and sufficient for separability, too.

3 Entanglement witnesses

An entanglement witness acting on the Hilbert space $\mathcal{H} = \mathcal{H}_2 \otimes \mathcal{H}_2 \otimes \mathcal{H}_2$ is a Hermitian operator $W = W^\dagger$, that satisfies $Tr(W\rho_s) \geq 0$ for any separable state ρ_s in $\boldsymbol{B}(\mathcal{H})$ (Hilbert space of bounded operators), and has at least one negative eigenvalue. If a density matrix ρ satisfies $Tr(W\rho) < 0$, then ρ is an entangled state and we say that W detects entanglement of the density matrix ρ. Note that in the aforementioned definition of EWs, we are not worry about the kind of entanglement of the quantum state and we are rather looking for EWs which possess nonnegative expectation values over all separable states despite of the fact that they possess some negative eigenvalues. The existence of an EW for any entangled state is a direct consequence of Hahn-Banach theorem [20] and the fact that the subspace of separable density operators is convex and closed [21]. Geometrically, EWs can be viewed as hyper planes which separate some entangled states from the set of separable states and hyper plane indicated as a line corresponds to the state with $Tr[W\rho] = 0$.

Based on the notion of partial transpose, the EWs are classified into two classes: decomposable EWs (d-EW) and non-decomposable EWs (nd-EW). An EW W is called decomposable if there exist positive operators P, Q_K so that

$$W = P + Q_1^{T_A} + Q_2^{T_B} + Q_3^{T_c}, \tag{3.25}$$

where T_K, $K = A, B, C$ denotes the partial transposition with respect to subsystems A, B and C, respectively. W is called non-decomposable if it can not be written in this form [22]. Clearly a d-EW can not detect bound entangled states (entangled states with positive partial transpose (PPT) with respect to all subsystems) whereas there are some bound entangled states which can be detected by a nd-EW.

Usually one is interested in finding optimal EWs W which detect entangled states in an optimal way. An EW W is said to be optimal, if for all positive operators P and $\varepsilon > 0$, the new Hermitian operator

$$W' = (1+\varepsilon)W - \varepsilon P \tag{3.26}$$

is not anymore an EW [23]. Suppose that there is a positive operator P and $\epsilon \geq 0$ such that $W' = (1+\varepsilon)W - \varepsilon P$ is yet an EW ($Tr(W'\rho_s) \geq 0$ for all separable states ρ_s). This means that if $Tr(W\rho_s) = 0$, then $Tr(P\rho_s) = 0$, for all separable states ρ_s which indicates that, the operator P is necessarily orthogonal to the kernel of W denoted by $Ker(W)$. By using the fact that every separable state is convex combination of pure product states, one can take ρ_s as a pure product state $|\psi\rangle\langle\psi|$. Also, one can assume that the positive operator P is a pure projection operator, since an arbitrary positive operator can be written as convex combination of pure projection operators with positive coefficients.

3.1 EWs detecting bound MUB diagonal density matrices

By employing tensor products of pauli operators relevant to MUB-$(zzz)_G$ state of Table I of the Appendix A, we introduce the following linear three qubit EW [24]

$$W = A_0 III + A_1 \ \ I\sigma_z\sigma_z + A_2(\sigma_x\sigma_x\sigma_x + \sigma_x\sigma_y\sigma_y) + A_3(\sigma_y\sigma_x\sigma_y + \sigma_y\sigma_y\sigma_x), \tag{3.27}$$

where $A_0, A_2, A_3 \geq 0$ and A_1 can be negative or positive. Now evaluating the trace of EW (3.27) over a pure product state,

$$\rho_s = |\alpha\rangle\langle\alpha| \otimes |\beta\rangle\langle\ \beta| \otimes |\gamma\rangle\langle\gamma|,$$

we get

$$Tr[W\rho_s] = A_0 + A_1 b_3 c_3 + A_2(a_1 b_1 c_1 + a_1 b_2 c_2) + A_3(a_2 b_1 c_2 + a_2 b_2 c_1),$$

where $a_i b_j c_k := Tr[\sigma_i\sigma_j\sigma_k\rho_s]$ for $i, j, k = 0, 1, 2, 3$ with $a_0 = b_0 = c_0 = 1$. We parameterize points on the unit sphere S^2 using traditional spherical coordinates, so that θ and φ stand for the angles of colatitude and longitude, respectively ($\theta \in [0, \pi], \varphi \in [0, 2\pi]$). Thus, the points

$a = (a_1, a_2, a_3)$, $b = (b_1, b_2, b_3)$ and $c = (c_1, c_2, c_3)$, can be uniquely represented as the unit vectors with the following coordinates

$$a_1 = \sin\theta_1 \cos\varphi_1, \quad a_2 = \sin\theta_1 \sin\varphi_1, \quad a_3 = \cos\theta_1$$

$$b_1 = \sin\theta_2 \cos\varphi_2, \quad b_2 = \sin\theta_2 \sin\varphi_2, \quad b_3 = \cos\theta_2$$

$$c_1 = \sin\theta_3 \cos\varphi_3, \quad c_2 = \sin\theta_3 \sin\varphi_3, \quad c_3 = \cos\theta_3,$$

so that, we obtain

$$Tr[W\rho_s] = A_0 + A_1 \cos\theta_3 \cos\theta_2 + \sin\theta_1 \sin\theta_2 \sin\theta_3 (A_2 \cos\varphi_1 \cos(\varphi_2 - \varphi_3) + A_3 \sin\varphi_1 \sin(\varphi_2 + \varphi_3)).$$

By appropriate choice of the angles, one can minimize the above expression. In fact, in the Appendix B, it has been proved that by taking $A_0 = \sqrt{A_2^2 + A_3^2}$ and $A_1 = -\sqrt{A_2^2 + A_3^2}$, the minimum value of $Tr[W\rho_s]$ is attained to zero, i.e., we obtain

$$min(Tr[W\rho_s]) = 0.$$

Consequently, EW (3.27) takes the following form

$$W^{(\psi)} = \sqrt{A_2^2 + A_3^2}(III - \quad I\sigma_z\sigma_z + \cos\psi(\sigma_x\sigma_x\sigma_x + \sigma_x\sigma_y\sigma_y) + \sin\psi(\sigma_y\sigma_x\sigma_y + \sigma_y\sigma_y\sigma_x)), \quad (3.28)$$

where

$$\cos\psi = \frac{A_2}{\sqrt{A_2^2 + A_3^2}}, \quad \sin\psi = \frac{A_3}{\sqrt{A_2^2 + A_3^2}}.$$

In the following, we discuss the optimality of the obtained linear EW W_ψ.

3.2 Optimality of the linear EW $W^{(\psi)}$

According to the arguments about optimal EWs given in section 3, in order to prove the optimality of the EW $W^{(\psi)}$ given in (3.28), it suffices to show that there exists no positive operator P such that $W' := (1 + \varepsilon)W^{(\psi)} - \varepsilon P$ be an EW, namely it must be proved that for any pure product state $|\nu\rangle$ so that $Tr(W^{(\psi)}|\nu\rangle\langle\nu|) = 0$, there exists no positive operator P

with the constraint $Tr(P|\nu\rangle\langle\nu|) = 0$. By considering a general three qubit pure product state as

$$|\nu\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} \cos\left(\frac{\theta_1}{2}\right) \\ e^{i\varphi_1}\sin\left(\frac{\theta_1}{2}\right) \end{pmatrix} \otimes \begin{pmatrix} \cos\left(\frac{\theta_2}{2}\right) \\ e^{i\varphi_2}\sin\left(\frac{\theta_2}{2}\right) \end{pmatrix} \otimes \begin{pmatrix} \cos\left(\frac{\theta_3}{2}\right) \\ e^{i\varphi_3}\sin\left(\frac{\theta_3}{2}\right) \end{pmatrix}, \tag{3.29}$$

one can evaluate

$$Tr[W^{(\psi)}\rho_s] = 1 - \cos\theta_2\cos\theta_3 - \sin\theta_1\sin\theta_2\sin\theta_3(\cos\psi\cos\varphi_1\cos(\varphi_2-\varphi_3) + \sin\psi\sin\varphi_1\sin(\varphi_2+\varphi_3)),$$

where $\rho_s = |\nu\rangle\langle\nu|$. Now, it is easily seen that by choosing the angles θ and φ as follows

$$(1): \begin{cases} \cos(\varphi_2-\varphi_3) = 1 \\ \sin(\varphi_2+\varphi_3) = 1 \end{cases} \Rightarrow \varphi_2 = \varphi_3 = \frac{\pi}{4}, \varphi_1 = \psi, \theta_1 = \frac{\pi}{2}, \theta_2 = \theta_3,$$

$$(2): \begin{cases} \cos(\varphi_2-\varphi_3) = 1 \\ \sin(\varphi_2+\varphi_3) = -1 \end{cases} \Rightarrow \varphi_2 = \varphi_3 = -\frac{\pi}{4}, \varphi_1 = -\psi, \theta_1 = \frac{\pi}{2}, \theta_2 = \theta_3,$$

$$(3): \begin{cases} \cos(\varphi_2-\varphi_3) = -1 \\ \sin(\varphi_2+\varphi_3) = -1 \end{cases} \Rightarrow \varphi_2 = \frac{\pi}{4}, \varphi_3 = -\frac{3\pi}{4}, \varphi_1 = \psi-\pi, \theta_1 = \frac{\pi}{2}, \theta_2 = \theta_3,$$

$$(4): \begin{cases} cos(\varphi_2-\varphi_3) = -1 \\ \sin(\varphi_2+\varphi_3) = 1 \end{cases} \Rightarrow \varphi_2 = \frac{3\pi}{4}\varphi_3 = -\frac{\pi}{4}, \varphi_1 = \pi-\psi, \theta_1 = \frac{\pi}{2}, \theta_2 = \theta_3, \tag{3.30}$$

we obtain $Tr[W^{(\psi)}\rho_s] = 0$. Now, in order to prove that $W^{(\psi)}$ is an optimal EW, we proceed as follows: Let P be a pure projection operator that one can subtract from $W^{(\psi)}$, so that $(1+\epsilon)W^{(\psi)} - \epsilon P$ is an EW for some $\epsilon > 0$. From Eq. (3.28), one can easily see that, any pure state of the form $|\Psi\rangle = |\alpha\rangle|z_+z_+\rangle + |\beta\rangle|z_-z_-\rangle$, (where, $|\alpha\rangle$ and $|\beta\rangle$ are arbitrary states) belongs to the $Ker(W^{(\psi)})$, i.e., we have $Tr[W^{(\psi)}|\Psi\rangle\langle\Psi|] = 0$. Then, due to the fact that, the pure projection operator P must be orthogonal to $Ker(W^{(\psi)})$ (and so orthogonal to $|\Psi\rangle\langle\Psi|$), we have $P = |\Phi\rangle\langle\Phi|$ with

$$|\Phi\rangle = |\alpha\rangle|z_+z_-\rangle + |\beta\rangle|z_-z_+\rangle \tag{3.31}$$

Now, the pure projection operator defined as above, must be orthogonal to pure product states $|\nu^{(i)}\rangle$, $i = 1, 2, 3, 4$ obtained by substituting the angles given by (3.30) in (3.29), since these states belong to $Ker(W^{(\psi)})$. But, this is possible only if $\alpha_1, \alpha_2, \beta_1$ and β_2 satisfy the following equations:

$$\langle\nu_1|\Phi\rangle = (\alpha_1 + \alpha_2 e^{-i\psi}) + (\beta_1 + \beta_2 e^{-i\psi}) = 0,$$

$$\langle\nu_2|\Phi\rangle = (\alpha_1 + \alpha_2 e^{+i\psi}) + (\beta_1 + \beta_2 e^{+i\psi}) = 0,$$

$$\langle\nu_3|\Phi\rangle = -(\alpha_1 - \alpha_2 e^{-i\psi}) + (\beta_1 - \beta_2 e^{-i\psi}) = 0,$$

$$\langle\nu_4|\Phi\rangle = -(\alpha_1 - \alpha_2 e^{+i\psi}) + (\beta_1 - \beta_2 e^{+i\psi}) = 0.$$

Above equations imply that for

$$\psi \neq 0, \pi$$

we have

$$\alpha_1 = \alpha_2 = \beta_1 = \beta_2 = 0.$$

Therefore, there is no positive operator P to subtract from $W^{(\psi)}$.

In general, linear optimal EWs can be written as

$$W^{(\psi)}_{\pm i,\pm(j,k),(l,m)} = III \pm O_i + \cos\psi(O_j \pm O_k) + \sin\psi(O_l \pm O_m), \tag{3.32}$$

where $i = 1, 2, 3$ while the indices $j \neq k \neq l \neq m$ take values between $4, 5, 6, 7$.

The observables O_i for $i = 1, 2, 3$ and O_j for $j = 4, 5, 6, 7$ are defined as

$$O_1 = I\sigma_z\sigma_z, \quad O_2 = \sigma_z I\sigma_z, \quad O_3 = \sigma_z\sigma_z I,$$

$$O_4 = \sigma_x\sigma_x\sigma_x, \quad O_5 = \sigma_x\sigma_y\sigma_y, \quad O_6 = \sigma_y\sigma_x\sigma_y, \; O_7 = \sigma_y\sigma_y\sigma_x.$$

4 Non-linear optimal EWs

Actually with a given entangled density matrix, one can associate a non-linear EW, simply by defining a non-linear functional, so that it is nonnegative valued over all separable density matrices, but it is negative valued over the density matrix. In other words, we optimize $Tr[W^{(\psi)}_{\pm i,\pm(j,k),(l,m)}\rho]$ where, $W^{(\psi)}_{\pm i,\pm(j,k),(l,m)}$ are the linear optimal EWs given by (3.32) and ρ is the MUB-$(zzz)_G$ diagonal density matrix given by (2.4). Then, one can easily get

$$Tr[W^{(\psi)}_{\pm i,\pm(j,k),(l,m)}\rho] = (1 \pm r_i) + (r_j + r_k)\cos\psi + (r_l + r_m)\sin\psi,$$

which indicates that, by appropriate choice of the parameter ψ as a functional of ρ, one can obtain a non-linear function of the parameters of ρ which is nonnegative over all separable states. To this aim, we define

$$\cos\theta = \frac{r_j + r_k}{\sqrt{(r_j + r_k)^2 + (r_l + r_m)^2}},$$

then $Tr[W^{(\psi)}_{\pm i,\pm(j,k),(l,m)}\rho]$ can be written as

$$Tr[W^{(\psi)}_{\pm i,\pm(j,k),(l,m)}\rho] = 1 \pm r_i + \sqrt{(r_j + r_k)^2 + (r_l + r_m)^2}cos(\psi - \theta).$$

Now, by choosing $(\psi - \theta) = \pi$, we obtain

$$Tr[W_{\pm i,\pm(j,k),(l,m)}\rho] = 1 \pm r_i - \sqrt{(r_j + r_k)^2 + (r_l + r_m)^2}. \qquad (4.33)$$

The above expression is the required non-linear function in terms of the parameters of ρ and it is definitely nonnegative valued function of separable states, hence it is the non-linear optimal EW associated with ρ (since it is obtained from optimal linear EWs).

4.1 Non-linear EWs as an envelop of family of linear EWs

As the parameter ψ of linear EW's $W^{(\psi)}_{\pm i,\pm(j,k),(l,m)}$ varies, the envelope of hyper planes defined by

$$Tr[W^{(\psi)}_{\pm i,\pm(j,k),(l,m)}\rho_s] = 0, \qquad (4.34)$$

namely their intersections, define the boundary of PPT bound entangled states that can be detected by the linear EWs. Obviously, the envelope of these curves can be obtained simply by eliminating the parameter ψ from the Eq.(4.34). To this aim, we need to determine $\cos\psi$ and $\sin\psi$ by solving above equation together with the equation that can be obtained by taking its derivative with respect to ψ equal to zero, i.e., we consider

$$\begin{cases} Tr[W^{(\psi)}_{\pm i,+(4,5),(6,7)}\rho] = (1\pm r_i) + (r_4+r_5)\cos\psi + (r_6+r_7)\sin\psi = 0, \\ \frac{d}{d\psi}(Tr[W^{(\psi)}_{\pm i,+(4,5),(6,7)}\rho]) = -\sin\psi(r_4+r_5) + \cos\psi(r_6+r_7) = 0. \end{cases}$$

By solving the above equations one can obtain

$$\cos\psi = -\frac{(r_j+r_k)(1\pm r_i)}{(r_j+r_k)^2+(r_l+r_m)^2},$$

$$\sin\psi = -\frac{(r_l+r_m)(1\pm r_i)}{(r_j+r_k)^2+(r_l+r_m)^2}.$$

Now, using the identity $\cos^2\psi + \sin^2\psi = 1$ we obtain the required envelope of curves defined by the following equations

$$(1\pm r_i)^2 = (r_j+r_k)^2 + (r_l+r_m)^2.$$

5 Bound entangled MUB diagonal density matrices

In this section, we consider three main categories of bound entangled states according to equations (B-i) and (B-ii) given in the Appendix B. In these categories, the relations $|(r_j \pm r_k)| \leq (1\pm r_i)$, are always satisfied since if we consider for example the inequality

$$|(r_4 - r_7)| > (1 + r_1),$$

then we conclude the inequality $p_2 + p_4 < 0$ which is clearly impossible.

5.1 First category

The first interesting family of three qubit bound entangled states is introduced for the choices of the parameters r_i so that:

$$1\pm r_1 = r_5 \pm r_6, 1\pm r_1 = r_4 \mp r_7, 1\pm r_2 = r_5 \pm r_7,$$

$$1 \pm r_2 = r_4 \mp r_6, 1 \pm r_3 = r_6 \pm r_7, 1 \pm r_3 = r_4 \mp r_5, \tag{5.35}$$

for example, if we consider $1 + r_1 = r_4 - r_7$, then we obtain $p_2 = p_4 = 0$. Then, the PPT conditions (2.6)-(2.11) lead to $p_1 = p_3$, and triangle inequalities for the cases (p_1, p_5, p_6) and (p_1, p_7, p_8) are established. This state can be detected by non-linear EW $W_{+1,-(4,7),(5,6)}$, since by using the result (4.33), we have

$$Tr[W_{+1,-(4,7),(5,6)}\rho] = (1 + r_1) - \sqrt{(1 + r_1)^2 + (r_5 - r_6)^2}, \tag{5.36}$$

which indicates that for $r_5 \neq r_6$, $Tr[W_{+1,-(4,7),(5,6)}\rho] < 0$.

On the other hand, by imposing the condition $(r_5 - r_6) = p_5 - p_6 - p_7 + p_8 = 0$, the state ρ will be separable, since we have

$$p_5 - p_6 - p_7 + p_8 = 0 \Rightarrow p_5 + p_8 = p_6 + p_7.$$

So, by using the relations (2.5), one can see that if $r_2 > 0$ ($r_2 = 2(p_6 - p_8)$ since we have $p_1 = p_3$ and $p_2 = p_4 = 0$), then we get $p_6 > p_8$ and therefore we have

$$\rho = (1 - r_2)III + (r_1 + r_2)I\sigma_z\sigma_z + r_2[(III - \sigma_z\sigma_z I)(III + \sigma_z I\sigma_z)] + r_4\sigma_x\sigma_x\sigma_x + r_5\sigma_x\sigma_y\sigma_y$$

with

$$r_4 - r_7 = 4p_1$$

$$r_1 + r_2 = 2(p_1 - p_7 - p_8)$$

$$r_4 - r_7 - (r_1 + r_2) = 4p_1 - 2p_1 + 2p_7 + 2p_8 = 2(p_1 + p_7 + p_8)$$

$$1 - r_2 = 1 - 2p_6 + 2p_8 = 2(p_1 + p_7 + p_8)$$

$$1 - r_2 - (r_1 + r_2) + r_4 - r_7 = 4(p_1 + p_7 + p_8) \leq 1,$$

which is separable state.

If $r_2 < 0$ then we will have $p_8 > p_6$ and

$$\rho = (1 + r_2)III + (r_1 - r_2)I\sigma_z\sigma_z - r_2[(III - \sigma_z\sigma_z I)(III + \sigma_z I\sigma_z)] + r_4\sigma_x\sigma_x\sigma_x + r_5\sigma_x\sigma_y\sigma_y$$

with

$$r_1 - r_2 = 2(p_1 - p_5 - p_6) \leq 0$$

$$r_4 - r_7 - (r_1 - r_2) = 2(p_1 + p_5 + p_6) \geq 0$$

$$1 + r_2 = 2(p_1 + p_5 + p_6) \geq 0$$

$$(1 + r_2) + r_4 - r_7 - (r_1 - r_2) = 4(p_1 + p_5 + p_6) \leq 1.$$

For the above cases we had $p_2 = p_4 = 0$, so, this category consists two vanishing non-paired (p_2 and p_4 belong to different pairs) parameters. The other cases in (5.35) can be discussed similarly.

A special case

As a special case, if we consider ρ in (2.4) with the following parameters

$$p_4 = p_8 = p_6 = 0,$$

$$p_3 = p_5 = p_7 = p,$$

we get $r_1 = r_2 = r_3$ and $r_5 = r_6 = r_7$. Then, ρ can be written as

$$\rho = \frac{1}{8}[III + r_1(I\sigma_z\sigma_z + \sigma_z I\sigma_z + \sigma_z\sigma_z I) + r_4\sigma_x\sigma_x\sigma_x + r_5(\sigma_x\sigma_y\sigma_y + \sigma_y\sigma_x\sigma_y + \sigma_y\sigma_y\sigma_x)]. \quad (5.37)$$

Concerning the following PPT and normalization conditions

$$p_1 + p_2 - p_3 \geq 0$$

$$p_1 - p_2 + p_3 \geq 0$$

$$-p_1 + p_2 + p_3 \geq 0$$

$$\sum_{i=1}^{8} p_i = 1 \Rightarrow p_1 + p_2 + 3p_3 = 1$$

we construct the convex hull of the following boundary planes

$p_1 + p_2 - p_3 = 0$

$p_1 + p_2 + 3p_3 = 1 \Rightarrow 4p_3 = 1 \; p_3 = \frac{1}{4}$

$p_1 - p_2 + p_3 = 0$

$p_1 + p_2 + 3p_3 = 1 \Rightarrow 2p_1 + 4p_3 = 1$

$-p_1 + p_2 + p_3 = 0$

$p_1 + p_2 + 3p_3 = 1 \Rightarrow 2p_2 + 4p_3 = 1,$

which define a triangular bound entangled region in (p_1, p_2, p_3) space (as it is shown in Fig.4). With the boundary defined by the following lines where the boundaries of triangular region corresponding to the lines passing through the points $(\frac{1}{4}, 0, \frac{1}{4}), (0, \frac{1}{4}, \frac{1}{4})$ and $(\frac{1}{2}, \frac{1}{2}, 0)$, where the states corresponding to the sides defined by the thick line passing through the points $(\frac{1}{4}, 0, \frac{1}{4})$ and $(\frac{1}{2}, \frac{1}{2}, 0)$ are separable.

5.2 Second category

Another interesting family for bound entangled states is obtained by considering the following cases:

$$\begin{aligned}
&1 \pm r_1 = r_4 + r_5, 1 \pm r_1 = r_4 - r_5, 1 \pm r_1 = r_6 + r_7, 1 \pm r_1 = r_6 - r_7, \\
&1 \pm r_1 = r_4 + r_6, 1 \pm r_1 = r_4 - r_6, 1 \pm r_1 = r_5 + r_7, 1 \pm r_1 = r_5 - r_7, \\
&1 \pm r_2 = r_4 + r_5, 1 \pm r_2 = r_4 - r_5, 1 \pm r_2 = r_6 + r_7, 1 \pm r_2 = r_6 - r_7, \\
&1 \pm r_2 = r_4 + r_7, 1 \pm r_2 = r_4 - r_7, 1 \pm r_2 = r_5 + r_6, 1 \pm r_2 = r_5 - r_6, \\
&1 \pm r_3 = r_4 + r_6, 1 \pm r_3 = r_4 - r_6, 1 \pm r_3 = r_5 + r_7, 1 \pm r_3 = r_5 - r_7, \\
&1 \pm r_3 = r_4 + r_7, 1 \pm r_3 = r_4 - r_7, 1 \pm r_3 = r_5 + r_6, 1 \pm r_3 = r_5 - r_6.
\end{aligned} \tag{5.38}$$

If we choose one case such as $1 + r_1 = r_4 + r_6$, we obtain $p_7 = p_1 + p_2 + 2p_4 + p_8$. Then, by using PPT conditions we obtain

$$p_1 + p_2 - p_7 + p_8 \geq 0 \Rightarrow p_4 = 0, \tag{5.39}$$

$$p_3 - p_7 + p_8 \geq 0 \Rightarrow p_3 = p_1 + p_2, \tag{5.40}$$

and satisfy the triangle inequality for (p_3, p_5, p_6) case. So according to (5.39) and (5.40) we get

$$p_7 = p_3 + p_8. \tag{5.41}$$

Applying the EW $W_{+1,+(4,6),(5,7)}$ to the state (5.37), we obtain

$$Tr[W\rho] = (1 + r_1) - \sqrt{(1 + r_1)^2 + (r_5 + r_7)^2} < 0$$

the condition $(r_5 + r_7) = -p_1 + p_2 + p_5 - p_6 = 0$ corresponds to separable state.

By using the normalization condition

$$\sum_{i=1}^{8} p_i = 1 \Rightarrow 3p_3 + p_5 + p_6 + 2p_8 = 1$$

and

$$-p_1 + p_2 + p_5 - p_6 = 0 \Rightarrow p_1 + p_6 = p_2 + p_5,$$

we obtain for $r_2 > 0$

$$\rho = (1 - r_2)III + (r_1 + r_2)I\sigma_z\sigma_z + r_2[(III + \sigma_z I\sigma_z)(III - \sigma_z\sigma_z I)] + r_4\sigma_x\sigma_x\sigma_x + r_6\sigma_y\sigma_x\sigma_y$$

$$r_4 + r_6 = 4(p_1 + p_3) = 4p_3$$

$$r_1 + r_2 = -4p_8$$

$$r_4 + r_6 - (r_1 + r_2) = 4p_7$$

$$1 - r_2 = 4p_7$$

$$\Rightarrow (1 - r_2) + (r_4 + r_6) - (r_1 + r_2) = 8p_7$$

while for $r_2 < 0$, we get

$$\rho = (1 + r_2)III + (r_1 - r_2)I\sigma_z\sigma_z - r_2[(III + \sigma_z\sigma_z I)(III - \sigma_z I\sigma_z)] + r_4\sigma_x\sigma_x\sigma_x + r_6\sigma_y\sigma_x\sigma_y$$

$$r_1 - r_2 = 2(p_3 - p_5 - p_6) \leq 0$$

$$r_4 + r_6 - (r_1 - r_2) = 2(p_3 + p_5 + p_6) \geq 0$$

$$1 + r_2 = 2(1 - 2p_7) = 2(p_3 + p_5 + p_6) \geq 0$$

$$\Rightarrow (1 + r_2) + (r_4 + r_6) - (r_1 - r_2) = 4(p_3 + p_5 + p_6) \leq 1.$$

So, in this case according to (B-i), if we choose parameters as $p_i = p_j + p_k$, (p_i and p_j are in the same pairs) and p_k belong to another pairs, then we obtain second category of bound entangled states.

The other family (5.2) can be considered similarly.

5.3 Third category

The last category is given by the following cases:

$$1 \pm r_1 = r_4 \pm r_7, 1 \pm r_1 = r_5 \mp r_6, 1 \pm r_2 = r_4 \pm r_6,$$

$$1 \pm r_2 = r_5 \mp r_7, 1 \pm r_3 = r_4 \pm r_5, 1 \pm r_3 = r_6 \mp r_7. \tag{5.42}$$

If $1 - r_1 = r_4 - r_7$ then $p_1 + p_3 = p_2 + p_4 + p_5 + p_6 + p_7 + p_8 = \frac{1}{2}$ and $r_5 - r_6 = 2(p_5 - p_6 - p_7 + p_8)$. The PPT conditions for this case have been previously considered (section 2.4.2). Therefore, if $r_5 - r_6 \neq 0$ this state will be bound entangled and can be detected by $W_{-1,-(4,7),(5,6)}$; otherwise it is separable since we have

$$r_5 - r_6 = 0 \Rightarrow p_6 + p_7 = p_5 + p_8$$

and so from the PPT conditions we get

$$p_5 = p_7, p_6 = p_8$$

after calculation of r_i's, we obtain

$$\rho = 2p_2(III + \sigma_z\sigma_z I)(III + I\sigma_z\sigma_z) + 2p_4(III + \sigma_z\sigma_z I)(III - \sigma_z I\sigma_z)$$

$$+(1 - 2(p_2 + p_4))III + 2p_5\sigma_x\sigma_x\sigma_x - 4p_6\sigma_x\sigma_y\sigma_y.$$

We know that the first and second cases in the density matrix are separable and for other cases

$$|(1-2(p_2+p_4))|+|2p_5|+|-4p_6|\leq 1.$$

So, if we choose two parameters and add them as $p_i+p_j=\frac{1}{2}$,(p_i,p_j are in different pairs) then, the category consists the bound entangled states.

The other cases (5.2) can be discussed similarly.

6 Numerical analysis of three-qubit bound MUB diagonal entangled states

This section is devoted to some numerical studies of three-qubit bound MUB diagonal entangled states as follows: The feasible regions in (p_1,p_2) and (p_1,p_3) planes, defined by equations (2.12) and (2.14), are supported numerically. Using the nonlinear EWs, about 2.7% of bound MUB-$(zzz)_G$ diagonal density matrices are detected numerically. The numerical results are plotted in (p_1,p_3,p_5) , (p_2,p_4,p_8) , (p_6,p_7) and (p_1,p_3) , (p_2,p_4) , (p_5,p_6) , (p_7,p_8) phase spaces and the bound density matrix ($p_1=0.043425,p_2=0.15308,p_3=0.016132,p_4=0.19387,p_5=0.059793,p_6=0.24806,p_7=0.18207,p_8=0.10357$) is shown in Fig.5 and Fig.6, as a prototype of a bound MUB diagonal density matrix.

7 Conclusion

The feasible region of PPT *MUB*-$(zzz)_G$ diagonal density matrices is determined, where it is a convex polyatope due to linearity of PPT conditions. In order to detect three-qubit bound MUB diagonal entangled states, some nonlinear optimal EWs are manipulated, such that they form the envelope of the boundary hyper-planes defined by a family of optimal linear EWs. By using these nonlinear EWs, the region of bound entangled states and separable ones are determined analytically in some particular cases three categories, where the numerical analysis support them. The results thus obtained in this paper indicate that, the proposed methods in this work, can be used in studying entanglement of more general systems with linear PPT conditions such as multiqubit MUB diagonal systems. .

Appendix A

I. Mutually unbiased basis

Let V be a d-dimensional Hilbert space with two orthonormal basis

$$B_1 = \{|e_1\rangle, |e_2\rangle, ..., |e_d\rangle\} \quad \text{and}$$

$$B_2 = \{|f_1\rangle, |f_2\rangle, ..., |f_d\rangle\},$$

where $|e_i\rangle$ and $|f_i\rangle$ for $i = 1, 2, ..., d$ belong to $\mathbb{C}^d$ (the standard Hilbert space of dimension d endowed with usual inner product denoted by $\langle\ |\ \rangle$).

The basis B_1 and B_2 are called mutually unbiased if and only if

$$|\langle e_i|f_j\rangle| = \frac{1}{\sqrt{d}}. \tag{A-i}$$

As an example, for a two-level system there is such a set of bases that can be represented in terms of eigenvectors of the usual Pauli matrices $\sigma_x, \sigma_y, \sigma_z$ as follows

$$B_x = \{\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle), \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)\},$$

$$B_y = \{\frac{1}{\sqrt{2}}(|0\rangle + i|1\rangle), \frac{1}{\sqrt{2}}(|0\rangle - i|1\rangle)\} \quad \text{and}$$

$$B_z = \{|0\rangle, |1\rangle\}.$$

When d is a prime or power of a prime, the maximum number of such MUB's is equal to $d+1$, otherwise there is no clear number of sets.

According to Refs. [18, 19] and Table I, in the case of three qubits, we have nine sets of mutually unbiased bases and corresponding maximally commuting sets of observables, where we will refer to them as generalized Pauli matrices; each of these sets consist of seven commuting observables. In the Table I, the first three rows contains product common eigenvectors, $(xyz)_\pi, (yzx)_\pi$ and $(zxy)_\pi$ (subscript π means product state). For example, eight states for basis $(xyz)_\pi$ could be written as $|n_x n_y n_z\rangle$ where $n_i = 1$ and $n_i = 0$ correspond to spin down and spin up along the ith axis for $i = x, y, z$, respectively. These product states are separable so we will not use them for construction of EWs. Other bases consist of six maximally entangled states $(xxx)_{Gi}, (yyy)_G, (zzz)_G, (xzy)_G, (yxz)_G$ and $(zyx)_G$, here subscript G denotes a family of Greenberger-Horne-Zeilinger (GHZ) states. For example, eight states for basis $(zzz)_G$ and $(xxx)_{Gi}$ can be written as

$$(zzz)_G = |n_z n_z n_z, \pm\rangle = (|n_z n_z n_z\rangle \pm |\bar{n_z}\bar{n_z}\bar{n_z}\rangle), \quad n_z = 0, 1 \tag{A-ii}$$

$$(xxx)_{Gi} = |n_x n_x n_x, \pm\rangle = (|n_x n_x n_x\rangle \pm i|\bar{n_x}\bar{n_x}\bar{n_x}\rangle), \quad n_x = 0, 1 \tag{A-iii}$$

where labels bar show that if $n_z = 0$ or 1, then $\bar{n_z} = 1$ or 0, respectively. In section 2, we have considered only the state $(zzz)_G$; since the other cases can be obtained from this state by local unitary operations.

II. MUB sets for three qubit systems

We know MUB can be constructed using a number of methods that depend on the dimensionality of the space. These methods using for different case such as dimension space is prime, a product of primes, or a power of a prime, and if it is odd or even. We confine our study to the case of three qubits, that is, to an eight-dimensional Hilbert space, in this space there exist four MUB formation, where denotes sets of MUBs where the basis vectors are either separable , biseparable or entangled states. The four MUB formations are $(2, 3, 4)$ (here 2 means two separable states, 3 means there is three biseparable state, 4 means four maximally entangled states), $(0, 9, 0)$, $(3, 0, 6)$ and $(1, 6, 2)$. There are other MUB sets for three qubits but one can get them by local transformations from the previous ones. In this paper we work with table $(3,0,6)$, line (6) in order to introduce our EWs. This table is given by

1	$(xyz)_\pi$	$\sigma_x II$	$I\sigma_y I$	$II\sigma_z$	$\sigma_x\sigma_y\sigma_z$	$\sigma_x\sigma_y I$	$\sigma_x I\sigma_z$	$I\sigma_y\sigma_z$
2	$(yzx)_\pi$	$\sigma_y II$	$I\sigma_z I$	$II\sigma_x$	$\sigma_y\sigma_z\sigma_x$	$\sigma_y\sigma_z I$	$\sigma_y I\sigma_x$	$I\sigma_z\sigma_x$
3	$(zxy)_\pi$	$\sigma_z II$	$I\sigma_x I$	$II\sigma_y$	$\sigma_z\sigma_x\sigma_y$	$\sigma_z\sigma_x I$	$\sigma_z I\sigma_y$	$I\sigma_x\sigma_y$
4	$(xxx)_{Gi}$	$\sigma_y\sigma_z\sigma_z$	$\sigma_z\sigma_y\sigma_z$	$\sigma_z\sigma_z\sigma_y$	$\sigma_y\sigma_y\sigma_y$	$\sigma_x\sigma_x I$	$\sigma_x I\sigma_x$	$I\sigma_x\sigma_x$
5	$(yyy)_G$	$\sigma_z\sigma_x\sigma_x$	$\sigma_x\sigma_z\sigma_x$	$\sigma_x\sigma_x\sigma_z$	$\sigma_z\sigma_z\sigma_z$	$\sigma_y\sigma_y I$	$\sigma_y I\sigma_y$	$I\sigma_y\sigma_y$
6	$(zzz)_G$	$\sigma_x\sigma_y\sigma_y$	$\sigma_y\sigma_x\sigma_y$	$\sigma_y\sigma_y\sigma_x$	$\sigma_x\sigma_x\sigma_x$	$\sigma_z\sigma_z I$	$\sigma_z I\sigma_z$	$I\sigma_z\sigma_z$
7	$(xzy)_G$	$\sigma_z\sigma_x\sigma_z$	$\sigma_y\sigma_x\sigma_x$	$\sigma_y\sigma_y\sigma_z$	$\sigma_z\sigma_y\sigma_x$	$\sigma_x\sigma_z I$	$\sigma_x I\sigma_y$	$I\sigma_z\sigma_y$
8	$(yxz)_G$	$\sigma_x\sigma_y\sigma_x$	$\sigma_z\sigma_y\sigma_y$	$\sigma_z\sigma_z\sigma_x$	$\sigma_x\sigma_z\sigma_y$	$\sigma_y\sigma_x I$	$\sigma_y I\sigma_z$	$I\sigma_x\sigma_z$
9	$(zyx)_G$	$\sigma_y\sigma_z\sigma_y$	$\sigma_x\sigma_z\sigma_z$	$\sigma_x\sigma_x\sigma_y$	$\sigma_y\sigma_x\sigma_z$	$\sigma_z\sigma_y I$	$\sigma_z I\sigma_x$	$I\sigma_y\sigma_x$

Table 1: Nine sets of operators defining a (3,0,6) MUB .

In this table three states

$$(xxx)_{Gi}, (yyy)_G, (zzz)_G \tag{A-iv}$$

can be reversibly converted into each other by local unitary operations (permutation), (i.e. $\sigma_y \to \sigma_z \to \sigma_x$), and e.g., if we construct EW using $(zzz)_G$ then this EW can be converted by another EW for $(xxx)_G$ state by applying the local unitary transformation $\sigma_z \to \sigma_x$.

Another states

$$(xzy)_G, (yxz)_G, (zyx)_G \tag{A-v}$$

can be transformed into each other by local unitary operations, e.g., for state $(xzy)_G$ we have

$$(xzy)_G = |n_x^1 n_z^2 n_y^3, \pm\rangle = (|n_x^1 n_z^2 n_y^3\rangle \pm |\bar{n}_x^1 \bar{n}_z^2 \bar{n}_y^3\rangle), \tag{A-vi}$$

we can convert the states (A-v) into other three maximally entangled states (A-iv) by the following local operations

$$U_{x\leftrightarrow z}=\frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix},\qquad U_{y\leftrightarrow x}=\begin{pmatrix}e^{\frac{i\pi}{4}} & 0\\ 0 & e^{-\frac{i\pi}{4}}\end{pmatrix},U_{y\leftrightarrow z}=\frac{1}{\sqrt{2}}\begin{pmatrix}1 & i\\ i & 1\end{pmatrix}.$$

where, we have applied the permutation $x\leftrightarrow z$ to the first qubit, $y\leftrightarrow x$ to the middle qubit and $y\leftrightarrow z$ to the rightmost qubit.

The above discussion was used for table $(3,0,6)$, but if we choose table $(2,3,4)$, we will obtain maximally entangled states $((xzy)_G,(yyz)_G,(yxy)_G,(zyx)_{Gi})$ so that, according to the following local operators and permutations we can convert the states (A-v) into other three maximally entangled states.

$(yyz)_G\rightarrow(yxy)_G$ with local operators $U(1)_{z\leftrightarrow x},U(2)_{y\leftrightarrow x},U(3)_{z\leftrightarrow y}$.(the notation $U(i)$ means that U acting on the (i)-th qubit)

$(xzy)_G\rightarrow(zyx)_{Gi}$ with permutation $(\sigma_x\rightarrow\sigma_z\rightarrow\sigma_y)$ only for first and second qubits and local operators $U(3)_{y\leftrightarrow x}$

$(xzy)_G\rightarrow(yyz)_G$ with local operators $U(1)_{x\leftrightarrow y},U(2)_{z\leftrightarrow y}$ and with permutation $(\sigma_y\rightarrow\sigma_z\rightarrow\sigma_x)$ for the rightmost qubit.

Appendix B

The following cases are used for construction of EWs:

$$r_4+r_5=2(p_3-p_4+p_5-p_6),r_6+r_7=2(-p_1+p_2+p_7-p_8)\qquad\text{(B-i)}$$

$$r_4-r_5=2(p_1-p_2+p_7-p_8),r_6-r_7=2(p_3-p_4-p_5+p_6)$$

$$r_4+r_6=2(p_3-p_4+p_7-p_8),r_5+r_7=2(-p_1+p_2+p_5-p_6)$$

$$r_4-r_6=2(p_1-p_2+p_5-p_6),r_5-r_7=2(p_3-p_4-p_7+p_8)$$

$$r_4+r_7=2(p_5-p_6+p_7-p_8),r_5+r_6=2(-p_1+p_2+p_3-p_4)$$

$$r_4 - r_7 = 2(p_1 - p_2 + p_3 - p_4), r_5 - r_6 = 2(p_5 - p_6 - p_7 + p_8).$$

We choose one the following cases for our EW:

$$1 + r_1 = 2(p_1 + p_2 + p_3 + p_4),\ 1 - r_1 = 2(p_5 + p_6 + p_7 + p_8) \tag{B-ii}$$

$$1 + r_2 = 2(p_1 + p_2 + p_5 + p_6),\ 1 - r_2 = 2(p_3 + p_4 + p_7 + p_8)$$

$$1 + r_3 = 2(p_1 + p_2 + p_7 + p_8),\ 1 - r_3 = 2(p_3 + p_4 + p_5 + p_6).$$

Proof for EWs detecting bound MUB-$(zzz)_G$ diagonal density matrices

For more detail, we have

$$Tr[W\rho_s] = A_0+A_1\cos\theta_3\cos\theta_2+\sin\theta_1\sin\theta_2\sin\theta_3(A_2\cos\varphi_1\cos(\varphi_2-\varphi_3)+A_3\sin\varphi_1\sin(\varphi_2+\varphi_3)).$$

Taking $\varphi_2=\varphi_3=\frac{\pi}{4}$, $\theta_1=\frac{\pi}{2}$

and according to relation $(-\sqrt{a^2+b^2}\leq a\sin\theta+b\cos\theta\leq\sqrt{a^2+b^2})$, we have

$$Tr[W\rho_s] = A_0+A_1\cos\theta_3\cos\theta_2\pm\sin\theta_2\sin\theta_3\sqrt{A_2^2+A_3^3},$$

according to $\cos\theta_3$, we obtain

$$Tr[W\rho_s] = A_0\pm\sqrt{A_1^2\cos{\theta_2}^2+\sin{\theta_2}^2(A_2^2+A_3^2)},$$

and from the condition $(A_2^2+A_3^2\geq A_1^2,\theta_2=\frac{\pi}{2})$, one can get

$$\Rightarrow Tr[W\rho_s] = A_0\pm\sqrt{A_2^2+A_3^2},$$

so , if

$$A_0=\sqrt{A_2^2+A_3^2},$$

$$Tr[W\rho_s]\geq 0,$$

$$W=\sqrt{A_2^2+A_3^2}III+A_1\quad I\sigma_z\sigma_z-A_2(\sigma_x\sigma_x\sigma_x+\sigma_x\sigma_y\sigma_y)+A_3(\sigma_y\sigma_x\sigma_y+\sigma_y\sigma_y\sigma_x),$$

then A_1 is an arbitrary number, therefore by taking $A_1=-\sqrt{A_2^2+A_3^2}$, we get

$$W=\sqrt{A_2^2+A_3^2}(III-\quad I\sigma_z\sigma_z-\frac{A_2}{\sqrt{A_2^2+A_3^2}}(\sigma_x\sigma_x\sigma_x+\sigma_x\sigma_y\sigma_y)+\frac{A_3}{\sqrt{A_2^2+A_3^2}}(\sigma_y\sigma_x\sigma_y+\sigma_y\sigma_y\sigma_x)).$$

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Figure Captions

Figure-1: Shows the feasible region in (p_1, p_2) plane defined by Eq.(2.12).

Figure-2: Shows the feasible region in (p_1, p_3) plane defined by Eq.(2.14).

Figure-3: The two colored triangles show the feasible region obtained by the condition $p_1 + p_3 = \frac{1}{2}$, where the light gray-colored triangle determines the region in (p_3, p_4) plane and (according to the PPT conditions) the dark gray-colored triangle indicates the region in (p_1, p_2) plane. The dotted line represents parametric equation (2.15) which has been drawn for two regions, i.e, from PPT conditions, dotted line in (p_3, p_4) plane corresponds to the dotted line in (p_1, p_2) plane.

Figure-4: The gray-colored triangle shows the region of bound entangled states in (p_1, p_2, p_3) phase space and thick line shows the region of separable states.

Figure-5:(a): Perspective of the region of bound entangled states in (p_1, p_3) plane obtained by numerical analysis. (b): Perspective of the region of bound entangled states in (p_2, p_4) plane obtained by numerical results. (c): Perspective of the region of bound entangled states in (p_5, p_6) plane obtained by numerical analysis. (d): Perspective of the region of bound entangled states in (p_7, p_8) plane obtained by numerical analysis.

Figure-6:.(a): Perspective of the region of bound entangled states in (p_1, p_3, p_5) phase space obtained by numerical analysis. (b): Perspective of the region of bound entangled states in (p_2, p_4, p_8) phase space obtained by numerical analysis. (c): Perspective of the region of bound entangled states in (p_6, p_7) plane obtained by numerical analysis.