A class of Bell diagonal states and entanglement witnesses

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Abstract

We analyze special class of bipartite states – so called Bell diagonal states. In particular we provide new examples of bound entangled Bell diagonal states and construct the class of entanglement witnesses diagonal in the magic basis.

1 Introduction

In recent years, due to the rapid development of quantum information theory [1] the necessity of classifying entangled states as a physical resource is of primary importance. It is well known that it is extremely hard to check whether a given density matrix describing a quantum state of the composite system is separable or entangled. There are several operational criteria which enable one to detect quantum entanglement (see e.g. [2] for the recent review). The most famous Peres-Horodecki criterion is based on the partial transposition: if a state ρ is separable then its partial transposition $(\mathbb{1} \otimes \tau)\rho$ is positive. States which are positive under partial transposition are called PPT states. Clearly each separable state is necessarily PPT but the converse is not true. We stress that it is easy to test wether a given state is PPT, however, there is no general methods to construct PPT states.

In [3] (see also [4]) we proposed a class of bipartite states which is based on certain decomposition of the total Hilbert space $\mathbb{C}^d \otimes \mathbb{C}^d$ into direct sum of d-dimensional subspaces. This decomposition is controlled by some cyclic property, that is, knowing one subspace, say Σ_0, the remaining subspaces $\Sigma_1, \ldots, \Sigma_{d-1}$ are uniquely determined by applying a cyclic shift to elements from Σ_0. Now, we call a density matrix ρ a *circulant state* if ρ is a convex combination of density matrices supported on Σ_α. The crucial observation is that a partial transposition of the circulant state has again a circular structure corresponding to another direct sum decomposition $\widetilde{\Sigma}_0 \oplus \ldots \oplus \widetilde{\Sigma}_{d-1}$. Interestingly, also realignment [5] leaves the circulant structure invariant. This class was generalized to multipartite systems [6]. Its separability properties were analyzed in [7].

The class of circulant states contains a subclass of states which are diagonal in the basis of generalized Bell states in $\mathbb{C}^d \otimes \mathbb{C}^d$. The corresponding rank-1 projectors define d^2–dimensional simplex known in the literature as *magic simplex*. Several properties of Bell diagonal states were analyzed [8, 9, 10, 11, 12]. In the present paper we perform further studies of this special class of bipartite states. In particular we provide new examples of bound entangled Bell diagonal states and analyzed the class of entanglement witnesses diagonal in the magic basis.

2 Circulant states for two qudits

Consider a class of states living in $\mathbb{C}^d \otimes \mathbb{C}^d$ constructed as follows: let $\{e_0, \ldots, e_{d-1}\}$ denotes an orthonormal basis in $\mathbb{C}^d$ and let $S : \mathbb{C}^d \to \mathbb{C}^d$ be a shift operator defined as follows

$$Se_k = e_{k+1} \ , \quad (\text{mod } d) \ . \tag{1}$$

One introduces d d-dimensional subspaces in $\mathbb{C}^d \otimes \mathbb{C}^d$:

$$\Sigma_0 = \text{span}\{e_0 \otimes e_0, \ldots, e_{d-1} \otimes e_{d-1}\} \ , \tag{2}$$

and

$$\Sigma_n = (\mathbb{I} \otimes S^n)\Sigma_0 \ , \quad n = 1, \ldots, d-1 \ . \tag{3}$$

It is clear that Σ_m and Σ_n are mutually orthogonal for $m \neq n$ and hence the collection $\{\Sigma_0, \ldots, \Sigma_{d-1}\}$ defines direct sum decomposition of $\mathbb{C}^d \otimes \mathbb{C}^d$

$$\mathbb{C}^d \otimes \mathbb{C}^d = \Sigma_0 \oplus \ldots \oplus \Sigma_{d-1} \ . \tag{4}$$

To construct a circulant state corresponding to this decomposition let us introduce d positive $d \times d$ matrices $a^{(n)} = [a^{(n)}_{ij}]$; $n = 0, 1, \ldots, d-1$. Now, define d positive operators ρ_n supported on Σ_n via the following formula

$$\rho_n = \sum_{i,j=0}^{d-1} a^{(n)}_{ij} \, e_{ij} \otimes S^n \, e_{ij} \, S^{*n} \ = \ \sum_{i,j=0}^{d-1} a^{(n)}_{ij} \, e_{ij} \otimes e_{i+n,j+n} \ . \tag{5}$$

Finally, we define the circulant density operator

$$\rho = \rho_0 + \rho_1 + \ldots + \rho_{d-1} \ . \tag{6}$$

Normalization of ρ, that is, $\text{Tr}\, \rho = 1$, is equivalent to the following condition for matrices $a^{(n)}$

$$\text{Tr}\, \left(a^{(0)} + a^{(1)} + \ldots + a^{(d-1)} \right) = 1 \ .$$

The crucial property of circulant states is based on the following observation [3]: the partially transposed circulant state ρ displays similar circulant structure, that is,

$$(\text{id} \otimes \tau)\rho = \widetilde{\rho}_0 \oplus \ldots \oplus \widetilde{\rho}_{d-1} \ , \tag{7}$$

where the operators $\widetilde{\rho}_n$ are supported on the new collection of subspaces $\widetilde{\Sigma}_n$ which are defined as follows:

$$\widetilde{\Sigma}_0 = \text{span}\{e_0 \otimes e_{\pi(0)}, e_1 \otimes e_{\pi(1)}, \ldots, e_{d-1} \otimes e_{\pi(d-1)}\} \ , \tag{8}$$

where π is a permutation defined by

$$\pi(k) = -k \ , \quad (\mathrm{mod}\ d) \ . \tag{9}$$

It means that

$$\pi(0) = 0, \ \pi(1) = d-1, \ \ldots, \pi(d-1) = 1 \ .$$

The remaining subspaces $\widetilde{\Sigma}_n$ are defined by a cyclic shift

$$\widetilde{\Sigma}_n = (\mathbb{I} \otimes S^n)\widetilde{\Sigma}_0 \ , \quad n = 1, \ldots, d-1 \ . \tag{10}$$

Again, the collection $\{\widetilde{\Sigma}_0, \ldots, \widetilde{\Sigma}_{d-1}\}$ defines direct sum decomposition of $\mathbb{C}^d \otimes \mathbb{C}^d$

$$\mathbb{C}^d \otimes \mathbb{C}^d = \widetilde{\Sigma}_0 \oplus \ldots \oplus \widetilde{\Sigma}_{d-1} \ . \tag{11}$$

Moreover, operators $\widetilde{\rho}_n$ are defined as follows

$$\widetilde{\rho}_n = \sum_{i,j=0}^{d-1} \widetilde{a}_{ij}^{(n)} \, e_{ij} \otimes S^n \, e_{\pi(i)\pi(j)} \, S^{*n} \ = \sum_{i,j=0}^{d-1} \widetilde{a}_{ij}^{(n)} \, e_{ij} \otimes e_{\pi(i)+n,\pi(j)+n} \ , \tag{12}$$

with

$$\widetilde{a}^{(n)} \ = \sum_{m=0}^{d-1} a^{(n+m)} \circ (\Pi S^m) \ , \qquad (\mathrm{mod}\ d) \ , \tag{13}$$

where Π is a permutation matrix corresponding to π, that is

$$\Pi_{kl} = \delta_{k,\pi(l)} \ , \tag{14}$$

and $A \circ B$ denotes the Hadamard product of $d \times d$ matrices A and B.

Theorem 1 *A circulant state ρ is PPT iff $\widetilde{a}^{(n)} \geq 0$, for $n = 0, 1, \ldots, d-1$.*

It is clear that any circulant state ρ gives rise to the completely positive map $\Lambda : M_d(\mathbb{C}) \to M_d(\mathbb{C})$ defined as follows

$$\rho = (\mathrm{id} \otimes \Lambda) P_d^+ \ , \tag{15}$$

where P_d^+ denotes the maximally entangled state in $\mathbb{C}^d \otimes \mathbb{C}^d$, that is,

$$P_d^+ = \frac{1}{d} \sum_{k,l=0}^{d-1} e_{kl} \otimes e_{kl} \ . \tag{16}$$

One easily finds the following formula for the action of Λ:

$$\Lambda(e_{kl}) = \sum_{n=0}^{d-1} a_{kl}^{(n)} e_{k+n,l+n} \ . \tag{17}$$

We call Λ a circulant quantum channel if Λ is unital, i.e. $\Lambda(\mathbb{I}) = \mathbb{I}$. It implies the following condition upon the collection of positive matrices $a^{(n)}$:

$$\sum_{k=0}^{d-1}\sum_{n=0}^{d-1} a^{(n)}_{kk} e_{k+n,k+n} = \mathbb{I} \ . \tag{18}$$

Note, that a dual map $\Lambda^\#$ defined by $\mathrm{Tr}(\rho\Lambda(X)) = \mathrm{Tr}(X\Lambda^\#(\rho))$, is defined as follows

$$\Lambda^\#(e_{kl}) = \sum_{n=0}^{d-1} a^{(n)}_{lk} e_{k+n,l+n} \ , \tag{19}$$

i.e. it is defined by the collection of $a^{(n)T}$. It is well known that if $\Lambda^\#$ is unital, then the original map Λ is trace preserving. Note, that in general Λ is neither unital nor trace preserving. In the next section we shall consider a special class of circulant states which give rise to unital and trace preserving circulant quantum channels.

Example 1 A circulant state of 2 qubits has the following form

$$\rho = \left(\begin{array}{cc|cc} a_{00} & \cdot & \cdot & a_{01} \\ \cdot & b_{00} & b_{01} & \cdot \\ \hline \cdot & b_{10} & b_{11} & \cdot \\ a_{10} & \cdot & \cdot & a_{11} \end{array} \right) \ . \tag{20}$$

where for a more transparent presentation we introduced matrices $a := a^{(0)} \geq 0$ and $b := a^{(1)} \geq 0$. Note, that a circulant state (31) is usually called X-state in quantum optics community [14]. One easily finds for the partial transposition

$$\rho^\Gamma = \left(\begin{array}{cc|cc} \widetilde{a}_{00} & \cdot & \cdot & \widetilde{a}_{01} \\ \cdot & \widetilde{b}_{00} & \widetilde{b}_{01} & \cdot \\ \hline \cdot & \widetilde{b}_{10} & \widetilde{b}_{11} & \cdot \\ \widetilde{a}_{10} & \cdot & \cdot & \widetilde{a}_{11} \end{array} \right) \ , \tag{21}$$

where the matrices $\widetilde{a} = [\widetilde{a}_{ij}]$ and $\widetilde{b} = [\widetilde{b}_{ij}]$ read as follows

$$\widetilde{a} = \left(\begin{array}{cc} a_{00} & b_{01} \\ b_{10} & a_{11} \end{array} \right) \ , \quad \widetilde{b} = \left(\begin{array}{cc} b_{00} & a_{01} \\ a_{10} & b_{11} \end{array} \right) \ . \tag{22}$$

Hence, ρ defined in (31) is PPT iff

$$\widetilde{a} \geq 0 \quad \text{and} \quad \widetilde{b} \geq 0 \ , \tag{23}$$

and hence

$$a_{00}a_{11} \geq |b_{01}|^2 \ , \qquad b_{00}b_{11} \geq |a_{01}|^2 \ . \tag{24}$$

Example 2 A circulant state of 2 qutrits has the following form

$$\rho = \left(\begin{array}{ccc|ccc|ccc} a_{00} & \cdot & \cdot & \cdot & a_{01} & \cdot & \cdot & \cdot & a_{02} \\ \cdot & b_{00} & \cdot & \cdot & \cdot & b_{01} & b_{02} & \cdot & \cdot \\ \cdot & \cdot & c_{00} & c_{01} & \cdot & \cdot & \cdot & c_{02} & \cdot \\ \hline \cdot & \cdot & c_{10} & c_{11} & \cdot & \cdot & \cdot & c_{12} & \cdot \\ a_{10} & \cdot & \cdot & \cdot & a_{11} & \cdot & \cdot & \cdot & a_{12} \\ \cdot & b_{10} & \cdot & \cdot & \cdot & b_{11} & b_{12} & \cdot & \cdot \\ \hline \cdot & b_{20} & \cdot & \cdot & \cdot & b_{21} & b_{22} & \cdot & \cdot \\ \cdot & \cdot & c_{20} & c_{21} & \cdot & \cdot & \cdot & c_{22} & \cdot \\ a_{20} & \cdot & \cdot & \cdot & a_{21} & \cdot & \cdot & \cdot & a_{22} \end{array}\right) , \tag{25}$$

where $a := a^{(0)} \geq 0$, $b := a^{(1)} \geq 0$ and $c := a^{(2)} \geq 0$. One easily finds for the partial transposition

$$\rho^\Gamma = \left(\begin{array}{ccc|ccc|ccc} \widetilde{a}_{00} & \cdot & \cdot & \cdot & \cdot & \widetilde{a}_{01} & \cdot & \widetilde{a}_{02} & \cdot \\ \cdot & \widetilde{b}_{00} & \cdot & \widetilde{b}_{01} & \cdot & \cdot & \cdot & \cdot & \widetilde{b}_{02} \\ \cdot & \cdot & \widetilde{c}_{00} & \cdot & \widetilde{c}_{01} & \cdot & \widetilde{c}_{02} & \cdot & \cdot \\ \hline \cdot & \widetilde{b}_{10} & \cdot & \widetilde{b}_{11} & \cdot & \cdot & \cdot & \cdot & \widetilde{b}_{12} \\ \cdot & \cdot & \widetilde{c}_{10} & \cdot & \widetilde{c}_{11} & \cdot & \widetilde{c}_{12} & \cdot & \cdot \\ \widetilde{a}_{10} & \cdot & \cdot & \cdot & \cdot & \widetilde{a}_{11} & \cdot & \widetilde{a}_{12} & \cdot \\ \hline \cdot & \cdot & \widetilde{c}_{20} & \cdot & \widetilde{c}_{21} & \cdot & \widetilde{c}_{22} & \cdot & \cdot \\ \widetilde{a}_{20} & \cdot & \cdot & \cdot & \cdot & \widetilde{a}_{21} & \cdot & \widetilde{a}_{22} & \cdot \\ \cdot & \widetilde{b}_{20} & \cdot & \widetilde{b}_{21} & \cdot & \cdot & \cdot & \cdot & \widetilde{b}_{22} \end{array}\right) , \tag{26}$$

where the matrices $\widetilde{a} = [\widetilde{a}_{ij}]$, $\widetilde{b} = [\widetilde{b}_{ij}]$ and $\widetilde{c} = [\widetilde{c}_{ij}]$ read as follows

$$\widetilde{a} = \begin{pmatrix} a_{00} & c_{01} & b_{02} \\ c_{10} & b_{11} & a_{12} \\ b_{20} & a_{21} & c_{22} \end{pmatrix} , \quad \widetilde{b} = \begin{pmatrix} b_{00} & a_{01} & c_{02} \\ a_{10} & c_{11} & b_{12} \\ c_{20} & b_{21} & a_{22} \end{pmatrix} , \quad \widetilde{c} = \begin{pmatrix} c_{00} & b_{01} & a_{02} \\ b_{10} & a_{11} & c_{12} \\ a_{20} & c_{21} & b_{22} \end{pmatrix} . \tag{27}$$

For more examples see [3]. Interestingly, circulant structure is preserved under realignment.

Proposition 1 *The realignment of the circulant bipartite operator*

$$A = \sum_{n,i,j=0}^{d-1} a_{ij}^{(n)} e_{ij} \otimes e_{i+n,j+n} , \tag{28}$$

reads

$$\mathrm{R}(A) = \sum_{n,i,j=0}^{d-1} R_{ij}^{(n)} e_{ij} \otimes e_{i+n,j+n} , \tag{29}$$

where

$$R_{ij}^{(n)} = a_{i+n,j}^{(j-i)} . \tag{30}$$

Example 3 The realignment of ρ defined in (31) leads to

$$\mathrm{R}(\rho) = \left(\begin{array}{cc|cc} a_{00} & \cdot & \cdot & b_{00} \\ \cdot & a_{10} & b_{10} & \cdot \\ \hline \cdot & b_{01} & a_{01} & \cdot \\ b_{11} & \cdot & \cdot & a_{11} \end{array} \right) . \tag{31}$$

Hence in this case one has

$$R^{(0)} = \left(\begin{array}{cc} a_{00} & b_{00} \\ b_{11} & a_{11} \end{array} \right) , \quad R^{(1)} = \left(\begin{array}{cc} a_{10} & b_{10} \\ b_{01} & a_{01} \end{array} \right) . \tag{32}$$

Example 4 The realignment of ρ defined in (25) leads to the circulant structure with

$$R^{(0)} = \left(\begin{array}{ccc} a_{00} & b_{00} & c_{00} \\ c_{11} & a_{11} & b_{11} \\ b_{22} & c_{22} & a_{22} \end{array} \right) , \quad R^{(1)} = \left(\begin{array}{ccc} a_{10} & b_{10} & c_{10} \\ c_{21} & a_{21} & b_{21} \\ b_{02} & c_{02} & a_{02} \end{array} \right) , \quad R^{(2)} = \left(\begin{array}{ccc} a_{20} & b_{20} & c_{20} \\ c_{01} & a_{01} & b_{01} \\ b_{12} & c_{12} & a_{12} \end{array} \right) , \tag{33}$$

and it my be easily generalized arbitrary dimension d.

3 Generalized Bell diagonal states

Consider now a simplex of Bell diagonal states [8, 10, 11, 12] defined by

$$\rho = \sum_{m,n=0}^{d-1} p_{mn} P_{mn} , \tag{34}$$

where $p_{mn} \geq 0$, $\sum_{m,n} p_{mn} = 1$ and

$$P_{mn} = (\mathbb{I} \otimes U_{mn})\, P_d^+ \,(\mathbb{I} \otimes U_{mn}^\dagger) , \tag{35}$$

with U_{mn} being the collection of d^2 unitary matrices defined as follows

$$U_{mn} e_k = \lambda^{mk} S^n e_k = \lambda^{mk} e_{k+n} , \tag{36}$$

with

$$\lambda = e^{2\pi i/d} . \tag{37}$$

The matrices U_{mn} define an orthonormal basis in the space $M_d(\mathbb{C})$ of complex $d \times d$ matrices. One easily shows

$$\mathrm{Tr}(U_{mn} U_{rs}^\dagger) = d\, \delta_{mr} \delta_{ns} . \tag{38}$$

Some authors [13] call U_{mn} generalized spin matrices since for $d = 2$ they reproduce standard Pauli matrices:

$$U_{00} = \mathbb{I} , \; U_{01} = \sigma_1 , \; U_{10} = i\sigma_2 , \; U_{11} = \sigma_3 . \tag{39}$$

Let us observe that Bell diagonal states (34) are circulant states in $\mathbb{C}^d \otimes \mathbb{C}^d$. Indeed, maximally entangled projectors P_{mn} are supported on Σ_n, that is,

$$\Pi_n = P_{0n} + \ldots + P_{d-1,n} \ , \tag{40}$$

defines a projector onto Σ_n, i.e.

$$\Sigma_n = \Pi_n(\mathbb{C}^d \otimes \mathbb{C}^d) \ . \tag{41}$$

One easily shows that the corresponding matrices $a^{(n)}$ are given by

$$a^{(n)} = HD^{(n)}H^* \ , \tag{42}$$

where H is a unitary $d \times d$ matrix defined by

$$H_{kl} := \frac{1}{\sqrt{d}}\,\lambda^{kl} \ , \tag{43}$$

and $D^{(n)}$ is a collection of diagonal matrices defined by

$$D^{(n)}_{kl} := p_{kn}\delta_{kl} \ . \tag{44}$$

One has

$$a^{(n)}_{kl} = \frac{1}{d}\sum_{m=0}^{d-1} p_{mn}\lambda^{m(k-l)} \ , \tag{45}$$

and hence it defines a circulant matrix

$$a^{(n)}_{kl} = f^{(n)}_{k-l} \ , \tag{46}$$

where the vector $f^{(n)}_m$ is the inverse of the discrete Fourier transform of p_{mn} (n is fixed).

Consider now partial transposition of Bell diagonal states. One has the following

Theorem 2 *If d is odd all matrices $\widetilde{a}^{(n)}$ are unitary equivalent*

$$\widetilde{a}^{(n)} = S^n \widetilde{a}^{(0)} S^{\dagger\, n} \ , \tag{47}$$

for $n = 0, 1, \ldots, d-1$. If d is even one has two groups of unitary equivalent matrices:

$$\widetilde{a}^{(2k)} = S^k \widetilde{a}^{(0)} S^{\dagger\, k} \ , \tag{48}$$

and

$$\widetilde{a}^{(2k+1)} = S^k \widetilde{a}^{(1)} S^{\dagger\, k} \ , \tag{49}$$

for $k = 0, 1, \ldots, d/2 - 1$.

Therefore

Corollary 1 *Bell diagonal state is PPT if*

- $\widetilde{a}^{(0)} \geq 0$ *for d odd,*

- $\widetilde{a}^{(0)} \geq 0$ *and* $\widetilde{a}^{(1)} \geq 0$ *for* d *even.*

The corresponding completely positive map $\Lambda : M_n(\mathbb{C}) \to M_n(\mathbb{C})$ is defined by the following Kraus representation

$$\Lambda(X) = \sum_{m,n=0}^{d-1} p_{mn} U_{mn} X U_{mn}^\dagger \ , \tag{50}$$

where $p_{mn} \geq 0$ and $\sum_{m,n} p_{mn} = 1$. One has $\Lambda(\mathbb{I}) = \sum_{m,n} p_{mn}\, \mathbb{I} = \mathbb{I}$, which proves that Λ is unital. Note, that the dual map

$$\Lambda^{\#}(X) = \sum_{m,n=0}^{d-1} p_{mn} U_{mn}^\dagger X U_{mn} \ , \tag{51}$$

is unital as well. Hence, Λ defines unital and trace preserving quantum channel (doubly stochastic completely positive map).

4 Special cases

In this section we analyze special classes of Bell diagonal states.

4.1 $d = 2$

For 2-qubit case one obtains the following density operator

$$a^{(n)} = \begin{pmatrix} x_n & y_n \\ y_n & x_n \end{pmatrix} \ , \tag{52}$$

where

$$x_n = \frac{1}{2}(p_{0n} + p_{1n}) \ , \quad y_n = \frac{1}{2}(p_{0n} - p_{1n}) \ , \tag{53}$$

for $n = 0, 1$. The state is PPT if and only if

$$x_0^2 \geq |y_1|^2 \ , \qquad x_1^2 \geq |y_0|^2 \ . \tag{54}$$

The above conditions imply well known result that 2-qubit Bell diagonal state is PPT (and hence separable) if and only if

$$p_{mn} \leq \frac{1}{2} \ . \tag{55}$$

4.2 $d = 3$

For $d = 3$ the Bell diagonal state is defined by the collection of 3 matrices

$$a^{(n)} = \begin{pmatrix} x_n & z_n & \overline{z}_n \\ \overline{z}_n & x_n & z_n \\ z_n & \overline{z}_n & x_n \end{pmatrix} \ , \quad n = 0, 1, 2 \ , \tag{56}$$

where

$$x_n = \frac{1}{3}(p_{0n} + p_{1n} + p_{2n}) \ , \tag{57}$$

and

$$z_n = \frac{1}{3}(p_{0n} + \lambda p_{1n} + \overline{\lambda} p_{2n}) \ . \tag{58}$$

Now, the PPT condition reduces to the positivity of $\widetilde{a}^{(0)}$

$$\widetilde{a}^{(0)} = \left(\begin{array}{ccc} x_0 & z_2 & \overline{z}_1 \\ \overline{z}_2 & x_1 & z_0 \\ z_1 & \overline{z}_0 & x_2 \end{array} \right) \ \geq \ 0 \ , \tag{59}$$

which is equivalent to the following conditions

$$x_0 x_1 \geq |z_2|^2 \ , \tag{60}$$

and

$$x_0 x_1 x_2 + 2\mathrm{Re}\, z_0 z_1 z_2 \geq x_0 |z_0|^2 + x_1 |z_1|^2 + x_2 |z_2|^2 \ . \tag{61}$$

Hence, even for $d = 3$ the PPT condition is by no means simple. It might considerably simplify if we specify x_n and z_n. Assume for example that $z_0 = 0$. Then (60)–(61) imply

$$x_0 x_1 x_2 \geq x_1 |z_1|^2 + x_2 |z_2|^2 \ . \tag{62}$$

4.3 $d = 4$

For $d = 4$ the Bell diagonal state is defined by the collection of 4 matrices

$$a^{(n)} = \left(\begin{array}{cccc} x_n & z_n & y_n & \overline{z}_n \\ \overline{z}_n & x_n & z_n & y_n \\ y_n & \overline{z}_n & x_n & z_n \\ z_n & y_n & \overline{z}_n & x_n \end{array} \right) \ , \quad n = 0,1,2,3 \ , \tag{63}$$

where

$$\begin{aligned} x_n &= \frac{1}{4}(p_{0n} + p_{1n} + p_{2n} + p_{3n}) \ , \\ y_n &= \frac{1}{4}(p_{0n} - p_{1n} + p_{2n} - p_{3n}) \ , \\ z_n &= \frac{1}{4}(p_{0n} + ip_{1n} - p_{2n} - ip_{3n}) \ . \end{aligned} \tag{64}$$

Bell diagonal state of two qutrits is PPT iff

$$\widetilde{a}^{(0)} = \left(\begin{array}{cccc} x_0 & z_4 & y_2 & \overline{z}_1 \\ \overline{z}_4 & x_2 & z_1 & y_0 \\ y_2 & \overline{z}_1 & x_0 & z_4 \\ z_1 & y_0 & \overline{z}_4 & x_2 \end{array} \right) \ \geq \ 0 \ , \quad \text{and} \quad \widetilde{a}^{(1)} = \left(\begin{array}{cccc} x_1 & z_0 & y_3 & \overline{z}_2 \\ \overline{z}_0 & x_3 & z_2 & y_1 \\ y_3 & \overline{z}_2 & x_1 & z_0 \\ z_2 & y_1 & \overline{z}_0 & x_3 \end{array} \right) \ \geq \ 0 \ . \tag{65}$$

4.4 Special form of p_{mn}

Consider now special examples of Bell diagonal states by specifying the structure of probability distribution p_{mn}. Let

$$p_{mn} = \delta_{mk}\pi_n \ , \tag{66}$$

with $\pi_0 + \ldots + \pi_{d-1} = 1$. It gives rise to

$$\rho = \sum_{n=0}^{d-1} \pi_n P_{kn} \ . \tag{67}$$

For example if $d = 2$ and $k = 0$ one obtains

$$\rho = \frac{1}{2} \left(\begin{array}{cc|cc} \pi_0 & \cdot & \cdot & \pi_0 \\ \cdot & \pi_1 & \pi_1 & \cdot \\ \hline \cdot & \pi_1 & \pi_1 & \cdot \\ \pi_0 & \cdot & \cdot & \pi_0 \end{array} \right) \ . \tag{68}$$

This state is separable if and only if $\pi_0 = \pi_1 = 1/2$. One easily generalizes this observation as follows

Proposition 2 *Bell diagonal state (67) is separable if and only if*

$$\pi_0 = \ldots = \pi_{d-1} = \frac{1}{d} \ . \tag{69}$$

Another characteristic class corresponds to

$$p_{mn} = q_m p_n \ , \tag{70}$$

i.e. p_{mn} represents the product distribution. One has

$$\rho = \sum_{k,l=0}^{d-1} p_{kl} P_{kl} = \rho_0 \oplus \ldots \oplus \rho_{d-1} \ , \tag{71}$$

where

$$\rho_n = p_n \sum_{m=0}^{d-1} q_m P_{mn} \ . \tag{72}$$

Note, that matrices $a^{(n)}$ are related as follows

$$a^{(n)} = p_n a \ , \tag{73}$$

where the matrix a reads

$$a_{kl} = \frac{1}{d} \sum_{m=0}^{d-1} \lambda^{m(k-l)} \, q_m \ . \tag{74}$$

Proposition 3 *Bell diagonal state (71) is separable if and only if*

$$p_0 = \ldots = p_{d-1} = \frac{1}{d} \ . \tag{75}$$

4.5 Generalized lattice states

Consider now a family of unitary operators acting on N copies of $\mathbb{C}^d$

$$U_{\boldsymbol{mn}} = U_{m_1 n_1} \otimes \ldots \otimes U_{m_N n_N} \ , \tag{76}$$

where $\mathbf{m} = (m_1, \ldots, m_N)$ and $\mathbf{n} = (n_1, \ldots, n_N)$. It is clear that $U_{\boldsymbol{mn}}$ defines a family of $D^2 = d^{2N}$ unitary operators in in $\mathbb{C}^D = \mathbb{C}^{d \otimes N}$. Note that

$$\mathrm{Tr}(U_{\boldsymbol{mn}} U_{\boldsymbol{kl}}^\dagger) = D\, \delta_{\boldsymbol{mk}} \delta_{\boldsymbol{nl}} \ . \tag{77}$$

Now, let $|\psi_D^+\rangle$ denote a maximally entangled state in $\mathbb{C}^D \otimes \mathbb{C}^D$ defined by

$$\psi_D^+ = \frac{1}{\sqrt{D}} \sum_{\boldsymbol{k}} e_{\boldsymbol{k}} \otimes e_{\boldsymbol{k}} \ , \tag{78}$$

where

$$e_{\boldsymbol{k}} = e_{k_1} \otimes \ldots \otimes e_{k_N} \ . \tag{79}$$

One defines a family of maximally entangled states by

$$|\psi_{\boldsymbol{mn}}\rangle = (\mathbb{I} \otimes U_{\boldsymbol{mn}}) |\psi_D^+\rangle \ . \tag{80}$$

These states are parameterized a point $(\mathbf{m}, \mathbf{n})$ in the N-dimensional lattice $L_{(N)}^{(d)}$ consisting of D^2 points. Now, a generalized lattice state is defined by a collection of points from $L_{(N)}^{(d)}$: for any subset $I \subset L_{(N)}^{(d)}$ one defines

$$\rho_I = \frac{1}{|I|} \sum_{(\boldsymbol{m},\boldsymbol{n}) \in I} P_{\boldsymbol{mn}} \ , \tag{81}$$

where $P_{\boldsymbol{mn}} = |\psi_{\boldsymbol{mn}}\rangle\langle\psi_{\boldsymbol{mn}}|$ and $|I|$ stands for the cardinality of I. Clearly, $1 \leq |I| \leq |L_{(N)}^{(d)}| = D^2$. Let us observe that the above construction generalized a class of lattice states presented in [15, 16, 17]. Lattice states of Benatti et. al. correspond to $d = 2$. In this case U_{mn} are defined in terms of Pauli matrices (see formula (39)).

5 Bound entangled Bell diagonal states

5.1 Two qutrits

Consider the following family of Bell diagonal states

$$\rho_\varepsilon = N_\varepsilon (P_{00} + \varepsilon \Pi_1 + \varepsilon^{-1} \Pi_2) \ , \quad \varepsilon > 0 \ , \tag{82}$$

where the projectors Π_k are defined in (40) and the normalization factor reads

$$N_\varepsilon = \frac{1}{1 + \varepsilon + \varepsilon^{-1}} \ . \tag{83}$$

It corresponds to (cf. formulae (64) and (58))

$$x_0 = \frac{N_\varepsilon}{3} \ , \quad x_1 = \frac{N_\varepsilon}{3}\, \varepsilon \ , \quad x_2 = \frac{N_\varepsilon}{3}\, \varepsilon^{-1} \ , \tag{84}$$

and

$$z_0 = \frac{N_\varepsilon}{3} \ , \quad z_1 = z_2 = 0 \ . \tag{85}$$

Hence, conditions (60)–(61) are trivially satisfied showing that (82) defines a family of PPT states. Now, it is well known [21] that ρ_ε is separable if and only if $\varepsilon = 1$. Hence, for $\varepsilon \neq 1$ it defines a family of bound entangled state in $\mathbb{C}^3 \otimes \mathbb{C}^3$. The entanglement of ρ_ε can be detected by using a realignment criterion [5]. In the next section we show that it can be detected also by the Bell diagonal entanglement witness. Note, that asymptotically

$$\lim_{\varepsilon \to 0} \rho_\varepsilon = \frac{1}{3}\, \Pi_2 \ , \quad \lim_{\varepsilon \to \infty} \rho_\varepsilon = \frac{1}{3}\, \Pi_1 \ , \tag{86}$$

that is, one obtains separable states defined by normalized separable projectors onto Σ_2 and Σ_1, respectively.

5.2 Two qudits

Consider a family of states in $\mathbb{C}^d \otimes \mathbb{C}^d$ defined by [18, 20]

$$\rho_\gamma = \frac{1}{N_\gamma} \sum_{i,j=0}^{d-1} e_{ij} \otimes A^\gamma_{ij} \, , \tag{87}$$

where $d \times d$ matrices

$$A^\gamma_{ij} = \left\{ \begin{array}{cl} e_{ij} & \text{for } i \neq j \, , \\ e_{00} + a_\gamma e_{11} + \sum_{\ell=2}^{d-2} e_{\ell\ell} + b_\gamma e_{d-1,d-1} & \text{for } i = j = 0 \, , \\ S^{j-1} A^\gamma_{00} S^{\dagger j-1} & \text{for } i = j \neq 1 \end{array} \right. \tag{88}$$

with

$$a_\gamma = \frac{1}{d}(\gamma^2 + d - 1) \, , \qquad b_\gamma = \frac{1}{d}(\gamma^{-2} + d - 1) \ , \tag{89}$$

and the normalization factor reads

$$N_\gamma = d^2 - 2 + \gamma^2 + \gamma^{-2} \ . \tag{90}$$

It gives the following spectral decomposition

$$\rho_\gamma = \frac{1}{N_\gamma} \left(dP_{00} + a_\gamma \Pi_1 + \sum_{\ell=2}^{d-2} \Pi_\ell + b_\gamma \Pi_{d-1} \right) \ . \tag{91}$$

In particular for $d = 3$ one obtains the following matrix representation:

$$\rho_\gamma = \frac{1}{N_\gamma} \left(\begin{array}{ccc|ccc|ccc} 1 & \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot & 1 \\ \cdot & a_\gamma & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & b_\gamma & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \hline \cdot & \cdot & \cdot & b_\gamma & \cdot & \cdot & \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot & \cdot & \cdot & a_\gamma & \cdot & \cdot & \cdot \\ \hline \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & a_\gamma & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & b_\gamma & \cdot \\ 1 & \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot & 1 \end{array} \right) = \frac{1}{N_\gamma}(3P_{00} + a_\gamma \Pi_1 + b_\gamma \Pi_2) \ , \tag{92}$$

with $a_\gamma = \frac{1}{3}(\gamma^2 + 2)$, $b_\gamma = \frac{1}{3}(\gamma^{-2} + 2)$ and the normalization factor $N_\gamma = 7 + \gamma^2 + \gamma^{-2}$.

6 Bell diagonal entanglement witnesses

Interestingly many well known entanglement witnesses displaying circulant structure are Bell diagonal. It is well known that any entanglement witness W can be represented as a difference $W = W_+ - W_-$, where both W_+ and W_- are semi-positive operators in $\mathcal{B}(\mathbb{C}^d \otimes \mathbb{C}^d)$. However, there is no general method to recognize that W defined by $W_+ - W_-$ is indeed an EW. An interesting class of such witnesses may be constructed using their spectral properties [22, 23]. Let ψ_α ($\alpha = 0, 1, \ldots, d^2 - 1$) be an orthonormal basis in $\mathbb{C}^d \otimes \mathbb{C}^d$ and denote by P_α the corresponding projector $P_\alpha = |\psi_\alpha\rangle\langle\psi_\alpha|$. Now, take d^2 semi-positive numbers $\lambda_\alpha \geq 0$ such that λ_α is strictly positive for $\alpha > L$, and define

$$W_- = \sum_{\alpha=0}^{L} \lambda_\alpha P_\alpha \ , \quad W_+ = \sum_{\alpha=L}^{d^2-1} \lambda_\alpha P_\alpha \ , \tag{93}$$

where L is an arbitrary integer $0 < L < d^2 - 1$. This construction guarantees that W_+ is strictly positive and all zero modes and strictly negative eigenvalues of W are encoded into W_-. Consider normalized vector $\psi \in \mathbb{C}^d \otimes \mathbb{C}^d$ and let $s_1(\psi) \geq \ldots \geq s_d(\psi)$ denote its Schmidt coefficients. For any $1 \leq k \leq d$ one defines k-norm of ψ by the following formula

$$||\psi||_k^2 = \sum_{j=1}^{k} s_j^2(\psi) \ . \tag{94}$$

It is clear that

$$||\psi||_1 \leq ||\psi||_2 \leq \ldots \leq ||\psi||_d \ . \tag{95}$$

Note that $||\psi||_1$ gives the maximal Schmidt coefficient of ψ, whereas due to the normalization, $||\psi||_d^2 = \langle\psi|\psi\rangle = 1$. One proves [22] the following

Theorem 3 *Let* $\sum_{\alpha=0}^{L-1} ||\psi_\alpha||_k^2 < 1$ *. If the following spectral conditions are satisfied*

$$\lambda_\alpha \geq \mu_k \ , \quad \alpha = L, \ldots, d^2 - 1 \ , \tag{96}$$

where

$$\mu_\ell := \frac{\sum_{\alpha=0}^{L-1} \lambda_\alpha ||\psi_\alpha||_\ell^2}{1 - \sum_{\alpha=0}^{L-1} ||\psi_\alpha||_\ell^2} \ , \tag{97}$$

then W is an k-EW. If moreover $\sum_{\alpha=1}^{L} ||\psi_\alpha||_{k+1}^2 < 1$ and

$$\mu_{k+1} > \lambda_\alpha \ , \quad \alpha = L, \ldots, d^2 - 1 \ , \tag{98}$$

then W being k-EW is not $(k+1)$-EW.

Let us observe that if ψ is maximally entangled then

$$||\psi||_k^2 = \frac{k}{d} \ . \tag{99}$$

Consider, therefore, the family of Bell diagonal states ψ_{mn}. On has the following

Corollary 2 *If $L < d$ and*

$$\lambda_\alpha \geq \mu_1 \ , \quad \alpha = L, \ldots, d^2 - 1 \ , \tag{100}$$

with $\mu_1 = \frac{1}{d-L} \sum_{\alpha=0}^{L-1} \lambda_\alpha$, then $W = W_+ - W_-$ defines Bell diagonal entanglement witness.

Example 5 Consider well known entanglement witness in $d = 2$ represented by the flip operator

$$F = \left(\begin{array}{cc|cc} 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot \\ \hline \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 \end{array} \right) \ . \tag{101}$$

Note that

$$F = P_{00} + P_{10} + P_{01} - P_{11} \ , \tag{102}$$

which proves that F is Bell diagonal and possesses single negative eigenvalue.

Example 6 A family of EWs in $\mathbb{C}^3 \otimes \mathbb{C}^3$ defined by [24]

$$W[a,b,c] \ = \left(\begin{array}{ccc|ccc|ccc} a & \cdot & \cdot & \cdot & -1 & \cdot & \cdot & \cdot & -1 \\ \cdot & b & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & c & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \hline \cdot & \cdot & \cdot & c & \cdot & \cdot & \cdot & \cdot & \cdot \\ -1 & \cdot & \cdot & \cdot & a & \cdot & \cdot & \cdot & -1 \\ \cdot & \cdot & \cdot & \cdot & \cdot & b & \cdot & \cdot & \cdot \\ \hline \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & b & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & c & \cdot \\ -1 & \cdot & \cdot & \cdot & -1 & \cdot & \cdot & \cdot & a \end{array} \right) \ , \tag{103}$$

with $a, b, c \geq 0$. Necessary and sufficient conditions for $W[a,b,c]$ to be an EW are

1. $0 \leq a < 2$,

2. $a+b+c \geq 2$,

3. if $a \leq 1$, then $bc \geq (1-a)^2$.

A family $W[a,b,c]$ generalizes celebrated Choi indecomposable witness corresponding to $a=b=1$ and $c=0$. One finds the following spectral representation

$$W[a,b,c] = (a-2)P_{00} + (a+1)(P_{10}+P_{20}) + b\Pi_1 + c\Pi_2 \ , \tag{104}$$

which shows that $W[a,b,c]$ is Bell diagonal with a single negative eigenvalue '$a-2$'.

Example 7 Consider a family of EWs defined by [20]

$$W_{\lambda,\mu} \ = \left(\begin{array}{ccc|ccc|ccc} 1 & \cdot & \cdot & \cdot & -1 & \cdot & \cdot & \cdot & -1 \\ \cdot & 1+\mu & \cdot & \cdot & \cdot & \mu & \mu & \cdot & \cdot \\ \cdot & \cdot & \lambda & \lambda & \cdot & \cdot & \cdot & \lambda & \cdot \\ \hline \cdot & \cdot & \lambda & \lambda & \cdot & \cdot & \cdot & \lambda & \cdot \\ -1 & \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot & -1 \\ \cdot & \mu & \cdot & \cdot & \cdot & 1+\mu & \mu & \cdot & \cdot \\ \hline \cdot & \mu & \cdot & \cdot & \cdot & \mu & 1+\mu & \cdot & \cdot \\ \cdot & \cdot & \lambda & \lambda & \cdot & \cdot & \cdot & \lambda & \cdot \\ -1 & \cdot & \cdot & \cdot & -1 & \cdot & \cdot & \cdot & 1 \end{array} \right) \ , \tag{105}$$

with $\lambda,\mu \geq 0$. Note that $W_{0,0} = W[1,1,0]$. One obtains for the spectral decomposition

$$W_{\lambda,\mu} = -3P_{00} + 2\Pi_0 + \Pi_1 + 3\mu P_{01} + 3\lambda P_{02} \ . \tag{106}$$

Let $\gamma > 0$. One shows [20] that for

$$\lambda < \frac{1-\gamma^2}{2+\gamma^{-2}} \ , \tag{107}$$

and

$$\mu < \frac{1-\gamma^2 - \lambda(2+\gamma^{-2})}{2+\gamma^2} \ , \tag{108}$$

$W_{\lambda,\mu}$ defines an indecomposable EW due to $\mathrm{Tr}(W_{\lambda,\mu}\rho_\gamma) < 0$.

Example 8 Entanglement witness corresponding to the reduction map $\Lambda(X) = \mathbb{I}\mathrm{Tr}X - X$ in $M_d(\mathbb{C})$. One has

$$W = \frac{1}{d}\,\mathbb{I}\otimes\mathbb{I} - P^+_d = \frac{1}{d}\sum_{k,l=0}^{d-1} P_{kl} - P_{00} \ , \tag{109}$$

which shows that W is Bell diagonal with a single negative eigenvalue $(1-d)/d$.

Example 9 A family of EWs in $\mathbb{C}^d \otimes \mathbb{C}^d$ defined by [18, 20]

$$W_{d,k} = \sum_{i,j=0}^{d-1} e_{ij} \otimes X^{d,k}_{ij} \ , \tag{110}$$

where the $d \times d$ matrices $X_{ij}^{d,k}$ are defined as

$$X_{ij}^{d,k} = \begin{cases} (d-k-1)e_{ii} + \sum_{\ell=1}^{k} S^\ell \, e_{ii} \, S^\ell & \text{for } i = j \,, \\ -e_{ij} & \text{for } i \neq j \,, \end{cases} \tag{111}$$

It is well known [18] that $W_{d,k}$ defines an indecomposable EW for $k = 1, 2, \ldots, d-2$. For $k = d-1$ it reproduces the witness corresponding to the reduction map. Note that for $d = 3$ and $k = 1$ it reproduces $W[a, b, c]$ with $a = b = 1$ and $c = 0$. On easily finds the following spectral representation

$$W_{d,k} = (d-k)\Pi_0 + \sum_{\ell=1}^{k} \Pi_k - dP_{00} \ , \tag{112}$$

showing that $W_{d,k}$ is Bell diagonal and the single negative eigenvalue corresponds to the maximally entangled state P_{00}.

7 Conclusions

We analyzed a class of bipartite circulant states which are diagonal with respect to generalized Bell (magic) basis. Such states are characterized by an elegant symmetry which considerably simplifies their analysis. We analyzed several examples of bound entangled states and provided corresponding entanglement witnesses which are Bell diagonal.

Acknowledgments

This work was partially supported by the Polish Ministry of Science and Higher Education Grant No 3004/B/H03/2007/33.

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