Investigating a class of $2\otimes2\otimes d$ bound entangled density matrices via linear and nonlinear entanglement witnesses constructed by exact convex optimization

M. A. Jafarizadeh,[1,2,3,*] Y. Akbari,[1,2,†] K. Aghayar,[1,‡] A. Heshmati,[1,§] and M. Mahdian[1,∥]
[1]*Department of Theoretical Physics and Astrophysics, University of Tabriz, Tabriz 51664, Iran*
[2]*Institute for Studies in Theoretical Physics and Mathematics, Tehran 19395-1795, Iran*
[3]*Research Institute for Fundamental Sciences, Tabriz 51664, Iran*
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Here we consider a class of $2\otimes2\otimes d$ density matrices which have positive partial transposes with respect to all subsystems. The entanglement witness approach is used to investigate the entanglement of these density matrices. To demonstrate the approach, the three-qubit case is considered in detail. For constructing entanglement witnesses (EWs) detecting these density matrices, we attempt to convert the problem to an exact convex optimization problem. To this aim, we map the convex set of separable states into a convex region, named feasible region, and consider the cases in which the exact geometrical shape of the feasible region can be obtained. In this way, various linear and nonlinear EWs are constructed. The optimality and decomposability of some of the introduced EWs are also considered. Furthermore, the detection of the density matrices by the introduced EWs are discussed analytically and numerically.

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I. INTRODUCTION

Bound entangled states, states with positive partial transposes with respect to all subsystems, are of great importance in quantum information processes [1–5]. One class of bound entangled states is the three-qubit states considered in [6] where the authors have used a separability criterion due to Horodecki to show the boundness of such states. The boundness of these states for some range of parameters is also investigated in [7] using entanglement witnesses (EWs) and in [8] from the perspective of convex optimization. Another class of three-qubit bound entangled states has been discussed in [9] again by using EWs. The EWs are of special interest since it has been proved that for any entangled state there exists at least one EW detecting it. The EWs are Hermitian operators which have non-negative expectation values over all separable states while they have negative expectation values over, that is, they are able to detect, some entangled states [10,11].

In this paper, first we consider a generalized form of the above bound entangled states for the $2\otimes2\otimes2$ case and use EWs approach to analyze their entanglement. As these states are 8×8 matrices like a chessboard, hereafter we will refer to them as chessboard density matrices. Then we extend them for the $2\otimes2\otimes d$ case and also refer to them as chessboard density matrices for simplicity. For constructing the relevant EWs, we attempt to convert the problem to an exact convex optimization problem. This method is general and one can apply it for multiqubits in a similar way. Just with a few changes in notation, all of the $2\otimes2\otimes2$ witnesses constructed in this way are also applicable in the $2\otimes2\otimes d$ case. As the dimension d of the third subsystem increases, the number and categories of EWs increase while the procedure is the same in general. Convex optimization techniques have been widely used in quantum information problems recently [12–23]. In Refs. [24–28] the problem of constructing EWs was converted to a linear programming problem, a special case of a convex optimization problem, exactly or approximately. To this aim, the convex set of separable states was mapped into a convex region, named feasible region (FR). The FR may be a polygon by itself or it may not. When FR was not a polygon, it was approximated by a polygon. In this way, the problem was converted to a linear programming problem whose linear constraints came from the exact or approximated boundary surfaces of FR.

Here we consider the cases that the geometrical shape of FR can be obtained exactly and hence convert the problem to an exact convex optimization problem. Any hyperplane tangent to the FR corresponds to a linear EW. According to the geometrical shape of FR, we can or cannot construct nonlinear EWs. It is shown that when the geometrical shape of FR is a polygon, all EWs are linear; otherwise it is possible to construct nonlinear EWs. In the previous works where a nonpolygonal FR was approximated by a polygonal one, the number of obtained linear EWs was not sufficient for constructing nonlinear EWs. However, in the present work where we consider the exact geometrical shape of a nonpolygonal FR, any hyperplane tangent to the surface of FR is a linear EW. Therefore, there exist innumerable linear EWs which are enough for constructing a nonlinear EW as the envelope of linear functionals arising from them. By construction, a nonlinear EW plays the role of innumerable linear EWs as a whole and hence it may detect bound entangled states. Our approach is typical and can be applied in all cases where the exact geometrical shape of FR is known.

The paper is organized as follows. In Sec. II, we review the basic notions and definitions of EWs relevant to our study and describe our approach of constructing EWs. Then we present a generalized form of a class of three-qubit den-

*jafarizadeh@tabrizu.ac.ir
†akbari@tabrizu.ac.ir
‡aghayar@tabrizu.ac.ir
§heshmati@tabrizu.ac.ir
∥mahdian@tabrizu.ac.ir

sity matrices of [6]. In Sec. III, we consider the construction of linear and nonlinear EWs that can detect the mentioned density matrices. Section IV is devoted to an analysis of optimality of the introduced EWs. It is proved that some of the introduced EWs are optimal. In Sec. V, we consider the detection of a mentioned density matrix by introducing EWs analytically and numerically. Section VI is devoted to the comparison of our results with those of the other works. In Sec. VII, we extend the three-qubit case to the $2\otimes 2\otimes d$ case and we show that the method is general and one can also apply it for multipartite chessboard density matrices. This extension neither changes the structure of positive partial transpose (PPT) conditions nor the structure of EWs. In Sec. VIII, we analyze the detection ability of the introduced EWs for $2\otimes 2\otimes 2$ and $2\otimes 2\otimes 3$ chessboard density matrices numerically.

II. PRELIMINARIES

A. A class of three-qubit density matrices with positive partial transposes

Here we consider a generalized form of a class of three-qubit density matrices presented in [6],

$$\rho=\frac{1}{n}\begin{pmatrix} a & 0 & 0 & 0 & 0 & 0 & 0 & r_1e^{i\varphi_1} \\ 0 & b & 0 & 0 & 0 & 0 & r_2e^{i\varphi_2} & 0 \\ 0 & 0 & c & 0 & 0 & r_3e^{i\varphi_3} & 0 & 0 \\ 0 & 0 & 0 & d & r_4e^{i\varphi_4} & 0 & 0 & 0 \\ 0 & 0 & 0 & r_4e^{-i\varphi_4} & \frac{1}{d} & 0 & 0 & 0 \\ 0 & 0 & r_3e^{-i\varphi_3} & 0 & 0 & \frac{1}{c} & 0 & 0 \\ 0 & r_2e^{-i\varphi_2} & 0 & 0 & 0 & 0 & \frac{1}{b} & 0 \\ r_1e^{-i\varphi_1} & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{a} \end{pmatrix}, \tag{2.1}$$

where a,b,c,d are non-negative parameters, $0\leqslant r_i\leqslant 1$ for $i=1,2,3,4$, and $n=(a+b+c+d+\frac{1}{a}+\frac{1}{b}+\frac{1}{c}+\frac{1}{d})$. It is easy to see that this density matrix has positive partial transposes with respect to all subsystems, i.e., it is a PPT state. The density matrix of [6] is a special case of ρ where $\varphi_1=0$, $r_1=1$, $r_2=r_3=r_4=0$, and $a=1$. We want to show that for some values of the parameters, ρ is a PPT entangled state. To this aim, we will construct various linear and nonlinear nondecomposable EWs that are able to detect it.

Written in the Pauli matrices basis, ρ has the form

$$\begin{aligned}\rho=\frac{1}{8}[&III+r_{300}\sigma_zII+r_{030}I\sigma_zI+r_{003}II\sigma_z+r_{330}\sigma_z\sigma_zI\\&+r_{303}\sigma_zI\sigma_z+r_{033}I\sigma_z\sigma_z+r_{333}\sigma_z\sigma_z\sigma_z+r_{111}\sigma_x\sigma_x\sigma_x\\&+r_{112}\sigma_x\sigma_x\sigma_y+r_{121}\sigma_x\sigma_y\sigma_x+r_{211}\sigma_y\sigma_x\sigma_x+r_{122}\sigma_x\sigma_y\sigma_y\\&+r_{212}\sigma_y\sigma_x\sigma_y+r_{221}\sigma_y\sigma_y\sigma_x+r_{222}\sigma_y\sigma_y\sigma_y],\end{aligned} \tag{2.2}$$

where the coefficients r_{ijk} are given in Appendix B. We will try to construct our nondecomposable EWs by using Pauli group operators appearing in the ρ. But before this, let us review the basic notions and definitions of EWs relevant to our study.

B. Entanglement witnesses

Let us first recall the definition of entanglement and separability [29]. By definition, an n-partite quantum mixed state $\rho\in\mathcal{B}(\mathcal{H})$ (the Hilbert space of bounded operators acting on the Hilbert space $\mathcal{H}=\mathcal{H}_{d_1}\otimes\cdots\otimes\mathcal{H}_{d_n}$) is called fully separable if it can be written as a convex combination of pure product states, that is,

$$\rho=\sum_i p_i|\alpha_i^{(1)}\rangle\langle\alpha_i^{(1)}|\otimes|\alpha_i^{(2)}\rangle\langle\alpha_i^{(2)}|\otimes\cdots\otimes|\alpha_i^{(n)}\rangle\langle\alpha_i^{(n)}|, \tag{2.3}$$

where $|\alpha_i^{(j)}\rangle$ are arbitrary but normalized vectors lying in the $\mathcal{H}_{d_j}$, and $p_i\geqslant 0$ with $\Sigma_i p_i=1$. Otherwise, ρ is called entangled. Throughout the paper, by separability we mean fully separable.

An entanglement witness (EW) W is a Hermitian operator which has non-negative expectation value over all separable states ρ_s and its expectation value over, at least, one entangled state ρ_e is negative. The existence of an EW for any entangled state is a direct consequence of the Hahn-Banach theorem [30] and the fact that the subspace of separable density operators is convex and closed.

Based on the notion of partial transpose map, the EWs are classified into two classes: decomposable (d-EW) and nondecomposable (nd-EW). An EW W is called decomposable if there exist positive operators $\mathcal{P}$, $\mathcal{Q}_K$ such that

$$W=\mathcal{P}+\sum_{K\subset\mathcal{N}}\mathcal{Q}_K^{T_K}, \tag{2.4}$$

where $\mathcal{N}:=\{1,2,3,\ldots,n\}$ and T_K denotes the partial transpose with respect to partite $K\subset\mathcal{N}$ and it is nondecomposable if it cannot be written in this form [31]. Clearly, d-EWs cannot 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 an nd-EW.

A nonlinear EW associated to an entangled density matrix ϱ is simply a nonlinear functional of ϱ such that it is nonnegative valued over all separable states, but has negative value over the density matrix ϱ. A nonlinear EW can be viewed as the envelope of a set of linear functionals $\mathrm{Tr}(W\varrho)$ that arise from the corresponding linear EWs W.

Usually one is interested in finding EWs W which detect entangled states in an optimal way. An EW W is called an optimal EW if there exists no other EW which detects more entangled states than W. It is shown that the necessary and sufficient condition for optimality of an EW W is that there exist no positive operator $\mathcal{P}$ and $\epsilon>0$ such that $W'=W-\epsilon\mathcal{P}$ be again an EW [32].

C. Constructing EWs via exact convex optimization

Let us consider a set of given Hermitian operators Q_i. By using these operators, we will attempt to construct various linear and nonlinear EWs. To this aim, for any separable state ρ_s we introduce the maps

$$P_i=\mathrm{Tr}(Q_i\rho_s), \tag{2.5}$$

which map the convex set of separable states into a convex region named the feasible region (FR). Any hyperplane tangent to the FR corresponds to a linear EW, since such hyperplanes separate the FR from entangled states. Hence, we need to determine the geometrical shape of FR. In general, determining the geometrical shape of FR is a difficult task. However, one may choose the Hermitian operators Q_i in such a way that the exact geometrical shape of FR can be obtained rather simply. By such a choice, when the FR is a polygon, its surface corresponds to linear EWs which are linear combinations of the operators Q_i; otherwise, linear EWs come from any hyperplane tangent to the surface of FR. When the FR is not a polygon, besides the linear EWs it is possible to obtain nonlinear EWs for the given density matrix.

To obtain the geometrical shape of FR, we note that every separable mixed state ρ_s can be written as a convex combination of pure product states, so the subspace of separable states $\mathcal{S}$ can be considered as a convex hull of the set of all pure product states $\mathcal{D}$. Thus first we specify the geometrical shape of a region obtained from mapping of $\mathcal{D}$ under the P_i's. If the resulted region is convex by itself, we get the FR, otherwise we have to take the convex hull of that region as FR.

In this paper, the operators Q_i are chosen as linear combinations of Hermitian operators in the Pauli group $\mathcal{G}_n$, a group consisting of tensor products of the identity I_2 and the usual Pauli matrices σ_x,σ_y and σ_z together with an overall phase ±1 or $\pm i$ [33–35].

III. CLASS OF THREE-QUBIT EWS

In this section, we want to introduce various nd-EWs for the density matrix ρ of Eq. (2.1). To simplify the analysis, let us classify these EWs according to the shape of relevant FRs: polygonal, conical, cylindrical, and spherical. Hereafter, we will use the following notation for the three-qubit Pauli group operators:

$$O_{ijk}=\sigma_i\otimes\sigma_j\otimes\sigma_k,\quad i,j,k=0,1,2,3, \tag{3.1}$$

where σ_0, σ_1, σ_2, and σ_3 stand for the 2×2 identity matrix I_2 and single qubit Pauli matrices σ_x, σ_y, and σ_z, respectively. Let us begin with the polygonal case.

A. EWs with polygonal FR

Let us consider the following operators:

$$Q_1^{\mathrm{Po}}=O_{333},\quad Q_2^{\mathrm{Po}}=O_{111}+(-1)^iO_{122},$$

$$Q_3^{\mathrm{Po}}=O_{212}+(-1)^{i+1}O_{221},\quad i=0,1,$$

and try to construct nd-EWs from them for detecting ρ. To this end, we define the maps

$$P_j=\mathrm{Tr}(Q_j^{\mathrm{Po}}|\alpha\rangle|\beta\rangle|\gamma\rangle\langle\alpha|\langle\beta|\langle\gamma|),\quad j=1,2,3$$

for any pure product state $|\alpha\rangle|\beta\rangle|\gamma\rangle$. In this case, the FR is a polygon whose boundary planes are as follows:

$$(-1)^{j_1}P_1+(-1)^{j_2}P_2+(-1)^{j_3}P_3=1,\quad (j_1,j_2,j_3)\in\{0,1\}^3 \tag{3.2}$$

(for a proof, see Appendix A). These planes can be rewritten as

$$\min_{|\alpha\rangle|\beta\rangle|\gamma\rangle}\mathrm{Tr}([III-(-1)^{j_1}Q_1^{\mathrm{Po}}-(-1)^{j_2}Q_2^{\mathrm{Po}}-(-1)^{j_3}Q_3^{\mathrm{Po}}]|\alpha\rangle|\beta\rangle|\gamma\rangle \times\langle\alpha|\langle\beta|\langle\gamma|)=0.$$

It is seen that the operators in brackets have non-negative expectation values over all pure product states, hence they give rise to the following linear EWs:

$$\begin{aligned}{}^1W^{\mathrm{Po}}_{i_1i_2i_3i_4}=III&+(-1)^{i_1}O_{333}+(-1)^{i_2}O_{111}+(-1)^{i_3}O_{122}\\&+(-1)^{i_4}O_{212}+(-1)^{i_2+i_3+i_4+1}O_{221},\end{aligned} \tag{3.3}$$

where $(i_1,i_2,i_3,i_4)\in\{0,1\}^4$. Besides the above 16 EWs, we can construct other 16 EWs by using the fact that local unitary operators take an EW to another EW. For this purpose, we enact the phase-shift gate

$$M=\begin{pmatrix}1&0\\0&i\end{pmatrix}$$

locally on the first qubit which takes $\sigma_x\to\sigma_y$, $\sigma_y\to-\sigma_x$, and $\sigma_z\to\sigma_z$ under conjugation, and get

$$^{2}W^{\rm Po}_{i_1i_2i_3i_4}=MII(W^{\rm Po}_{i_1i_2i_3i_4})M^{\dagger}II=III+(-1)^{i_1}O_{333}+(-1)^{i_2}O_{111}+(-1)^{i_3}O_{122}+(-1)^{i_4+1}O_{212}+(-1)^{i_2+i_3+i_4}O_{221}. \quad (3.4)$$

We could replace $Q_1^{\rm Po}$ with the operator $\sigma_z\sigma_z I$ or any cyclic permutation of it, but since these lead to d-EWs we do not consider such cases here. In this way, we have constructed 32 linear EWs with polygonal FR.

B. EWs with conical FR

For this case, we consider the following Hermitian operators:

$$Q_1^{\rm Co}=O_{k'j'l'},\quad Q_2^{\rm Co}=O_{111}+(-1)^iO_{kjl},$$

$$Q_3^{\rm Co}=O_{lkj}+(-1)^iO_{jlk},\quad i=0,1,$$

where $k'j'l'$ is one of the triples 333, 330, 303, 033, and kjl is one of the triples 122, 212, 221. Now we try to determine the exact shape of the FR. The FR is a cone given by

$$(1\pm P_1)^2=P_2^2+P_3^2 \quad (3.5)$$

(for a proof, see Appendix A), where

$$P_j=\mathrm{Tr}(Q_j^{\rm Co}|\alpha\rangle|\beta\rangle|\gamma\rangle\langle\alpha|\langle\beta|\langle\gamma|),\quad j=1,2,3.$$

We assert that any plane tangent to the FR corresponds to an EW. To show this, we maximize the function

$$f(P_1,P_2,P_3)=A_1P_1+A_2P_2+A_3P_3, \quad (3.6)$$

where A_i are real parameters, under the constraint (3.5). This is a convex optimization problem since the function and its constraint are both convex functions. Using the Lagrange multiplier method shows that this maximum is $\pm A_1$ provided that $A_1^2=A_2^2+A_3^2$. It is easy to see that the plane $A_1P_1+A_2P_2+A_3P_3=\pm A_1$ is tangent to the surface (3.5) at the point $(-A_1\pm 1,A_2,A_3)$. This plane can be rewritten as

$$\min_{|\alpha\rangle|\beta\rangle|\gamma\rangle}\mathrm{Tr}\{[A_1III\pm A_1Q_1^{\rm Co}\pm(A_2Q_2^{\rm Co}+A_3Q_3^{\rm Co})]|\alpha\rangle|\beta\rangle|\gamma\rangle\langle\alpha|\times\langle\beta|\langle\gamma|\}=0.$$

Thus the operator

$$W_{\pm}^{\rm Co}=A_1III\pm A_1Q_1^{\rm Co}\pm(A_2Q_2^{\rm Co}+A_3Q_3^{\rm Co})$$

has a non-negative expectation value over all pure product states, hence it can be a linear EW. By defining $\cos\psi=\frac{A_2}{A_1}$ and $\sin\psi=\frac{A_3}{A_1}$, $W_{\pm}^{\rm Co}$ is rewritten as

$$^{k'j'l'}W^{\rm Co}_{kjl,i\pm}=III\pm O_{k'j'l'}+\cos\psi[O_{111}+(-1)^iO_{kjl}]+\sin\psi[O_{lkj}+(-1)^iO_{jlk}], \quad (3.7)$$

where $i=0,1$. Now we obtain nonlinear functionals of ρ, hence nonlinear EWs, by optimizing $\mathrm{Tr}[(^{k'j'l'}W^{\rm Co}_{kjl,i\pm})\rho]$ with an appropriate choice of the parameter ψ as a functional of ρ. We note that

$$\mathrm{Tr}[(^{k'j'l'}W^{\rm Co}_{kjl,i\pm})\rho]=1\pm r_{k'j'l'}+\cos\psi[r_{111}+(-1)^ir_{kjl}]+\sin\psi[r_{lkj}+(-1)^ir_{jlk}].$$

By defining

$$\cos\eta=\frac{r_{111}+(-1)^ir_{kjl}}{\sqrt{[r_{111}+(-1)^ir_{kjl}]^2+[r_{lkj}+(-1)^ir_{jlk}]^2}},$$

$\mathrm{Tr}[(^{k'j'l'}W^{\rm Co}_{kjl,i\pm})\rho]$ can be rewritten as

$$\mathrm{Tr}[(^{k'j'l'}W^{\rm Co}_{kjl,i\pm})\rho]=1\pm r_{k'j'l'}+\sqrt{[r_{111}+(-1)^ir_{kjl}]^2+[r_{lkj}+(-1)^ir_{jlk}]^2}\cos(\psi-\eta),$$

which takes its minimum value for $\psi-\eta=\pi$.

$$^{k'j'l'}F^{\rm Co}_{kjl,i\pm}(\rho)=\min\mathrm{Tr}[(^{k'j'l'}W^{\rm Co}_{kjl,i\pm})\rho]=1\pm r_{k'j'l'}-\sqrt{[r_{111}+(-1)^ir_{kjl}]^2+[r_{lkj}+(-1)^ir_{jlk}]^2}. \quad (3.8)$$

These are the required nonlinear functionals, hence nonlinear EWs, associated with ρ. It is seen that the number of such nonlinear EWs is 48.

We can obtain other 48 linear EWs from $^{k'j'l'}W^{\rm Co}_{kjl,i\pm}$ by conjugating them with MII. This gives further 48 nonlinear EWs of the conical case as follows:

$$^{k'j'l'}F'^{\rm Co}_{kjl,i\pm}(\rho)=\min\mathrm{Tr}[MII(^{k'j'l'}W^{\rm Co}_{kjl,i\pm})M^{\dagger}II\rho]=1\pm r_{k'j'l'}-\sqrt{[r_{222}+(-1)^ir_{kjl}]^2+[r_{lkj}+(-1)^ir_{jlk}]^2}. \quad (3.9)$$

Here kjl is one of the triples 211, 121, and 112.

In this way, we have constructed 96 nonlinear EWs with conical FR.

C. EWs with cylindrical FR

The second type of nonlinear EWs for ρ can be derived by considering the following operators:

$$Q_1^{\rm Cy}=O_{k'j'l'},\quad Q_2^{\rm Cy}=O_{111}+(-1)^iO_{kjl},$$

$$Q_3^{\mathrm{Cy}} = O_{lkj} + (-1)^{i+1} O_{jlk}, \quad i = 0,1,$$

where $k'j'l'$ is one of the triples 300,030,003, and kjl is one of the triples 122,212,221. It can be shown that the FR has the cylindrical shape

$$P_1^2 + (P_2 + P_3)^2 = 1. \tag{3.10}$$

The maximum value of the function (3.6) under the constraint (3.10) is $\sqrt{A_1^2+A_2^2}$ provided that $A_2=A_3$ and this leads to the linear EWs

$$^{k'j'l'}W^{\mathrm{Cy}}_{kjl;i_1i_2} = III + (\cos\psi)O_{k'j'l'} + \sin\psi[O_{111} + (-1)^{i_1}O_{kjl} + (-1)^{i_2}O_{lkj} + (-1)^{i_1+i_2+1}O_{jlk}]. \tag{3.11}$$

where $\cos\psi=A_1/\sqrt{A_1^2+A_2^2}$ and $i_1,i_2=0,1$. Similar arguments as above show that $^{k'j'l'}W^{\mathrm{Cy}}_{kjl;i_1i_2}$ give rise to nonlinear EWs for ρ as follows:

$$^{k'j'l'}F^{\mathrm{Cy}}_{kjl;i_1i_2}(\rho) = \min \mathrm{Tr}[(^{k'j'l'}W^{\mathrm{Cy}}_{kjl;i_1i_2})\rho] = 1 - \sqrt{r^2_{k'j'l'} + [r_{111} + (-1)^{i_1}r_{kjl} + (-1)^{i_2}r_{lkj} + (-1)^{i_1+i_2+1}r_{jlk}]^2}. \tag{3.12}$$

The number of these nonlinear EWs is 36. We obtain other 36 nonlinear EWs of this type by conjugating $^{k'j'l'}W^{\mathrm{Cy}}_{kjl,i_1i_2}$ with MII as follows:

$$^{k'j'l'}F^{\mathrm{Cy}}_{kjl;i_1i_2}(\rho) = \min \mathrm{Tr}[MII(^{k'j'l'}W^{\mathrm{Cy}}_{kjl,i_1i_2})M^\dagger II\rho] = 1 - \sqrt{r^2_{k'j'l'} + [r_{222} + (-1)^{i_1}r_{kjl} + (-1)^{i_2}r_{lkj} + (-1)^{i_1+i_2+1}r_{jlk}]^2}. \tag{3.13}$$

Here kjl is one of the triples 211, 121, and 112, and $i_1,i_2=0,1$. In this way, we have constructed 72 nonlinear EWs with cylindrical FR.

D. EWs with spherical FR

The third type of nonlinear EWs for ρ follows from the operators

$$Q_1^{\mathrm{Sp}} = O_{k'j'l'}, \quad Q_2^{\mathrm{Sp}} = O_{111} + (-1)^i O_{kjl},$$

$$Q_3^{\mathrm{Sp}} = O_{lkj} + (-1)^i O_{jlk}, \quad i = 0,1,$$

where $k'j'l'$ is one of the triples 300, 030, 003, and kjl is one of the triples 122, 212, 221. In this case, the FR is of spherical shape

$$P_1^2 + P_2^2 + P_3^2 = 1. \tag{3.14}$$

The maximum value of the function (3.6) under the constraint (3.14) is $\sqrt{A_1^2+A_2^2+A_3^2}$ and this leads to the linear EWs

$$^{k'j'l'}W^{\mathrm{Sp}}_{kjl,i} = III + (\sin\eta\cos\zeta)O_{k'j'l'} + \sin\eta\sin\zeta[O_{111} + (-1)^i O_{kjl}] + \cos\eta[O_{lkj} + (-1)^i O_{jlk}], \tag{3.15}$$

where

$$\sin\eta\cos\zeta = \frac{A_1}{\sqrt{A_1^2+A_2^2+A_3^2}}, \quad \sin\eta\sin\zeta = \frac{A_2}{\sqrt{A_1^2+A_2^2+A_3^2}}, \quad \cos\eta = \frac{A_3}{\sqrt{A_1^2+A_2^2+A_3^2}}.$$

The 18 nonlinear EWs which correspond to $^{k'j'l'}W^{\mathrm{Sp}}_{kjl,i}$ are

$$^{k'j'l'}F^{\mathrm{Sp}}_{kjl;i}(\rho) = \min \mathrm{Tr}[(^{k'j'l'}W^{\mathrm{Sp}}_{kjl,i})\rho] = 1 - \sqrt{r^2_{k'j'l'} + [r_{111} + (-1)^i r_{kjl}]^2 + [r_{lkj} + (-1)^i r_{jlk}]^2}. \tag{3.16}$$

We obtain other 18 nonlinear EWs of this type by conjugating $^{k'j'l'}W^{\mathrm{Sp}}_{kjl,i}$ with MII as follows:

$$^{k'j'l'}F^{\mathrm{Sp}}_{kjl;i}(\rho) = \min \mathrm{Tr}[MII(^{k'j'l'}W^{\mathrm{Sp}}_{kjl,i})M^\dagger II\rho] = 1 - \sqrt{r^2_{k'j'l'} + [r_{222} + (-1)^i r_{kjl}]^2 + [r_{lkj} + (-1)^i r_{jlk}]^2}. \tag{3.17}$$

Here kjl is one of the triples 211, 121, and 112. In this way, we have constructed 36 nonlinear EWs with spherical FR.

IV. OPTIMALITY OF THE EWS

In this section we discuss the optimality of the EWs introduced so far. Let us recall that if there exist $\epsilon>0$ and a positive operator $\mathcal{P}$ such that $W'=W-\epsilon\mathcal{P}$ be again an EW, the EW W is not optimal, otherwise it is. Every positive operator can be expressed as a sum of pure projection operators with positive coefficients, i.e., $\mathcal{P}=\sum_i\lambda_i|\psi_i\rangle\langle\psi_i|$ with all $\lambda_i\geqslant 0$, so we can take $\mathcal{P}$ as pure projection operator $\mathcal{P}=|\psi\rangle\langle\psi|$. If W' is to be an EW, then $|\psi\rangle$ must be orthogonal to all pure product states that the expectation value of W over them is zero. The eigenstates of each three-qubit Pauli group operator can be chosen as pure product states, half with eigenvalue +1 and the other half with eigenvalue −1. In EWs introduced so far, there exists no pair of locally commuting Pauli group operators, so the expectation value of such Pauli group operators vanishes over the pure product eigenstates of one of them. Regarding the above facts, we are now ready to discuss the optimality of introduced EWS.

A. Optimality of EWs with polygonal FR

Let us begin with EWs of Eq. (3.3). We discuss two cases $i_1=0$ and $i_1=1$ separately. For the case $i_1=0$, note that we can take the pure product states

$$|z;+\rangle|z;+\rangle|z;+\rangle, \quad |z;+\rangle|z;-\rangle|z;-\rangle,$$

$$|z;-\rangle|z;+\rangle|z;-\rangle, \quad |z;-\rangle|z;-\rangle|z;+\rangle, \tag{4.1}$$

as eigenstates of the operator $\sigma_z\sigma_z\sigma_z$ with eigenvalue +1 and the following ones:

$$|z;+\rangle|z;+\rangle|z;-\rangle, \quad |z;+\rangle|z;-\rangle|z;+\rangle,$$

$$|z;-\rangle|z;+\rangle|z;+\rangle, \quad |z;-\rangle|z;-\rangle|z;-\rangle, \tag{4.2}$$

as eigenstates with eigenvalue −1. The EWs $W^{\mathrm{Po}}_{0i_2i_3i_4}$ have zero expectation values over the states of Eq. (4.2), so if there exists a pure projection operator $|\psi\rangle\langle\psi|$ that can be subtracted from EWs $W^{\mathrm{Po}}_{0i_2i_3i_4}$, the state $|\psi\rangle$ ought to be of the form

$$|\psi\rangle = a_{+++}|z;+\rangle|z;+\rangle|z;+\rangle + a_{+--}|z;+\rangle|z;-\rangle|z;-\rangle + a_{-+-}|z;-\rangle|z;+\rangle|z;-\rangle + a_{--+}|z;-\rangle|z;-\rangle|z;+\rangle. \tag{4.3}$$

Expectation values of $W^{\mathrm{Po}}_{00i_3i_4}$ over pure product eigenstates of the operator $\sigma_x\sigma_x\sigma_x$ with eigenvalue −1 are zero, so $|\psi\rangle$ should be orthogonal to these eigenstates. Applying the orthogonality constraints gives the following equations:

$$\langle x;+|\langle x;+|\langle x;-||\psi\rangle = \frac{1}{2\sqrt{2}}(a_{+++}-a_{+--}-a_{-+-}+a_{--+})=0,$$

$$\langle x;+|\langle x;-|\langle x;+||\psi = \frac{1}{2\sqrt{2}}(a_{+++}-a_{+--}+a_{-+-}-a_{--+})=0,$$

$$\langle x;-|\langle x;+|\langle x;+||\psi\rangle = \frac{1}{2\sqrt{2}}(a_{+++}+a_{+--}-a_{-+-}-a_{--+})=0,$$

$$\langle x;-|\langle x;-|\langle x;-||\psi\rangle = \frac{1}{2\sqrt{2}}(a_{+++}+a_{+--}+a_{-+-}+a_{--+})=0.$$

The solution of this system of four linear equations is $a_{++}=a_{+-}=a_{-+-}=a_{-+}=0$. Thus $|\psi\rangle=0$; that is, there exists no pure projection operator $|\psi\rangle\langle\psi|$, hence no positive operator $\mathcal{P}$, which can be subtracted from $W^{\mathrm{Po}}_{00i_3i_4}$ and leave them EWs again. So the EWs $W^{\mathrm{Po}}_{00i_3i_4}$ are optimal. Similar argument proves the optimality of EWs $W^{\mathrm{Po}}_{01i_3i_4}$.

As for EWs $W^{\mathrm{Po}}_{1i_2i_3i_4}$, the state $|\psi\rangle$ (if it exists) ought to be of the form

$$|\psi\rangle = a_{++-}|z;+\rangle|z;+\rangle|z;-\rangle + a_{+-+}|z;+\rangle|z;-\rangle|z;+\rangle + a_{-++}|z;-\rangle|z;+\rangle|z;+\rangle + a_{---}|z;-\rangle|z;-\rangle|z;-\rangle. \tag{4.4}$$

The same argument as above shows the impossibility of the existence of such $|\psi\rangle$. Therefore, the EWs $W^{\mathrm{Po}}_{1i_2i_3i_4}$ are also optimal.

B. Optimality of EWs with conical FR

The optimality of EWs ${}^{330}W^{\mathrm{Co}}_{122,i\pm}$ has been proved in [36], so we talk about the optimality of EWs ${}^{333}W^{\mathrm{Co}}_{122,i\pm}$. Let us first find pure product states that the expectation value of ${}^{333}W^{\mathrm{Co}}_{122,i\pm}$ over them vanishes. For this purpose, we consider a pure product state as follows:

$$|\nu\rangle = \bigotimes_{j=1}^{3}\left[\cos\left(\frac{\theta_j}{2}\right)|z;+\rangle + \exp(i\varphi_j)\sin\left(\frac{\theta_j}{2}\right)|z;-\rangle\right], \tag{4.5}$$

and attempt to choose parameters θ_j and φ_j such that $\mathrm{Tr}[({}^{333}W^{\mathrm{Co}}_{122,i\pm})|\nu\rangle\langle\nu|]=0$. By direct calculation, this trace is

$$\begin{aligned}\mathrm{Tr}[({}^{333}W^{\mathrm{Co}}_{122,i\pm})|\nu\rangle\langle\nu|] = 1 &\pm \cos\theta_1\cos\theta_2\cos\theta_3 \\ &+ \sin\theta_1\sin\theta_2\sin\theta_3 \\ &\times\{\cos\psi\cos\varphi_1\cos[\varphi_2+(-1)^{i+1}\varphi_3] \\ &+ \sin\psi\sin\varphi_1\sin[\varphi_2+(-1)^{i}\varphi_3]\}.\end{aligned} \tag{4.6}$$

It is easy to see that the following four choices of parameters θ_j and φ_j lead to zero value for the trace of ${}^{333}W^{\mathrm{Co}}_{122,0\pm}$:

$$|\nu_{1+}\rangle: \quad \theta_2=\theta_3=\frac{\pi}{2}, \quad \theta_1=\frac{3\pi}{2}, \quad \varphi_1=\psi, \quad \varphi_2=\varphi_3=\frac{\pi}{4},$$

$$|\nu_{2+}\rangle: \quad \theta_1=\theta_3=\frac{\pi}{2}, \quad \theta_2=\frac{3\pi}{2}, \quad \varphi_1=\psi, \quad \varphi_2=\varphi_3=\frac{\pi}{4},$$

$$|\nu_{3+}\rangle: \quad \theta_2=\theta_3=\frac{\pi}{2}, \quad \theta_1=\frac{3\pi}{2}, \quad \varphi_1=-\psi, \quad \varphi_2=\varphi_3=-\frac{\pi}{4},$$

$$|\nu_{4+}\rangle: \quad \theta_1=\theta_3=\frac{\pi}{2}, \quad \theta_2=\frac{3\pi}{2}, \quad \varphi_1=-\psi, \quad \varphi_2=\varphi_3=-\frac{\pi}{4}.$$

For ${}^{333}W^{\mathrm{Co}}_{122,0+}$, the state $|\psi\rangle$ (if it exists) must be of the form (4.3) and be orthogonal to the above four states, i.e.,

$$\langle\nu_{1+}|\psi\rangle=\frac{1}{2\sqrt{2}}\left\{-a_{+++}+ia_{+--}+\exp\left[-i\left(\psi+\frac{\pi}{4}\right)\right]\times(a_{-+-}+a_{--+})\right\}=0,$$

$$\langle\nu_{2+}|\psi\rangle=\frac{1}{2\sqrt{2}}\left\{-a_{+++}-ia_{+--}-\exp\left[-i\left(\psi+\frac{\pi}{4}\right)\right]\times(a_{-+-}-a_{--+})\right\}=0,$$

$$\langle\nu_{3+}|\psi\rangle=\frac{1}{2\sqrt{2}}\left\{-a_{+++}-ia_{+--}+\exp\left[i\left(\psi+\frac{\pi}{4}\right)\right]\times(a_{-+-}+a_{--+})\right\}=0,$$

$$\langle\nu_{4+}|\psi\rangle=\frac{1}{2\sqrt{2}}\left\{-a_{+++}+ia_{+--}-\exp\left[i\left(\psi+\frac{\pi}{4}\right)\right]\times(a_{-+-}-a_{--+})\right\}=0.$$

The above system of four equations has the trivial solution $a_{++}=a_{+-}=a_{-+-}=a_{-+}=0$ provided that $\psi\neq\pm\frac{\pi}{4},\pm\frac{3\pi}{4}$. This proves the optimality of ${}^{333}W^{\mathrm{Co}}_{122,0+}$ for all but $\pm\frac{\pi}{4},\pm\frac{3\pi}{4}$ values of ψ. Similarly, the optimality of ${}^{333}W^{\mathrm{Co}}_{122,0-}$ is proved for the same values of ψ.

V. DETECTION OF ρ BY EWS

In this section, we consider the problem of detection of ρ by the introduced EWs.

A. Detection of ρ by the EWs with polygonal FR

First we begin with 16 EWs ${}^{1}W^{\mathrm{Po}}_{i_1i_2i_3i_4}$ of Eq. (3.3). For these EWs we have

$$\mathrm{Tr}({}^{1}W^{\mathrm{Po}}_{i_1i_2i_3i_4}\rho)=1+(-1)^{i_1}r_{333}+(-1)^{i_2}r_{111}+(-1)^{i_3}r_{122}+(-1)^{i_4}r_{212}+(-1)^{i_2+i_3+i_4+1}r_{221}. \quad (5.1)$$

It is seen that ρ is detectable by ${}^{1}W^{\mathrm{Po}}_{i_1i_2i_3i_4}$ if the parameters of ρ satisfy the following conditions:

$$b+c+\frac{1}{a}+\frac{1}{d}<\pm 4r_j\cos\varphi_j, \quad a+d+\frac{1}{b}+\frac{1}{c}<\pm 4r_j\cos\varphi_j, \quad j=1,2,3,4. \quad (5.2)$$

For the 16 EWs ${}^{2}W^{\mathrm{Po}}_{i_1i_2i_3i_4}$ of Eq. (3.4), we have

$$\mathrm{Tr}({}^{2}W^{\mathrm{Po}}_{i_1i_2i_3i_4}\rho)=1+(-1)^{i_1}r_{333}+(-1)^{i_2}r_{211}+(-1)^{i_3}r_{222}+(-1)^{i_4+1}r_{112}+(-1)^{i_2+i_3+i_4}r_{121}. \quad (5.3)$$

The detection condition imposes the following constraints on the parameters:

$$b+c+\frac{1}{a}+\frac{1}{d}<\pm 4r_j\sin\varphi_j, \quad a+d+\frac{1}{b}+\frac{1}{c}<\pm 4r_j\sin\varphi_j, \quad j=1,2,3,4. \quad (5.4)$$

B. Detection of ρ by the EWs with conical FR

The detection conditions obtained from 48 nonlinear EWs ${}^{k'j'l'}F^{\mathrm{Co}}_{kjl;i\pm}(\rho)$ of Eq. (3.8) together with 48 nonlinear EWs ${}^{k'j'l'}F^{\mathrm{Co}}_{kjl;i\pm}(\rho)$ of Eq. (3.9) are

$$\left(a+\frac{1}{a}+b+\frac{1}{b}\right)^2<4w, \quad \left(a+\frac{1}{a}+c+\frac{1}{c}\right)^2<4w,$$
$$\left(a+\frac{1}{a}+d+\frac{1}{d}\right)^2<4w, \quad \left(b+\frac{1}{b}+c+\frac{1}{c}\right)^2<4w,$$
$$\left(b+\frac{1}{b}+d+\frac{1}{d}\right)^2<4w, \quad \left(c+\frac{1}{c}+d+\frac{1}{d}\right)^2<4w,$$
$$\left(a+\frac{1}{b}+d+\frac{1}{c}\right)^2<4w, \quad \left(b+\frac{1}{a}+c+\frac{1}{d}\right)^2<4w, \quad (5.5)$$

where $w=u_1,u_2,u_3;v_1,v_2,v_3$ and

$$u_1=(r_2\cos\varphi_2\pm r_3\cos\varphi_3)^2+(r_1\cos\varphi_1\mp r_4\cos\varphi_4)^2,$$
$$u_2=(r_1\cos\varphi_1\pm r_3\cos\varphi_3)^2+(r_2\cos\varphi_2\mp r_4\cos\varphi_4)^2,$$
$$u_3=(r_1\cos\varphi_1\pm r_2\cos\varphi_2)^2+(r_3\cos\varphi_3\mp r_4\cos\varphi_4)^2,$$
$$v_1=(r_2\sin\varphi_2\pm r_3\sin\varphi_3)^2+(r_1\sin\varphi_1\mp r_4\sin\varphi_4)^2,$$
$$v_2=(r_1\sin\varphi_1\pm r_3\sin\varphi_3)^2+(r_2\sin\varphi_2\mp r_4\sin\varphi_4)^2,$$
$$v_3=(r_1\sin\varphi_1\pm r_2\sin\varphi_2)^2+(r_3\sin\varphi_3\mp r_4\sin\varphi_4)^2. \quad (5.6)$$

C. Detection of ρ by the EWs with cylindrical FR

The detection conditions obtained from 36 nonlinear EWs ${}^{k'j'l'}F^{\mathrm{Cy}}_{kjl;i_1i_2}(\rho)$ of Eq. (3.12) together with 36 nonlinear EWs ${}^{k'j'l'}F^{\mathrm{Cy}}_{kjl;i_1i_2}(\rho)$ of Eq. (3.13) are

$$z_i<16r_j^2\cos^2\varphi_j, \quad z_i<16r_j^2\sin^2\varphi_j, \quad i=1,2,3;j=1,2,3,4, \quad (5.7)$$

where

$$z_1 = (a+b+c+d)\left(\frac{1}{a}+\frac{1}{b}+\frac{1}{c}+\frac{1}{d}\right),$$

$$z_2 = \left(a+b+\frac{1}{c}+\frac{1}{d}\right)\left(c+d+\frac{1}{a}+\frac{1}{b}\right),$$

$$z_3 = \left(a+c+\frac{1}{b}+\frac{1}{d}\right)\left(b+d+\frac{1}{a}+\frac{1}{c}\right). \qquad (5.8)$$

Unfortunately, as the following argument shows, the conditions (5.7) are not held for ρ. We can write

$$z_1 = 4 + \left(\frac{a}{b}+\frac{b}{a}\right)+\left(\frac{a}{c}+\frac{c}{a}\right)+\left(\frac{a}{d}+\frac{d}{a}\right)+\left(\frac{b}{c}+\frac{c}{b}\right) + \left(\frac{b}{d}+\frac{d}{b}\right)+\left(\frac{c}{d}+\frac{d}{c}\right).$$

The two terms in each set of parentheses are the inverse of each other, so the value of each expression in parentheses is greater than or equal to 2, and hence $z_1 \geqslant 16$, while according to Eq. (5.7) $z_1 < 16$. Similar arguments show that $z_2, z_3 \geqslant 16$, but according to Eq. (5.7) they are smaller than 16.

D. Detection of ρ by the EWs with spherical FR

Finally, the detection conditions obtained from 18 nonlinear EWs ${}^{k'j'l'}F^{\mathrm{Sp}}_{kjl;i}(\rho)$ of Eq. (3.16) together with 36 nonlinear EWs ${}^{k'j'l'}F^{\mathrm{Sp}}_{kjl;i}(\rho)$ of Eq. (3.17) are

$$z_i < 4u_j, \quad z_i < 4v_j, \quad i,j = 1,2,3,$$

where z_i, u_j, and v_j are defined as in Eqs. (5.8) and (5.6).

VI. COMPARISON WITH OTHER WORKS

If we put $a=b=c=d=1$, $r_1=r_2=1$, and $\varphi_1=\varphi_2=0$, the detection conditions (5.5) give

$$4 < 4 + (r_3 \cos \varphi_3 - r_4 \cos \varphi_4)^2.$$

Hence, this case is detected by our EWs unless $r_3 \cos \varphi_3 = r_4 \cos \varphi_4$. Further inspection shows that if in addition, $\varphi_3 = \varphi_4 = 0, \pi$, then ρ is separable. So for the choice of parameters as $a=b=c=d=1$, $r_1=r_2=1$, $\varphi_1=\varphi_2=0$, and $\varphi_3=\varphi_4=0,\pi$, the ρ is separable if and only if $r_3=r_4$, in agreement with Ref. [9].

For the case $a=1$, $0<b,c,\frac{1}{d}<1$, $r_1=1$, $\varphi_1=0$, and $r_2=r_3=r_4=0$, we have

$$\mathrm{Tr}({}^1W^{\mathrm{Po}}_{1101}\rho) = \frac{2\left(b+c+\frac{1}{d}-3\right)}{2+b+c+d+\frac{1}{b}+\frac{1}{c}+\frac{1}{d}}.$$

This trace attains its minimum value -0.3371 at $b=c=\frac{1}{d}=0.3798$ and hence improves the result -0.1069 at $b=c=\frac{1}{d}=0.3460$ of Ref. [7].

For the case $a=1$, $0<\frac{1}{b},\frac{1}{c},d<1$, $r_1=1$, $\varphi_1=0$, and $r_2=r_3=r_4=0$, we have

$$\mathrm{Tr}({}^1W^{\mathrm{Po}}_{0101}\rho) = \frac{2\left(\frac{1}{b}+\frac{1}{c}+d-3\right)}{2+b+c+d+\frac{1}{b}+\frac{1}{c}+\frac{1}{d}}.$$

This trace attains its minimum value -0.3371 at $\frac{1}{b}=\frac{1}{c}=d=0.3460$.

VII. $2\otimes 2\otimes d$ CHESSBOARD DENSITY MATRICES

In this section, we generalize previous three-qubit chessboard density matrices to the $2\otimes 2\otimes d$ case such that they satisfy PPT conditions. As a result of this extension, the form of EWs remains the same. It is enough to change the notation slightly. The approach can be applied even for higher dimensions and for multiqubits although the number and classifications of EWs increase. Using some new algebraic notation for the $2\otimes 2\otimes d$ case, we can write the relevant chessboard density matrices as follows:

$$\begin{aligned}\rho_{d,\alpha,\beta,\gamma} = \sum_{j=0}^{1}\Bigg(&\sum_{k=1}^{d} a^{jk}_{jk}|0jk\rangle\langle 0jk| + z^{j\alpha}_{\bar{j}\beta}|0j\alpha\rangle\langle 1\bar{j}\beta| + \bar{z}^{j\alpha}_{\bar{j}\beta}|1\bar{j}\beta\rangle \\ &\times\langle 0j\alpha| + z^{j\beta}_{\bar{j}\alpha}|0j\beta\rangle\langle 1\bar{j}\alpha| + \bar{z}^{j\beta}_{\bar{j}\alpha}|1\bar{j}\alpha\rangle\langle 0j\beta| + z^{j\gamma}_{\bar{j}\gamma}|0j\gamma\rangle \\ &\times\langle 1\bar{j}\gamma| + \bar{z}^{j\gamma}_{\bar{j}\gamma}|1\bar{j}\gamma\rangle\langle 0j\gamma| + \frac{1}{a^{j\alpha}_{j\alpha}}|1j\alpha\rangle\langle 1j\alpha| + \frac{1}{a^{j\beta}_{j\beta}}|1j\beta\rangle \\ &\times\langle 1j\beta| + \frac{1}{a^{j\gamma}_{j\gamma}}|1j\gamma\rangle\langle 1j\gamma|\Bigg). \end{aligned} \qquad (7.1)$$

Here $\bar{j}=0$ if $j=1$ and vice versa and

$$\alpha \neq \beta = 0,\ldots,d-1, \quad 0 \leqslant \alpha < \beta \leqslant d-1, \quad 0 \leqslant \gamma \leqslant d-1,$$

$$z^{j\nu}_{\bar{j}\mu} = r^{j\nu}_{\bar{j}\mu}\exp(i\varphi^{j\nu}_{\bar{j}\mu}), \quad \bar{z}^{j\nu}_{\bar{j}\mu} = r^{j\nu}_{\bar{j}\mu}\exp(-i\varphi^{j\nu}_{\bar{j}\mu}).$$

For a given α and β, if $r^{j\nu}_{\bar{j}\mu} \leqslant 1$ for every j,μ,ν then these density matrices have positive partial transposes with respect to all subsystems, i.e., they are PPT states. All of the three-qubit EWs discussed previously are also EWs for these density matrices if we make the replacements

$$I_2 \to I_d, \quad \sigma_x \to \sqrt{2}\lambda^{+}_{\alpha\beta}, \quad \sigma_y \to \sqrt{2}\lambda^{-}_{\alpha\beta}, \quad \sigma_z \to E_{\alpha\alpha} - E_{\beta\beta} \qquad (7.2)$$

in the operators acting on the third subsystem (see Appendix C). In the following subsections, we will use the replacements (7.2) to discuss the similar categories of EWs for the $2\otimes 2\otimes d$ case. Note that in all categories

$$\alpha \neq \beta = 0,\ldots,d-1 \quad \text{and} \quad 0 \leqslant \alpha < \beta \leqslant d-1.$$

A. Polygonal EWs

Using the above notations, for the polygonal case we have $32(\frac{d(d-1)}{2})$ EWs. In analogy with Eq. (3.3), the $16(\frac{d(d-1)}{2})$ of these EWs are

$$
\begin{aligned}
{}^{1}W^{\alpha,\beta}_{i_1i_2i_3i_4} &= I_2 I_2 I_d + (-1)^{i_1}\sigma_z\sigma_z(E_{\alpha\alpha}-E_{\beta\beta}) \\
&+ \sqrt{2}(-1)^{i_2}\sigma_x\sigma_x\lambda^{+}_{\alpha\beta} + \sqrt{2}(-1)^{i_3}\sigma_x\sigma_y\lambda^{-}_{\alpha\beta} \\
&+ \sqrt{2}(-1)^{i_4}\sigma_y\sigma_x\lambda^{-}_{\alpha\beta} + \sqrt{2}(-1)^{i_2+i_3+i_4+1}\sigma_y\sigma_y\lambda^{+}_{\alpha\beta},
\end{aligned} \tag{7.3}
$$

where $(i_1,i_2,i_3,i_4)\in\{0,1\}^4$. The remaining $16(\frac{d(d-1)}{2})$ polygonal EWs can be obtained by applying the phase-shift gate M locally on the first qubit. The result is

$$
\begin{aligned}
{}^{2}W^{\alpha,\beta}_{i_1i_2i_3i_4} &= I_2 I_2 I_d + (-1)^{i_1}\sigma_z\sigma_z(E_{\alpha\alpha}-E_{\beta\beta}) \\
&+ \sqrt{2}(-1)^{i_2}\sigma_x\sigma_x\lambda^{+}_{\alpha\beta} + \sqrt{2}(-1)^{i_3}\sigma_x\sigma_y\lambda^{-}_{\alpha\beta} \\
&+ \sqrt{2}(-1)^{i_4+1}\sigma_y\sigma_x\lambda^{-}_{\alpha\beta} + \sqrt{2}(-1)^{i_2+i_3+i_4}\sigma_y\sigma_y\lambda^{+}_{\alpha\beta}.
\end{aligned} \tag{7.4}
$$

B. Conical EWs

We can expand the density matrices (7.1) in terms of tensor products of Pauli matrices and the Lie algebra Su(d) generators (see Appendix C). In the following relations, r_{ijk} are coefficients of relevant operators appearing in the density matrices expansions, e.g., r_{ij1} is the coefficient of $\sqrt{2}\sigma_i\sigma_j\lambda^{+}_{\alpha\beta}$, r_{ij2} is the coefficient of $\sqrt{2}\sigma_i\sigma_j\lambda^{-}_{\alpha\beta}$, and r_{ij3} is the coefficient of $\sigma_i\sigma_j(E_{\alpha\alpha}-E_{\beta\beta})$. The $96(\frac{d(d-1)}{2})$ conical EWs [in analogy with Eqs. (3.8) and (3.9)] are

$$
\begin{aligned}
{}^{k'j'l'}F^{\mathrm{Co}}_{kjl,i\pm}(\rho) &= \min \mathrm{Tr}[({}^{k'j'l'}W^{\mathrm{Co}}_{kjl,i\pm})\rho] = 1 \pm r_{k'j'l'} \\
&- \sqrt{[r_{111}+(-1)^i r_{kjl}]^2 + [r_{lkj}+(-1)^i r_{jlk}]^2},
\end{aligned} \tag{7.5}
$$

where $k'j'l'$ is one of the triples 333, 330, 303, 033, and kjl is one of the triples 122, 212, 221. The remaining of the conical EWs are

$$
\begin{aligned}
{}^{k'j'l'}F'^{\mathrm{Co}}_{kjl,i\pm}(\rho) &= \min \mathrm{Tr}[MII({}^{k'j'l'}W^{\mathrm{Co}}_{kjl,i\pm})M^{\dagger}II\rho] \\
&= 1 \pm r_{k'j'l'} \\
&- \sqrt{[r_{222}+(-1)^i r_{kjl}]^2 + [r_{lkj}+(-1)^i r_{jlk}]^2}.
\end{aligned} \tag{7.6}
$$

Here kjl is one of the triples 211, 121, and 112. Cylindrical and spherical EWs for $2\otimes 2\otimes d$ chessboard density matrices can be constructed by this procedure and are in full analogy with Eqs. (3.12), (3.13), (3.16), and (3.17). Hence the overall number of EWs are $236(\frac{d(d-1)}{2})$.

C. $2\otimes 2\otimes 3$ Chessboard density matrices: An example

Now let us study the density matrix for $d=3$, $\alpha=0$, $\beta=2$, and $\gamma=1$ in some detail. In this case, we can expand this density matrix in terms of tensor products of Pauli matrices and Gell-Mann matrices $\Lambda_1,\ldots,\Lambda_8$ (see Appendix D), and all of the previous EWs for three-qubit case are also valid here if we make the replacements

$$
I_2 \to I_3, \quad \sigma_x \to \sqrt{2}\lambda^{+}_{02} = \Lambda_4, \quad \sigma_y \to \sqrt{2}\lambda^{-}_{02} = \Lambda_5,
$$

TABLE I. The percent of detection for introduced $2\otimes 2\otimes 3$ EWs. $\bar{R}$ indicates mean ratios and σ is standard deviation.

EWs	Percent of detection
All 236 EWs	$\bar{R}\pm\sigma=85.45\pm 3.336$

$$
\sigma_z \to E_{00} - E_{22} = \frac{1}{2}(\Lambda_3 + \sqrt{3}\Lambda_8) \tag{7.7}
$$

in the operators acting on the third subsystem. For example, using the above prescription, the polygonal EWs in Eq. (3.3) can be written as

$$
\begin{aligned}
{}^{1}W^{\mathrm{Po}}_{i_1i_2i_3i_4} &= I_2 I_2 I_3 + (-1)^{i_1}\sigma_z\sigma_z\left[\frac{1}{2}(\Lambda_3+\sqrt{3}\Lambda_8)\right] \\
&+ (-1)^{i_2}\sigma_x\sigma_x\Lambda_4 + (-1)^{i_3}\sigma_x\sigma_y\Lambda_5 + (-1)^{i_4}\sigma_y\sigma_x\Lambda_5 \\
&+ (-1)^{i_2+i_3+i_4+1}\sigma_y\sigma_y\Lambda_4.
\end{aligned} \tag{7.8}
$$

By similar substitution, all of 236 EWs can be constructed. The detection ratio (the ratio of entangled density matrices detected by all of our EWs to all randomly selected density matrices) is listed in Table I.

VIII. NUMERICAL ANALYSIS OF ENTANGLEMENT PROPERTY OF ρ

In this section we deal with some numerical analysis regarding the detection ability of introduced EWs for $2\otimes 2\otimes 2$ and $2\otimes 2\otimes 3$ chessboard density matrices. Numerical calculation is done on a random set of relevant PPT chessboard density matrices. Those density matrices detected by introduced EWs are counted and then the ratio is calculated. The percent of the volume of phase space that can be detected by introduced EWs is as listed in the Table II.

IX. CONCLUSION

In this paper, we have considered a class of three-partite PPT chessboard density matrices and via an exact convex optimization method, have constructed various linear and

TABLE II. The percent of detection for introduced EWs. "Not polygonal but conical" means the percent of the three-qubit PPT density matrices ρ that the polygonal EWs cannot detect but the conical ones can detect.

EWs	Percent of detection
Polygonal	28.3
Conical	18.3
Spherical	0.047
All EWs	28.62
Not polygonal but conical	0.44
Not polygonal but spherical	0.0275
Polygonal and spherical	0.0176
Conical and spherical	0.031

nonlinear EWs detecting them. The operators participating in constructing the EWs have been chosen in such a way that the geometrical shape of the corresponding feasible regions have been obtained exactly. The EWs have been classified according to the geometrical shape of relevant feasible regions. When the feasible region was not a polygon, nonlinear EWs were obtained. The optimality of the EWs with polygonal and conical feasible regions have been shown. The introduced EWs were all nondecomposable, since they were able to detect PPT entangled states. Even so, we have mainly discussed these methods for $2\otimes 2\otimes 2$ and $2\otimes 2\otimes d$ chessboard density matrices, but they are general and one can apply them for $d_1\otimes d_2\otimes d_3$ via some minor changes in notations and calculations. It was shown that the detection ability of the introduced EWs is often comparable with one of the EWs introduced elsewhere. In some cases, the detection ability of the EWs introduced here is better. Finally, the prescription of this work is applicable for multipartite PPT chessboard density matrices, which is under investigation.

APPENDIX A

Proving the inequalities

In the following proofs, we use the abbreviations

$$\mathrm{Tr}(\sigma_i^{(1)}|\alpha\rangle\langle\alpha|) = a_i,$$

$$\mathrm{Tr}(\sigma_i^{(2)}|\beta\rangle\langle\beta|) = b_i,$$

$$\mathrm{Tr}(\sigma_i^{(3)}|\gamma\rangle\langle\gamma|) = c_i. \tag{A1}$$

Since $a_1^2+a_2^2+a_3^2=1$ and also the similar relations hold for b_i's and c_i's, so the points a,b,c lie on a unit sphere and we can paramterize their coordinates by using spherical coordinates θ and φ as follows:

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

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

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

Envelope of a family of curves

The envelope of a one-parameter family of plane curves described implicitly by $F(x,y,c)=0$, or in parametric form by $(f(t,c),g(t,c))$, is a curve in which each point of it touches one member of the family [38,39]. In the case of implicit representation, the envelope is given by simultaneously solving

$$F(x,y,c) = 0 \quad \text{and} \quad \frac{\partial F}{\partial c} = 0.$$

In the case of parametric representation, the envelope is found by solving

$$\frac{\partial f}{\partial t}\frac{\partial g}{\partial c} - \frac{\partial f}{\partial c}\frac{\partial g}{\partial t} = 0.$$

Proof of Eq. (3.2)

To prove this equality, we note that

$$P_1 = a_3b_3c_3 = \cos\theta_1\cos\theta_2\cos\theta_3,$$

$$P_2 = a_1(b_1c_1 \pm b_2c_2) = \sin\theta_1\sin\theta_2\sin\theta_3\cos\varphi_1\cos(\varphi_3 \mp \varphi_2),$$

$$P_3 = a_2(b_1c_2 \mp b_2c_1) = \sin\theta_1\sin\theta_2\sin\theta_3\sin\varphi_1\sin(\varphi_3 \mp \varphi_2).$$

First we take θ_1, θ_2, and θ_3 to be constant and define

$$a = \sin\theta_1\sin\theta_2\sin\theta_3,\quad t = \varphi_1,\quad c = \varphi_3 \mp \varphi_2,$$

to get

$$P_2(t,c) = a\cos t\cos c,\quad P_3(t,c) = a\sin t\sin c.$$

Then we find the envelope of a family of curves represented parametrically by

$$(P_2(t,c),P_3(t,c)).$$

For this purpose, we solve

$$\frac{\partial P_2}{\partial t}\frac{\partial P_3}{\partial c} - \frac{\partial P_2}{\partial c}\frac{\partial P_3}{\partial t} = a^2(-\sin^2 t\cos^2 c + \cos^2 t\sin^2 c) = 0,$$

and obtain

$$\sin(t \pm c) = 0 \quad \text{or} \quad c = \pm t + n\pi,$$

where n is an integer. Substituting this back into $P_2(t,c)$ and $P_3(t,c)$, gives

$$P_2(t) = (-1)^n a\cos^2 t,\quad P_3(t) = \pm(-1)^n a\sin^2 t.$$

By using $\sin^2 t+\cos^2 t=1$, we get the envelope

$$P_2 + P_3 = \pm a = \pm\sin\theta_1\sin\theta_2\sin\theta_3,$$

$$P_2 - P_3 = \pm a = \pm\sin\theta_1\sin\theta_2\sin\theta_3.$$

In the next step, we take θ_3 to be constant and find the envelope of a family of curves given by

$$(P_1(\theta_1,\theta_2),(P_2 \pm P_3)(\theta_1,\theta_2)),$$

with

$$P_1(\theta_1,\theta_2) = \cos\theta_3\cos\theta_1\cos\theta_2,$$

$$P_2 \pm P_3 = \pm\sin\theta_3\sin\theta_1\sin\theta_2.$$

A similar argument as above, gives

$$P_1(\theta_1) = (-1)^n\cos^2\theta_1\cos\theta_3,$$

$$(P_2 \pm P_3)(\theta_1) = \pm(-1)^n\sin^2\theta_1\sin\theta_3.$$

Noting that $\sin^2\theta_1+\cos^2\theta_1=1$, we obtain the envelope

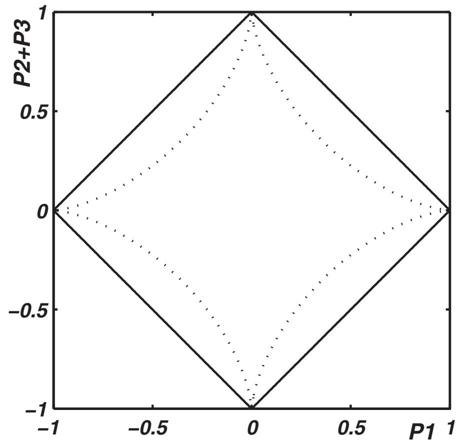

FIG. 1. The boundaries of feasible region for pure product states (dotted curves) which form an astroid and for mixed separable states (line segments) which form a rhombus, for EWs of relation (3.8). The P_i's are dimensionless.

$$F(P_1,P_2 \pm P_3,\theta_3) = \frac{P_1}{\cos\,\theta_3} + \frac{(P_2 \pm P_3)}{\sin\,\theta_3} \pm 1 = 0.$$

$$G(P_1,P_2 \pm P_3,\theta_3) = \frac{P_1}{\cos\,\theta_3} - \frac{(P_2 \pm P_3)}{\sin\,\theta_3} \pm 1 = 0. \tag{A2}$$

These are the implicit forms of a one-parameter family of curves with parameter θ_3.

Finally, to obtain the feasible region of pure product states, we find the envelope of the family of curves (A2). To this aim, we solve

$$\frac{\partial F}{\partial \theta_3} = 0 \quad \text{and} \quad \frac{\partial G}{\partial \theta_3} = 0$$

for θ_3, which yields

$$\frac{P_1}{\cos^3\,\theta_3} = \pm \frac{(P_2 \pm P_3)}{\sin^3\,\theta_3}.$$

Substituting these back into F and G, gives

$$\sin^3\,\theta_3 = \pm (P_2 \pm P_3), \quad \cos^3\,\theta_3 = \pm P_1.$$

By using the identity $\sin^2\,\theta_3+\cos^2\,\theta_3=1$, we get the envelope

$$P_1^{2/3} + (P_2 \pm P_3)^{2/3} = 1,$$

which is an astroid (dotted curves in Fig. 1). But, as Fig. 1 shows, this is a concave region. Since the feasible region of mixed separable states is the convex hull of the feasible region of pure product states, the boundaries of FR are the planes of Eq. (3.7), i.e., the edges of the rhombus in Fig. 1.

Proof of Eq. (3.5)

The proofs are similar, so we give the proof for the case $Q_1^{\mathrm{Co}}=O_{333}$ and $kjl=122$. We note that

$$P_1 = a_3b_3c_3 = \cos\,\theta_1 \cos\,\theta_2 \cos\,\theta_3,$$

$$P_2 = a_1(b_1c_1 \pm b_2c_2) = \sin\,\theta_1 \sin\,\theta_2 \sin\,\theta_3 \cos\,\varphi_1 \cos(\varphi_2 \mp \varphi_3),$$

$$P_3 = a_2(b_1c_2 \pm b_2c_1) = \sin\,\theta_1 \sin\,\theta_2 \sin\,\theta_3 \sin\,\varphi_1 \sin(\varphi_2 \pm \varphi_3).$$

As we want to obtain the boundaries of the feasible region, first we maximize the absolute values of P_2 and P_3 by taking $\varphi_2=\varphi_3=\frac{\pi}{4}$ or $\varphi_2=\frac{3\pi}{4}$ and $\varphi_3=\frac{\pi}{4}$. This choice gives

$$P_2 = \sin\,\theta_1 \sin\,\theta_2 \sin\,\theta_3 \cos\,\varphi_1,$$

$$P_3 = \sin\,\theta_1 \sin\,\theta_2 \sin\,\theta_3 \sin\,\varphi_1.$$

From these, we obtain

$$(P_2^2 + P_3^2)^{1/2} = \sin\,\theta_1 \sin\,\theta_2 \sin\,\theta_3.$$

Now we take θ_3 to be constant, rename $P=(P_2^2+P_3^2)^{1/2}$, and try to find the envelope of a family of curves represented parametrically by

$$(P_1(\theta_1,\theta_2),P(\theta_1,\theta_2)),$$

in which

$$P_1(\theta_1,\theta_2) = \cos\,\theta_1 \cos\,\theta_2 \cos\,\theta_3,$$

$$P(\theta_1,\theta_2) = \sin\,\theta_1 \sin\,\theta_2 \sin\,\theta_3.$$

To this aim, we solve

$$\frac{\partial P_1}{\partial \theta_1}\frac{\partial P}{\partial \theta_2} - \frac{\partial P_1}{\partial \theta_2}\frac{\partial P}{\partial \theta_1} = \sin\,\theta_3 \cos\,\theta_3(-\cos^2\,\theta_1 \sin^2\,\theta_2 + \sin^2\,\theta_1 \cos^2\,\theta_2) = 0,$$

which yields

$$\sin(\theta_1 \pm \theta_2) = 0 \quad \text{or} \quad \theta_2 = \pm \theta_1 + n\pi,$$

where n is an integer. Substituting this back into $P_1(\theta_1,\theta_2)$ and $P(\theta_1,\theta_2)$, gives

$$P_1(\theta_1) = (-1)^n \cos^2\,\theta_1 \cos\,\theta_3,$$

$$P(\theta_1) = \pm(-1)^n \sin^2\,\theta_1 \sin\,\theta_3.$$

From $\sin^2\,\theta_1+\cos^2\,\theta_1=1$, we get the envelope

$$\frac{P_1}{\cos\,\theta_3} + \frac{P}{\sin\,\theta_3} \pm 1 = 0, \quad \frac{P_1}{\cos\,\theta_3} - \frac{P}{\sin\,\theta_3} \pm 1 = 0.$$

Finally, taking the derivative with respect to θ_3 and using the identity $\sin^2\,\theta_3+\cos^2\,\theta_3=1$, gives the feasible region of pure product states

$$P_1^{2/3} + P^{2/3} = 1,$$

which is again an astroid (dotted curves in Fig. 1). But, as Fig. 1 shows, this is a concave curve in terms of variables P_1 and $P=(P_2^2+P_3^2)^{1/2}$. Since the mixed separable states are convex combinations of pure product states, the relations between these two variables are given by the lines (i.e., the edges of the rhombus in Fig. 1)

$$P_1+(P_2^2+P_3^2)^{1/2}=\pm 1, \quad P_1-(P_2^2+P_3^2)^{1/2}=\pm 1.$$

So the relations between P_1, P_2, and P_3 are as in relation (3.10).

If we take $Q_1^{\mathrm{Co}}=O_{330}$, the proof of Eq. (3.5) proceeds as follows. We note that in this case

$$P_1=a_3b_3=\cos\theta_1\cos\theta_2,$$

but P_2 and P_3 are as before. To maximize the absolute values of P_2 and P_3, we set $\theta_3=\frac{\pi}{2}$ and $\varphi_2=\varphi_3=\frac{\pi}{4}$, or $\varphi_2=\frac{3\pi}{4}$ and $\varphi_3=\frac{\pi}{4}$. This gives

$$P_2=\sin\theta_1\sin\theta_2\cos\varphi_1, \quad P_3=\sin\theta_1\sin\theta_2\sin\varphi_1.$$

From these, we obtain

$$(P_2^2+P_3^2)^{1/2}=\sin\theta_1\sin\theta_2.$$

Now we rename $P=(P_2^2+P_3^2)^{1/2}$ and try to find the envelope of a family of curves represented parametrically by

$$(P_1(\theta_1,\theta_2),P(\theta_1,\theta_2)).$$

A similar argument as above again leads to the relation (3.5).

APPENDIX B

Coefficients of Pauli operators appearing in ρ

$$r_{111}=\frac{2}{n}(r_1\cos\varphi_1+r_2\cos\varphi_2+r_3\cos\varphi_3+r_4\cos\varphi_4),$$

$$r_{112}=\frac{2}{n}(r_1\sin\varphi_1-r_2\sin\varphi_2+r_3\sin\varphi_3-r_4\sin\varphi_4),$$

$$r_{121}=\frac{2}{n}(r_1\sin\varphi_1+r_2\sin\varphi_2-r_3\sin\varphi_3-r_4\sin\varphi_4),$$

$$r_{211}=\frac{2}{n}(-r_1\sin\varphi_1-r_2\sin\varphi_2-r_3\sin\varphi_3-r_4\sin\varphi_4),$$

$$r_{122}=\frac{2}{n}(-r_1\cos\varphi_1+r_2\cos\varphi_2+r_3\cos\varphi_3-r_4\cos\varphi_4),$$

$$r_{212}=\frac{2}{n}(r_1\cos\varphi_1-r_2\cos\varphi_2+r_3\cos\varphi_3-r_4\cos\varphi_4),$$

$$r_{221}=\frac{2}{n}(r_1\cos\varphi_1+r_2\cos\varphi_2-r_3\cos\varphi_3-r_4\cos\varphi_4),$$

$$r_{222}=\frac{2}{n}(r_1\sin\varphi_1-r_2\sin\varphi_2-r_3\sin\varphi_3+r_4\sin\varphi_4),$$

$$r_{300}=\frac{1}{n}\left(a+b+c+d-\frac{1}{a}-\frac{1}{b}-\frac{1}{c}-\frac{1}{d}\right),$$

$$r_{030}=\frac{1}{n}\left(a+b-c-d-\frac{1}{a}-\frac{1}{b}+\frac{1}{c}+\frac{1}{d}\right),$$

$$r_{003}=\frac{1}{n}\left(a-b+c-d-\frac{1}{a}+\frac{1}{b}-\frac{1}{c}+\frac{1}{d}\right),$$

$$r_{330}=\frac{1}{n}\left(a+b-c-d+\frac{1}{a}+\frac{1}{b}-\frac{1}{c}-\frac{1}{d}\right),$$

$$r_{303}=\frac{1}{n}\left(a-b+c-d+\frac{1}{a}-\frac{1}{b}+\frac{1}{c}-\frac{1}{d}\right),$$

$$r_{033}=\frac{1}{n}\left(a-b-c+d+\frac{1}{a}-\frac{1}{b}-\frac{1}{c}+\frac{1}{d}\right),$$

$$r_{333}=\frac{1}{n}\left(a-b-c+d-\frac{1}{a}+\frac{1}{b}+\frac{1}{c}-\frac{1}{d}\right).$$

APPENDIX C

Every d-dimensional square matrix can be written in terms of square matrices E_{ij}, which show the value 1 at the position (i,j) and zeros elsewhere. Now one can define the Hermitian traceless basis for d-dimensional matrices as follows (see [37]).

The off-diagonal bases are

$$\lambda_{\alpha\beta}^{+}=\frac{1}{\sqrt{2}}(E_{\alpha\beta}+E_{\beta\alpha}),$$

$$\lambda_{\alpha\beta}^{-}=\frac{1}{i\sqrt{2}}(E_{\alpha\beta}-E_{\beta\alpha}),$$

and diagonal bases are

$$\lambda_0=\begin{pmatrix}1 & & & & 0\\ & -1 & & & \\ & & 0 & & \\ & & & \ddots & \\ 0 & & & & 0\end{pmatrix},$$

$$\lambda_1=\frac{1}{\sqrt{3}}\begin{pmatrix}1 & & & & 0\\ & 1 & & & \\ & & -2 & & \\ & & & \ddots & \\ 0 & & & & 0\end{pmatrix}, \quad \ldots,$$

$$\lambda_{d-2}=\sqrt{\frac{2}{d(d-1)}}\begin{pmatrix}1 & & & & 0\\ & 1 & & & \\ & & \ddots & & \\ & & & 1 & \\ 0 & & & & -d+1\end{pmatrix}.$$

In order to generalize the witnesses, we must write $E_{\alpha\alpha}$ in terms of I_d ($d\times d$ identity matrix) and λ_α's. Some calculation shows that

$$E_{ii} = E_{i+1,i+1} + \sqrt{\frac{i+2}{2(i+1)}}\lambda_i - \sqrt{\frac{i}{2(i+1)}}\lambda_{i-1},$$

$$0 \leqslant i \leqslant d-2$$

(recursion relation) and

$$E_{d-1,d-1} = \frac{1}{d}I_d - \sqrt{\frac{d-1}{2d}}\lambda_{d-2}.$$

Proving the inequalities for $2\otimes 2\otimes d$

The proof is almost the same as one explained in Appendix A. We use the abbreviations

$$\mathrm{Tr}(\sigma_i^{(1)}|\alpha\rangle\langle\alpha|) = a_i,$$

$$\mathrm{Tr}(\sigma_i^{(2)}|\beta\rangle\langle\beta|) = b_i,$$

$$\mathrm{Tr}(\sqrt{2}\lambda^{+}_{\alpha\beta}|\xi\rangle\langle\xi|) = c_1,$$

$$\mathrm{Tr}(\sqrt{2}\lambda^{-}_{\alpha\beta}|\xi\rangle\langle\xi|) = c_2,$$

$$\mathrm{Tr}[(E_{\alpha\alpha} - E_{\beta\beta})|\xi\rangle\langle\xi|] = c_3, \tag{C1}$$

where

$$|\xi\rangle = \frac{1}{\sqrt{r_0^2 + \cdots + r_{d-1}^2}}\begin{pmatrix} r_0 e^{i\theta_0} \\ \vdots \\ r_{d-1}e^{i\theta_{d-1}} \end{pmatrix}.$$

We have

$$a_1^2 + a_2^2 + a_3^2 = 1, \quad b_1^2 + b_2^2 + b_3^2 = 1,$$

and

$$c_1^2 + c_2^2 + c_3^2 = \frac{(r_\alpha^2 + r_\beta^2)^2}{(r_0^2 + \cdots + r_{d-1}^2)^2} = q.$$

If we set $q=1$ without loss of generality, then the points a,b,c lie on a unit sphere and we can parametrize their coordinates by using spherical coordinates θ and φ as follows:

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

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

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

APPENDIX D

Gell-Mann matrices

The analog of the Pauli matrices for su(3) are Gell-Mann matrices defined as

$$\Lambda_1 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \Lambda_2 = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \Lambda_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix},$$

$$\Lambda_4 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \quad \Lambda_5 = \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix}, \quad \Lambda_6 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix},$$

$$\Lambda_7 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \quad \Lambda_8 = \frac{1}{\sqrt{3}}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}.$$

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