Class of Bell-diagonal entanglement witnesses in $\mathbb{C}^4 \otimes \mathbb{C}^4$: Optimization and the spanning property

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Two classes of Bell-diagonal indecomposable entanglement witnesses in $\mathbb{C}^4 \otimes \mathbb{C}^4$ are considered. Within the first class, we find a generalization of the well-known Choi witness from $\mathbb{C}^3 \otimes \mathbb{C}^3$, while the second one contains the reduction map. Interestingly, contrary to the $\mathbb{C}^3 \otimes \mathbb{C}^3$ case, the generalized Choi witnesses are no longer optimal. We perform an optimization procedure of finding spanning vectors that eventually gives rise to optimal witnesses. Operators from the second class turn out to be optimal, however, without the spanning property. This analysis sheds light onto the intricate structure of optimal entanglement witnesses.

I. INTRODUCTION

Quantum entanglement is arguably the most peculiar feature of quantum theory that also demarcates it from the classical one [1–3]. It is a crucial ingredient in quantum information processing applications, such as (entanglement-based) quantum cryptography [4], quantum dense coding [5], quantum teleportation [6], measurement-based computation [7], and so on. However, despite tremendous progress in the understanding of entanglement, we still lack its full characterization, especially in terms of entanglement detection, i.e., methods that can faithfully discriminate between entangled and separable states. Indeed, a wealth of various operational entanglement criteria for bipartite quantum states already exist in the literature, in particular, the partial transposition criterion [8,9], the majorization criterion [10], the cross-norm or realignment criterion [11–13], and the covariance matrix criterion [14,15] to name a few. However, due to a very rich structure of entanglement, most of the currently available techniques are either only sufficient in characterization or restricted to a narrow class of states [1–3]. Therefore, it is of paramount importance to have robust ways of entanglement detection, in particular operational (i.e., measurable) tools are of special interest. One such method is based on the notion of entanglement witness (EW), an observable that is capable of detecting entangled states [9,16–18]. The central concept of EWs is based on the ideas of the Hahn-Banach theorem on normed linear spaces [19]. A special subclass of EWs called optimal entanglement witnesses (OEWs) is considered *the gold standard* for measurable entanglement detection since the observables that are OEWs allow to detect the largest set (in terms of its cardinality) of entangled states [20–22]. Thus, making them a suitable choice for investigation.

In addition to this, a few experiments were performed in the last two decades on whether a certain quantum state is entangled or separable. The authors of Ref. [23] proposed a procedure for measuring the entanglement of an unknown state by successively measuring witness operators, which was experimentally realized in Ref. [24]. The authors of Ref. [25] described a new method to detect the entanglement of quantum states, about which nothing is known except the dimension, using random local measurements. Moreover, the authors of Ref. [26] experimentally demonstrated the detection of entanglement polytopes in a four-qubit system. Additionally, quantum entanglement was extensively studied in terms of quantum resources [27–29], in particular, as a crucial ingredient for quantum computation [7,30,31], where multipartite entanglement is exploited (see, for example, the case of variational quantum algorithms [32,33]). The multipartite case is substantially more complex to analyze, however, some approximate methods already exist, even ones that are based on the extension of EWs. These extensions can be measured in quantum computing hardware [34] and allows to asses if this quantum resource is exploited in the computation, despite the detrimental effects of noise.

In this paper, we analyze a family of EWs in $\mathbb{C}^4 \otimes \mathbb{C}^4$, which are Bell diagonal and covariant w.r.t. the maximal commutative subgroup of the unitary group U(4). This is a highly symmetric family that can be analyzed in detail [35]. We consider a class of EWs in $\mathbb{C}^4 \otimes \mathbb{C}^4$ displaying a characteristic circular structure. Such a class of circulant witnesses in $\mathbb{C}^3 \otimes \mathbb{C}^3$ without any connection to entanglement theory was proposed in Ref. [36] as a generalization of a seminal indecomposable positive map of Choi [37]. Further analysis was provided in Refs. [38–40]. In particular, it was shown that these witnesses are optimal [38,40].

In our paper, we show that the corresponding class of circulant witness $\mathbb{C}^4 \otimes \mathbb{C}^4$ splits into two subclasses: one class provides a generalization of the Choi witnesses in $\mathbb{C}^3 \otimes \mathbb{C}^3$ and the other contains the witness corresponding to the reduction map. Interestingly, contrary to $\mathbb{C}^3 \otimes \mathbb{C}^3$ the generalized Choi witnesses are no longer optimal. Following a general

framework [20,21] (see also Ref. [22] for a slightly different approach) we perform an optimization procedure which eventually gives rise to optimal witnesses satisfying the spanning property. Due to the symmetry of the considered class, the optimization procedure can be performed analytically. We show that the witnesses from the second class are optimal, however, without the spanning property. We believe that our analysis in $\mathbb{C}^4 \otimes \mathbb{C}^4$ sheds a new light into the structure of optimal entanglement witnesses and can find applications in experimental entanglement detection.

This paper is organized as follows. In Sec. II, we briefly introduce the theory of the optimal entanglement witness. In Sec. III, we present the covariant Bell-diagonal entanglement witnesses in $\mathbb{C}^n \otimes \mathbb{C}^n$ and also describe the corresponding entanglement witness in $\mathbb{C}^3 \otimes \mathbb{C}^3$ and $\mathbb{C}^4 \otimes \mathbb{C}^4$. The main results on the optimality of the introduced classes is given in Sec. IV. Finally, in Sec. V we provide concluding remarks.

II. PRELIMINARIES

The most general approach to discriminate between separable and entangled states of a quantum composite system living in $\mathcal{H}_A \otimes \mathcal{H}_B$ is based on the notion of positive (but not completely positive) maps or equivalently entanglement witnesses (EWs) [2,3,9,16–18,41–43]. A state represented by a density operator ρ in $\mathcal{H}_A \otimes \mathcal{H}_B$ is separable iff it can be represented as a mixture of product states $\rho = \sum_k p_k \rho_A^{(k)} \otimes \rho_B^{(k)}$, with $\rho_A^{(k)}$ and $\rho_B^{(k)}$ being density operators of subsystems A and B, respectively [44]. Recall, that a Hermitian operator W acting on $\mathcal{H}_A \otimes \mathcal{H}_B$ is an EW [17,18] if $\langle \psi \otimes \phi | W | \psi \otimes \phi \rangle \geqslant 0$ but W is not a positive operator (cf. also Refs. [45,46] for the concept of the ultra EW and mirror EW, respectively). A state ρ is entangled if and only if there exists an EW W such that $\mathrm{Tr}(W\rho) < 0$. Equivalently, a bipartite state ρ living in $\mathcal{H}_A \otimes \mathcal{H}_B$ is entangled iff there exists a positive map Φ such that $(\mathbb{1}_A \otimes \Phi)\rho$ is no longer a positive operator ($\mathbb{1}_A$ denotes an identity map acting on subsystem A).

In the qubit-qubit or qubit-qutrit case the situation is fully solved: a state ρ is separable if and only if it is PPT, i.e., its partial transposition is positive [$\rho^\Gamma = (\mathbb{1}_A \otimes T)\rho \geqslant 0$] [8,47]. However, in general the so-called separability problem is notoriously hard, that is, there exist PPT states which are entangled (they belong to the class of so-called bound entangled states [2]).

Recall, that an EW W is decomposable if

$$W = A + B^\Gamma, \qquad (1)$$

where $A, B \geqslant 0$ and Γ denotes the partial transposition. It is clear from the definition that a decomposable EW is unable to detect an entangled PPT state. Therefore, it is more interesting to examine EWs that are of indecomposable form, i.e., they fail to be represented in the form of Eq. (1). Equivalently, a linear positive map Φ is decomposable if $\Phi = \Lambda_1 + \Lambda_2 \circ T$, where Λ_1, Λ_2 are completely positive and T denotes transposition.

Given an EW, one may define a set of entangled states $\mathcal{D}_W$ detected by W, that is, $\mathcal{D}_W = \{\rho \mid \mathrm{Tr}(W\rho) < 0\}$. It is straightforward that if $\mathcal{D}_W \supset \mathcal{D}_{\tilde{W}}$, then W is more effective than $\tilde{W}$ since it detects more entangled states than $\tilde{W}$ does. Following the authors of Refs. [20,21], an entanglement witness W is

optimal if there is no other EW W' such that $\mathcal{D}_W \subset \mathcal{D}_{W'}$. Therefore, the knowledge of optimal EWs is sufficient for the full characterization of separable or entangled states.

In this regard, the following sufficient condition for optimality was provided in Ref. [20]: if a set of product vectors $|\psi_k \otimes \phi_k\rangle$ satisfying

$$\langle \psi_k \otimes \phi_k | W | \psi_k \otimes \phi_k \rangle = 0, \qquad (2)$$

span $\mathcal{H}_A \otimes \mathcal{H}_B$, then W is optimal. Therefore, one can say that such W has the spanning property. Several examples of EWs satisfying (2) (hence optimal) already exist in the literature [38,48–53] (cf. also review papers [54,55]). Since the condition (2) is only sufficient, one may identify optimal EWs without the spanning property. In Ref. [56], the authors provided such an example for a decomposable case.

III. COVARIANT BELL-DIAGONAL ENTANGLEMENT WITNESSES IN $\mathbb{C}^n \otimes \mathbb{C}^n$

Let us consider an n-dimensional Hilbert space. By fixing a computational basis $\{|0\rangle, \ldots, |n-1\rangle\}$, we introduce a family of Weyl unitary operators U_{mk} defined via [57–59]

$$U_{mk}|\ell\rangle = \omega^{m\ell}|\ell + k\rangle \,(\mathrm{mod}\,n), \qquad (3)$$

with $\omega = e^{2\pi i/n}$. The Weyl operators (matrices) satisfy

$$U_{k\ell}U_{rs} = \omega^{ks}U_{k+r,\ell+s}, \qquad (4)$$

together with $U_{k\ell}^* = U_{-k\ell}$, $U_{k\ell}^\dagger = \omega^{k\ell}U_{-k,-\ell}$, and $\mathrm{Tr}(U_{k\ell}U_{rs}^\dagger) = n\,\delta_{kr}\delta_{\ell s}$ (with all index summations being modulo n). One can define the generalized Bell states in $\mathbb{C}^n \otimes \mathbb{C}^n$ via

$$|\psi_{k\ell}\rangle = \mathbb{1}_n \otimes U_{k\ell}|\psi_n^+\rangle, \qquad (5)$$

where $|\psi_n^+\rangle = 1/\sqrt{n} \sum_{k=0}^{n-1} |k \otimes k\rangle$ stands for the canonical maximally entangled states. A bipartite operator X in $\mathbb{C}^n \otimes \mathbb{C}^n$ is Bell diagonal if

$$X = \sum_{k,\ell=0}^{n-1} x_{k\ell} P_{k\ell}, \qquad (6)$$

where $P_{k\ell} = |\psi_{k\ell}\rangle\langle\psi_{k\ell}|$. Consider now a maximal commutative subgroup of $\mathrm{U}(n)$

$$T(n) = \left\{ \mathrm{U} \in \mathrm{U}(n) \,\middle|\, \mathrm{U} = \sum_{k=0}^{n-1} e^{i\phi_k}|k\rangle\langle k| \right\}, \qquad (7)$$

with $\phi_k \in \mathbb{R}$. Moreover, a bipartite operator X is said to be $T \otimes T^*$ covariant whenever

$$\mathrm{U} \otimes \mathrm{U}^* X (\mathrm{U} \otimes \mathrm{U}^*)^\dagger = X, \qquad (8)$$

for any $\mathrm{U} \in T(n)$. Actually, any covariant operator has the following structure

$$X = \sum_{k,\ell=0}^{n-1} A_{kl}|k\rangle\langle k| \otimes |\ell\rangle\langle \ell| + \sum_{k \neq \ell=0}^{n-1} B_{kl}|k\rangle\langle \ell| \otimes |k\rangle\langle \ell|, \quad (9)$$

with complex parameters $A_{k\ell}$ and $B_{k\ell}$. In this paper we are going to analyze the Hermitian Bell-diagonal operators which are $T \otimes T^*$ covariant. It turns out [58–60] that for such operators the Hermitian matrix $A_{k\ell}$ is circulant, i.e., $A_{k\ell} = \alpha_{k-\ell}$

for some real vector $(\alpha_0, \alpha_1, \ldots, \alpha_{n-1})$. Moreover, all B_{kl} are constant, i.e., $B_{k\ell} = \beta \in \mathbb{R}$.

Now the following Proposition provides the sufficient condition for the circulant matrix $A_{k\ell}$ and the parameter β that guarantee that Eq. (9) defines a legitimate entanglement witness.

Proposition 1. If the circulant matrix $A_{k\ell}$ satisfies the following constraints [61]

$$\alpha_0 + \alpha_1 + \ldots + \alpha_{n-1} = n - 1, \qquad (10)$$

together with

$$AA^T = \mathbb{I} + (n-2)\mathbb{J}, \qquad (11)$$

where $\mathbb{J}_{k\ell} = 1$, then

$$W = \sum_{k,\ell=0}^{n-1} \alpha_{k-l} |k\rangle\langle k| \otimes |\ell\rangle\langle\ell| - \sum_{k\neq\ell=0}^{n-1} |k\rangle\langle\ell| \otimes |k\rangle\langle\ell|, \quad (12)$$

defines an EW.

Introducing the following projectors

$$\Pi_k = P_{k0} + P_{k1} + \ldots + P_{k,n-1}, \qquad (13)$$

for $k = 0, 1, \ldots, n-1$, formula (12) can be rewritten in the compact form as

$$W = (\alpha_0 + 1)\Pi_0 + \alpha_1 \Pi_1 + \ldots + \alpha_{n-1}\Pi_{n-1} - nP_n^+, \quad (14)$$

where $P_n^+ = |\psi_n^+\rangle\langle\psi_n^+|$ stands for the projector onto the canonical maximally entangled state.

A. EWs in $\mathbb{C}^3 \otimes \mathbb{C}^3$

For $n = 3$ let us use the following notation $a = \alpha_0$, $b = \alpha_1$, $c = \alpha_2$ and hence the circulant matrix $A_{k\ell}$ has the structure

$$A = \begin{pmatrix} a & b & c \\ c & a & b \\ b & c & a \end{pmatrix}. \qquad (15)$$

Conditions (10) and (11) imply

$$a + b + c = 2, \qquad (16)$$

$$a^2 + b^2 + c^2 = 2, \qquad (17)$$

$$ab + bc + ca = 1, \qquad (18)$$

which, after simple algebra, gives rise to

$$a + b + c = 2, \quad a^2 + b^2 + c^2 = 2, \qquad (19)$$

or equivalently [36]

$$a + b + c = 2, \quad bc = (a-1)^2. \qquad (20)$$

The corresponding EW (14) reads as follows:

$$W[a, b, c] = (a+1)\Pi_0 + b\,\Pi_1 + c\,\Pi_2 - P_3^+. \qquad (21)$$

Hence the above class may be parameterized by a single parameter $\phi \in [0, 2\pi)$ [39,62]

$$a = \tfrac{2}{3}(1 + \cos\phi),$$
$$b = \tfrac{1}{3}(2 - \cos\phi - \sqrt{3}\sin\phi),$$
$$c = \tfrac{1}{3}(2 - \cos\phi + \sqrt{3}\sin\phi). \qquad (22)$$

One proves [38] (see also Ref. [40] for another proof) that if $a \leqslant 1$, then $W[a, b, c]$ defines an optimal EW. Moreover, if $a < 1$, then $W[a, b, c]$ enjoys spanning property [38,40]. However, for $a = 1$, two EWs correspond to Choi maps $W[1, 1, 0]$ and $W[1, 0, 1]$ for which there are only seven vectors $|\psi_k \otimes \phi_k\rangle$ satisfying $\langle\psi_k \otimes \phi_k|W[a, b, c]|\psi_k \otimes \phi_k\rangle = 0$.

B. EWs in $\mathbb{C}^4 \otimes \mathbb{C}^4$

For $n = 4$, one has the corresponding circulant matrix

$$A = \begin{pmatrix} a & b & c & d \\ d & a & b & c \\ c & d & a & b \\ b & c & d & a \end{pmatrix}, \qquad (23)$$

where $d = \alpha_3$. Conditions (10) and (11) imply

$$a + b + c + d = 3, \qquad (24)$$

$$a^2 + b^2 + c^2 + d^2 = 3, \qquad (25)$$

$$ac + bd = 1, \qquad (26)$$

$$(a + c)(b + d) = 2. \qquad (27)$$

Simple algebra provides two solutions: class I is characterized by the following condition

$$a + c = 2, \quad b + d = 1, \quad bd = (1-a)^2, \qquad (28)$$

whereas class II is characterized by the following condition

$$a + c = 1, \quad b + d = 2, \quad ac = (1-b)^2. \qquad (29)$$

The corresponding EW has the following form:

$$W[a, b, c, d] = (a+1)\Pi_0 + b\,\Pi_1 + c\,\Pi_2 + d\,\Pi_3 - P_4^+. \qquad (30)$$

In the next section, we provide the detailed analysis of these two classes of EWs.

IV. OPTIMALITY

The key question we address in this section is whether or not EWs constructed in the previous section for $n = 4$ are optimal.

A. Class I

For the class defined by Eq. (28), we introduce the following parametrization:

$$a = \tfrac{1}{2}(2 - \sin\theta),$$
$$b = \tfrac{1}{2}(1 + \cos\theta),$$
$$c = 2 - a,$$
$$d = 1 - b, \qquad (31)$$

with $\theta \in [0, \pi]$. With this parametrization of θ, we express the corresponding entanglement witness for this class I as $W_I(\theta)$. Here $\theta = 0$ corresponds to $W[1, 1, 1, 0]$ which is the generalization of the Choi EW from $M_3(\mathbb{C})$. Note that $M_3(\mathbb{C})$ denotes a set of 3×3 complex matrices. Similarly, for $\theta = \pi$, we get another Choi-like witness $W[1, 0, 1, 1]$. It is important to mention here that the witness $W[a, b, c, d]$ is decomposable

only if $b = d$ [60], which is equivalent to $\theta = \pi/2$. To check the optimality of the entanglement witness $W_I(\theta)$ for $\theta \neq \frac{\pi}{2}$, let us look for a family of vectors $|\psi_k \otimes \phi_k\rangle$ satisfying Eq. (2). For that purpose, we introduce a vector $|\psi\rangle \in \mathbb{C}^4$ given by

$$|\psi\rangle = \sum_{k=0}^{3} e^{i\beta_k}|k\rangle, \qquad (32)$$

for arbitrary (real) phases β_k, and we observe that

$$\langle\psi \otimes \psi^*|W[a,b,c,d]|\psi \otimes \psi^*\rangle = 0. \qquad (33)$$

One has the following

Proposition 2. The vectors $|\psi_k \otimes \psi_k^*\rangle \in \mathbb{C}^n \otimes \mathbb{C}^n$ with

$$|\psi_k\rangle = \sum_{\ell=0}^{n-1} e^{i\nu_{k\ell}}|\ell\rangle, \qquad (34)$$

with real ν_{kl}, span $n^2 - (n-1)$-dimensional space in $\mathbb{C}^n \otimes \mathbb{C}^n$.

For $n = 4$, it gives, therefore, 13 vectors. To have a spanning property, one still needs three additional linearly independent vectors satisfying Eq. (2). Interestingly, for $\theta = 0$ and $\theta = \pi$, i.e., for Choi-like witnesses, we found only these 13 vectors that satisfy Eq. (2). This is in a full analogy with the property of Choi witnesses for $n = 3$: in that case one has only $3^2 - 2 = 7$ linearly independent vectors [38,40]. Now we study the region $\theta \in (0, \pi)$, for which $a < 1$ and $b > 0$. Introducing the following vectors

$$|\psi_{14}\rangle = \sqrt{\sin(\theta/2)}|0\rangle + \sqrt{\cos(\theta/2)}|1\rangle,$$
$$|\varphi_{14}\rangle = \sqrt{\cos(\theta/2)}|0\rangle + \sqrt{\sin(\theta/2)}|1\rangle,$$
$$|\psi_{15}\rangle = \sqrt{\sin(\theta/2)}|1\rangle + \sqrt{\cos(\theta/2)}|2\rangle,$$

$$|\varphi_{15}\rangle = \sqrt{\cos(\theta/2)}|1\rangle + \sqrt{\sin(\theta/2)}|2\rangle,$$
$$|\psi_{16}\rangle = \sqrt{\sin(\theta/2)}|2\rangle + \sqrt{\cos(\theta/2)}|3\rangle,$$
$$|\varphi_{16}\rangle = \sqrt{\cos(\theta/2)}|2\rangle + \sqrt{\sin(\theta/2)}|3\rangle, \qquad (35)$$

one can show that

$$\langle\psi_k \otimes \varphi_k|W[a,b,c,d]|\psi_k \otimes \varphi_k\rangle = 0,$$

for $k = 14, 15, 16$. However, these 16 vectors span only 15-dimensional space in $\mathbb{C}^4 \otimes \mathbb{C}^4$. There exists no other linearly independent vectors in this subspace. We will show it by subtracting an amount of the projector onto its orthogonal complement and still obtaining an entanglement witness. Summarizing, for class I we have 15 linearly independent vectors for $0 < \theta < \pi$ and 13 linearly independent vectors for $\theta = 0, \pi$. Recall that, if $n = 3$, then for the Choi witness, we have only $7 (= n^2 - n + 1)$ linearly independent vectors.

B. Optimization for the class I

It turns out that EWs from class I are not optimal. Note that $W_I(\pi/2)$ is decomposable. Precisely, for this case, we obtain the following decomposition

$$W_I\left(\frac{\pi}{2}\right) = W\left[\frac{1}{2}, \frac{1}{2}, \frac{3}{2}, \frac{1}{2}\right] = 2P + A^\Gamma, \qquad (36)$$

where $P = |\Psi\rangle\langle\Psi|$ is a rank-1 projector onto the maximally entangled state in $\mathbb{C}^4 \otimes \mathbb{C}^4$ with

$$|\Psi\rangle = \frac{1}{2}\sum_{j=0}^{3}(-1)^{j+1}|j \otimes j\rangle, \qquad (37)$$

and A is a positive-definite matrix

$$A = \frac{1}{2}\begin{pmatrix} \cdot & 1 & \cdot & \cdot & -1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 3 & \cdot & \cdot & \cdot & \cdot & \cdot & -3 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & -1 & \cdot & \cdot & \cdot \\ \cdot & -1 & \cdot & \cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 1 & \cdot & \cdot & -1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 3 & \cdot & \cdot & \cdot & \cdot & \cdot & -3 & \cdot & \cdot \\ \cdot & \cdot & -3 & \cdot & \cdot & \cdot & \cdot & \cdot & 3 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & -1 & \cdot & \cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot & -1 & \cdot \\ \cdot & \cdot & \cdot & -1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & -3 & \cdot & \cdot & \cdot & \cdot & \cdot & 3 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & -1 & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix}, \qquad (38)$$

where we replaced all zeros by dots. It is therefore clear that $W_I(\frac{\pi}{2})$ is not optimal since we can subtract a positive operator $2P$, that is,

$$W_I\left(\frac{\pi}{2}\right) - 2P = A^\Gamma,$$

is an EW. Let us observe that $|\Psi\rangle$ defined in Eq. (37) is orthogonal to 15-dimensional subspace spanned

by

$$\{|\psi_k \otimes \psi_k^*\rangle, \; |\psi_\ell \otimes \varphi_\ell\rangle\},$$

for $k = 1, \ldots, 13$ and $\ell = 14, 15, 16$. Hence, following Refs. [20,21] one may try to optimize $W_I(\theta)$ subtracting a fraction of the projector P.

Theorem 1. The following operator

$$W_I'(\theta) = W_I(\theta) - \lambda P, \qquad (39)$$

with $P = |\Psi\rangle\langle\Psi|$ satisfying Eq. (37) and $\theta \in [0, \pi]$, is an entanglement witness if and only if $\lambda \leqslant 2$. Moreover, for $\lambda = 2$, the witness is optimal.

The proof is provided in Appendix A. Interestingly, the optimal witness $W_{\text{opt}}(\theta) = W_I(\theta) - 2P$ has the spanning property for $\theta \in (0, \pi)$. Indeed, we provide the full set of spanning vectors given in Eqs. (A39) to (A43) in Appendix A.

Now below by considering an example of a family of PPT states, we show that there are regions where these states are detected by optimal entanglement witness W_I', but not by W_I. The (unnormalized) state is in the following form:

$$\rho_\epsilon = \begin{pmatrix}
1 & . & . & . & . & 1 & . & . & . & . & 1 & . & . & . & . & 1 \\
. & \epsilon & . & . & 1 & . & . & . & . & . & . & . & . & . & . & . \\
. & . & 1 & . & . & . & . & . & 1 & . & . & . & . & . & . & . \\
. & . & . & \frac{1}{\epsilon} & . & . & . & . & . & . & . & . & 1 & . & . & . \\
. & 1 & . & . & \frac{1}{\epsilon} & . & . & . & . & . & . & . & . & . & . & . \\
1 & . & . & . & . & 1 & . & . & . & 1 & . & . & . & . & . & 1 \\
. & . & . & . & . & . & \epsilon & . & . & 1 & . & . & . & . & . & . \\
. & . & . & . & . & . & . & 1 & . & . & . & . & . & 1 & . & . \\
. & . & 1 & . & . & . & . & . & 1 & . & . & . & . & . & . & . \\
. & . & . & . & . & . & 1 & . & . & \frac{1}{\epsilon} & . & . & . & . & . & . \\
1 & . & . & . & . & 1 & . & . & . & . & 1 & . & . & . & . & 1 \\
. & . & . & . & . & . & . & . & . & . & . & \epsilon & . & . & 1 & . \\
. & . & . & 1 & . & . & . & . & . & . & . & . & \epsilon & . & . & . \\
. & . & . & . & . & . & . & 1 & . & . & . & . & . & 1 & . & . \\
. & . & . & . & . & . & . & . & . & . & . & 1 & . & . & \frac{1}{\epsilon} & . \\
1 & . & . & . & . & 1 & . & . & . & . & 1 & . & . & . & . & 1
\end{pmatrix}, \qquad (40)$$

with $\epsilon > 0$. One can easily verify

$$\mathrm{Tr}(W_I \rho_\epsilon) = \mathrm{Tr}(W_I' \rho_\epsilon) = 4\left(a + c + \epsilon b + \frac{1}{\epsilon}d - 3\right). \quad (41)$$

Let us find the critical value of ϵ satisfying $\mathrm{Tr}(W_I \rho_\epsilon) = 0$, which are $\epsilon_\pm = \frac{1 \pm \cos\theta}{1 + \cos\theta}$. Take any point between these ϵ_- and ϵ_+, e.g., $\epsilon^* = \frac{1}{2}(\epsilon_+ + \epsilon_-) = \frac{1}{1+\cos\theta}$. One finds for $\epsilon = \epsilon^*$

$$\mathrm{Tr}(W_I \rho_\epsilon) = -2\cos^2\theta < 0, \qquad (42)$$

that is, ρ_ϵ is detected both by W_I and W_I'. Now we consider a noisy state

$$\tilde{\rho}_{\epsilon,\gamma} = \rho_\epsilon + \gamma \, \mathbb{I}_4 \otimes \mathbb{I}_4, \qquad (43)$$

with $\gamma > 0$. Again, $\tilde{\rho}_{\epsilon,\gamma}$ is not normalized. For this state one finds

$$\mathrm{Tr}(W_I \tilde{\rho}_{\epsilon,\gamma}) = 2(6\gamma - \cos^2\theta),$$
$$\mathrm{Tr}(W_I' \tilde{\rho}_{\epsilon,\gamma}) = 2(5\gamma - \cos^2\theta). \qquad (44)$$

Therefore, in the region $\frac{1}{6}\cos^2\theta < \gamma < \frac{1}{5}\cos^2\theta$, we have $\mathrm{Tr}(W_I \tilde{\rho}_{\epsilon,\gamma}) > 0$ and $\mathrm{Tr}(W_I' \tilde{\rho}_{\epsilon,\gamma}) < 0$. Hence, a noisy state is still detected by the optimal witness W_I' but it is *not* detected by the original one W_I. It clearly shows that W_I' provides more efficient tools in the considered class.

C. Class II

In class II, obeying the condition (29), we have the following parametrization

$$a = \tfrac{1}{2}(1 + \cos\theta),$$
$$b = \tfrac{1}{2}(2 - \sin\theta),$$
$$c = 1 - a,$$
$$d = 2 - b, \qquad (45)$$

for $\theta \in [0, \pi]$. Similarly to class I, we express the corresponding entanglement witness with θ parametrization for this class II as $W_{II}(\theta)$. Note that for $\theta = \pi$, we find

$$W_{II}(\pi) = W[0, 1, 1, 1], \qquad (46)$$

which recovers the EW corresponding to the reduction map. This witness is optimal having the spanning property, that is, $\langle\phi \otimes \phi^*|W(\pi)|\phi \otimes \phi^*\rangle = 0$ for any $|\phi\rangle \in \mathbb{C}^4$ and these vectors span the whole 16-dimensional space. For $\theta = 0$, we get another decomposable witness

$$W_{II}(0) = W[1, 1, 0, 1], \qquad (47)$$

with the following decomposition

$$W[1, 1, 0, 1] = B^\Gamma + 2(P_1 + P_2), \qquad (48)$$

where

$$B = \begin{pmatrix}
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & 1 & \cdot & \cdot & -1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & -1 & \cdot & \cdot & \cdot \\
\cdot & -1 & \cdot & \cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 1 & \cdot & -1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & -1 & \cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 1 & \cdot & \cdot & -1 & \cdot & \cdot \\
\cdot & \cdot & \cdot & -1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & -1 & \cdot & \cdot & 1 & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot
\end{pmatrix}, \qquad (49)$$

and $P_k = |\Psi_k\rangle\langle\Psi_k|$, $k = 1, 2$ with

$$|\Psi_1\rangle = \frac{1}{\sqrt{2}}(|0 \otimes 0\rangle - |2 \otimes 2\rangle), \qquad (50)$$

$$|\Psi_2\rangle = \frac{1}{\sqrt{2}}(|1 \otimes 1\rangle - |3 \otimes 3\rangle). \qquad (51)$$

Hence $W[1, 1, 0, 1]$ is not optimal.

Next we investigate what happens when $\theta > 0$.

Proposition 3. The expectation value of $W_{II}(\theta)$ vanishes on a product vector iff it is of the form $|\psi^* \otimes \psi\rangle$, where

$$|\psi_0| = |\psi_2|, \quad |\psi_1| = |\psi_3|. \qquad (52)$$

We prove this proposition in Appendix B. Moreover, we show that such vectors span 14-dimensional subspace of $\mathbb{C}^4 \otimes \mathbb{C}^4$.

Theorem 2. The witness $W_{II}(\theta)$ with $\theta \in (0, \pi)$ is optimal [with only 14 vectors satisfying Eq. (2)].

We provide a proof of this theorem in Appendix C. In summary, the class II consists of optimal EWs $W_{II}(\theta)$ for $\theta \in (0, \pi]$, where we have the spanning property only for $\theta = \pi$.

Now for the sake of the completeness of the paper, we consider the same example of a family of PPT states ρ_ϵ defined in Eq. (40), and show that there are completely disjointed region in which these states are detected by the two witnesses, W_I and W_{II} from the first and second classes, respectively. We already showed in Sec. IV B that $\mathrm{Tr}(W_I\rho_\epsilon) = 0$ [see Eq. (41)] implies the two roots of ϵ, which are $\epsilon_\pm = \frac{1\pm\cos\theta}{1+\cos\theta}$. In a similar way, for the second class, we obtain the roots from $\mathrm{Tr}(W_{II}\rho_\epsilon) = 0$, and these are $\epsilon_\pm = \frac{2\pm\sin\theta}{2-\sin\theta}$. Therefore in the region $\theta \in (0, \pi/2)$, it is evident that for class I, $0 \leqslant \epsilon_\pm \leqslant 1$ and for the class II, $1 \leqslant \epsilon_\pm \leqslant 3$. This implies that for $\theta \in (0, \pi/2)$, these two sets of $\epsilon_\pm$ from class I and II are disjointed except 1. Therefore we can say that if $\mathrm{Tr}(W_I\rho_\epsilon) < 0$, then $\mathrm{Tr}(W_{II}\rho_\epsilon) > 0$ and vice versa.

V. CONCLUSION

In this paper, we considered two one-parameter classes of the entanglement witnesses in $\mathbb{C}^4 \otimes \mathbb{C}^4$ that are diagonal in the Bell basis. Additionally, observables from these classes are covariant w.r.t. a maximal commutative subgroup of U(4). The investigated classes are a natural extension of a well-studied construction in $\mathbb{C}^3 \otimes \mathbb{C}^3$ of optimal witnesses described by a single parameter. Interestingly, the later case contains paradigmatic examples of EWs that are indecomposable Choi witnesses and the witness corresponding to the reduction map. Now in $\mathbb{C}^4 \otimes \mathbb{C}^4$, the situation is different: instead of a single class, one has two classes which display distinct properties and can serve as a playground for investigation of various features of entanglement witnesses.

Class I contains only EWs which are not optimal. This shows that a straightforward generalization of the Choi witness from $n = 3$ to $n = 4$ does not preserve optimality. Let us recall that for $n = 3$ the Choi witness is not only optimal, but even extremal [37,38]. Moreover, all EWs from this class posses 15 linearly independent vectors satisfying condition (2). The only exception is provided by Choi-like witnesses for which one has only 13 vectors. Following the optimization technique developed in Refs. [20,21], we showed that all EWs from class I can be optimized by subtracting a single projector. Interestingly, the optimized entanglement witnesses possess the spanning property [again with an exception of Choi-like witnesses for which we have now 14 vectors satisfying Eq. (2)].

Class II contains optimal EWs [with one exception $W_{II}(0)$, i.e., at $\theta = 0$]. However, these EWs do not have the spanning property [again with one exception $W(\pi)$ corresponding to the reduction map]. This result is quite unexpected since it shows that in the limit $\theta \to 0$ one obtains nonoptimal witness $W_{II}(0)$ out of optimal EWs $W_{II}(\theta)$.

It should be stressed that checking for optimality of a given EW is, in general, a difficult problem. This analysis sheds light into the structure of optimal entanglement witnesses. We show that two classes of EWs displaying the same symmetry posses very different properties: one is optimal and the other is not. Moreover, due to the symmetry of the problem, we were able to performed the full optimization procedure [20,21]. It would be interesting to find a general characterization for arbitrary n. Another interesting problem is the issue of extremality. For

$n = 3$ it is known that the considered class is already extremal. For $n > 3$ the problem is open.

ACKNOWLEDGMENTS

APPENDIX A: PROOF OF THEOREM 1

Due to the Choi-Jamiołkowski isomorphism, any entanglement witness W in $\mathbb{C}^n \otimes \mathbb{C}^n$ corresponds to a positive map $\Phi : M_n(\mathbb{C}) \otimes M_n(\mathbb{C})$ via the following relation:

$$W = \sum_{i,j=0}^{n-1} e_{ij} \otimes \Phi(e_{ij}), \tag{A1}$$

where $e_{ij} = |e_i\rangle\langle e_j|$, $\{e_0, e_1, \ldots, e_{n-1}\}$ denotes an orthonormal basis in $\mathbb{C}^n$. The map corresponding to Eq. (14) has the following form:

$$\Phi(e_{ii}) = \sum_{j=0}^{n-1} a_{ij} e_{jj},$$

$$\Phi(e_{ij}) = e_{ij}, \ i \neq j, \tag{A2}$$

where $a_{ij} = \alpha_{i-j} \geqslant 0$. One can easily find the inverse relation, which is

$$\Phi(|\chi\rangle\langle\chi|) = \mathrm{Tr}_1((|\chi\rangle\langle\chi|)^T \otimes \mathbb{I}_n W), \tag{A3}$$

where the transposition is performed with respect to $\{e_0, e_1, \ldots, e_{n-1}\}$. Now, to show the optimality of the Theorem 1, i.e., the entanglement witness $W_I'(\theta) = W_I(\theta) - 2P$ in first class, our idea is to find the 16 linearly independent vectors satisfying the spanning criteria for the EW $W_I'(\theta)$. For that purpose, we act with the corresponding map Φ on an arbitrary vector $|\psi\rangle = \{\psi_0, \psi_1, \psi_2, \psi_3\} \in \mathbb{C}^4$ and get

$$\Phi(|\psi\rangle\langle\psi|) = \mathrm{diag}\{y_0, y_1, y_2, y_3\} - |\psi\rangle\langle\psi| - 2D \circ |\psi\rangle\langle\psi| \overset{df}{=} A - B - C, \tag{A4}$$

where $\circ$ denotes the Hadamard product

$$D = \frac{1}{4}\begin{pmatrix} 1 & -1 & 1 & -1 \\ -1 & 1 & -1 & 1 \\ 1 & -1 & 1 & -1 \\ -1 & 1 & -1 & 1 \end{pmatrix}, \tag{A5}$$

and

$$y_0 = \left(1 + \frac{2 - \sin\theta}{2}\right)|\psi_0|^2 + \frac{1 + \cos\theta}{2}|\psi_1|^2 + \frac{2 + \sin\theta}{2}|\psi_2|^2 + \frac{1 - \cos\theta}{2}|\psi_3|^2, \tag{A6}$$

$$y_1 = \left(1 + \frac{2 - \sin\theta}{2}\right)|\psi_1|^2 + \frac{1 + \cos\theta}{2}|\psi_2|^2 + \frac{2 + \sin\theta}{2}|\psi_3|^2 + \frac{1 - \cos\theta}{2}|\psi_0|^2, \tag{A7}$$

$$y_2 = \left(1 + \frac{2 - \sin\theta}{2}\right)|\psi_2|^2 + \frac{1 + \cos\theta}{2}|\psi_3|^2 + \frac{2 + \sin\theta}{2}|\psi_0|^2 + \frac{1 - \cos\theta}{2}|\psi_1|^2, \tag{A8}$$

$$y_3 = \left(1 + \frac{2 - \sin\theta}{2}\right)|\psi_3|^2 + \frac{1 + \cos\theta}{2}|\psi_0|^2 + \frac{2 + \sin\theta}{2}|\psi_1|^2 + \frac{1 - \cos\theta}{2}|\psi_2|^2. \tag{A9}$$

Its determinant is equal to

$$\det[\Phi(|\psi\rangle\langle\psi|)] = \det[A_0|A_1|A_2|A_3] - \det[B_0|A_1|A_2|A_3] - \cdots - \det[A_0|A_1|A_2|B_3] - \det[C_0|A_1|A_2|A_3]$$

$$- \cdots - \det[A_0|A_1|A_2|C_3] + \det[B_0|C_1|A_2|A_3] + \det[C_0|B_1|A_2|A_3] + \ldots$$

$$+ \det[C_0|A_1|A_2|B_3] + \det[B_0|A_1|A_2|C_3]. \tag{A10}$$

This determinant is a multilinear function on columns, hence we obtain 4^3 summands, but most of them are zero; in each summand, there can be at most one column from B and at most one column from C (each of the two columns of B are linearly dependent and then the summand would be zero, the same holds for C). If one column from B and one column from C enter the summand, they have to be neighbors to produce a nonzero summand. Proceeding in this way, we get

$$\det[\Phi(|\psi\rangle\langle\psi|)] = y_0 y_1 y_2 y_3 - \frac{3}{2}|\psi_0|^2 y_1 y_2 y_3 - \cdots - \frac{3}{2}|\psi_1|^2 y_2 y_3 y_0 + 2|\psi_0|^2|\psi_1|^2 y_2 y_3 + 2|\psi_1|^2|\psi_2|^2 y_3 y_0 + 2|\psi_2|^2|\psi_3|^2 y_0 y_1$$

$$+ 2|\psi_3|^2|\psi_0|^2 y_1 y_2$$

$$= y_0 y_1 y_2 y_3 \left[1 - \frac{3}{2}\sum_{i=0}^{3}\frac{|\psi_i|^2}{y_i} + 2\left(\frac{|\psi_0|^2}{y_0} + \frac{|\psi_2|^2}{y_2}\right)\left(\frac{|\psi_1|^2}{y_1} + \frac{|\psi_3|^2}{y_3}\right)\right]. \tag{A11}$$

Now, we will show that the second factor in the above is nonnegative. Denoting

$$z_0 = \frac{|\psi_0|^2}{y_0} + \frac{|\psi_2|^2}{y_2}, \tag{A12}$$

$$z_1 = \frac{|\psi_1|^2}{y_1} + \frac{|\psi_3|^2}{y_3}. \tag{A13}$$

We have the following condition:

$$1 - \tfrac{3}{2}(z_0 + z_1) + 2z_0 z_1 \geqslant 0 \Rightarrow (4z_0 - 3)(4z_1 - 3) \geqslant 1, \tag{A14}$$

where

$$4z_0 - 3 = -\frac{(x_{0+} + 3x_{1+})(3x_{0+} + x_{1+}) + [(5 + 3s)x_{0-} - 3cx_{1-}][(1 - s)x_{0-} + cx_{1-}]}{(3x_{0+} + x_{1+})^2 - [(1 - s)x_{0-} + cx_{1-}]^2}, \tag{A15}$$

$$4z_1 - 3 = -\frac{(x_{0+} + 3x_{1+})(3x_{0+} + x_{1+}) + [(5 + 3s)x_{1-} + 3cx_{0-}][(1 - s)x_{1-} - cx_{0-}]}{(3x_{1+} + x_{0+})^2 - [(1 - s)x_{1-} - cx_{0-}]^2}. \tag{A16}$$

Note that we denote here $\sin\theta$ and $\cos\theta$ as s and c, respectively, and also

$$x_{0\pm} = |\psi_0|^2 \pm |\psi_2|^2, \tag{A17}$$

$$x_{1\pm} = |\psi_1|^2 \pm |\psi_3|^2. \tag{A18}$$

Using Eqs. (A15) and (A16) in Eq. (A14), we obtain

$$2(1 - s)(x_{0+} + 3x_{1+})(3x_{0+} + x_{1+})(x_{0-}^2 + x_{1-}^2) + (1 - s)[c(x_{1-}^2 - x_{0-}^2) - 2sx_{0-}x_{1-}][(5 + 3s)x_{0-} - 3cx_{1-}][(5 + 3s)x_{1-} + 3cx_{0-}]$$

$$\geqslant -(1 - s)(3x_{0+} + x_{1+})^2[(1 - s)x_{1-}^2 - 2cx_{0-}x_{1-} + (1 + s)x_{0-}^2]^2 - (1 - s)(3x_{1+} + x_{0+})^2$$

$$\times [(1 - s)x_{0-}^2 + 2cx_{0-}x_{1-} + (1 + s)x_{1-}^2]^2 + (1 - s)^2[c(x_{1-}^2 - x_{0-}^2) - 2sx_{1-}x_{0-}]^2, \tag{A19}$$

which implies

$$2(x_{0-}^2 + x_{1-}^2)(x_{0+} + x_{1+})^2 + s(x_{0-}^2 - x_{1-}^2)(x_{0+}^2 - x_{1+}^2) - c(2x_{0-}x_{1-})(x_{0+}^2 - x_{1+}^2)$$

$$+ c(1 + 4s + 2s^2)(2x_{0-}x_{1-})(x_{1-}^2 - x_{0-}^2) - s(1 + s)^2(2x_{0-}x_{1-})^2 - c^2(2 + s)(x_{1-}^2 - x_{0-}^2)^2 \geqslant 0,$$

$$\Rightarrow 2(x_{0-}^2 + x_{1-}^2)(x_{0+} + x_{1+})^2 - [s(x_{1-}^2 - x_{0-}^2) + c2x_{0-}x_{1-}](x_{0+}^2 - x_{1+}^2)$$

$$- [c(x_{1-}^2 - x_{0-}^2) - s2x_{0-}x_{1-}][c(2 + s)(x_{1-}^2 - x_{0-}^2) - (1 + s)2x_{0-}x_{1-}] \geqslant 0, \tag{A20}$$

Clearly here $x_{0+}, x_{1+} \geqslant 0$ and $x_{0-} \in [-x_{0+}, x_{0+}]$, $x_{1-} \in [-x_{1+}, x_{1+}]$. Now we convert our system into the polar coordinates (see Fig. 1) and rewrite the above equation in these new coordinates.
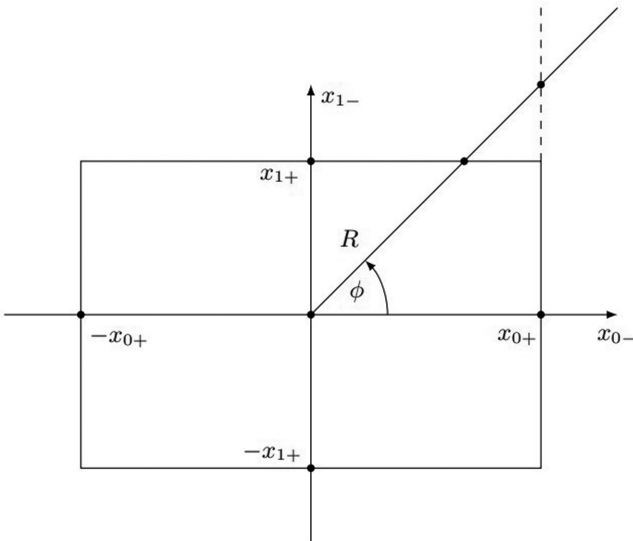
FIG. 1. The polar coordinates representation. Here $\phi \in [0, 2\pi)$.

In the new coordinate system, $R \in [0, \min\{\frac{x_{0+}}{|\cos\phi|}, \frac{x_{1+}}{|\sin\phi|}\}]$, and therefore the inequality (A20) can be written as

$$R^2[2(x_{0+} + x_{1+})^2 - \sin(2\phi - \theta)(x_{0+}^2 - x_{1+}^2)]$$

$$- R^4 \cos(2\phi - \theta)[\sin 2\phi + (2 + \sin\theta)\cos(2\phi - \theta)] \geqslant 0, \tag{A21}$$

and this equation has to be satisfied for all R mentioned in the above range. Hence

$$\cos(2\phi - \theta)[\sin 2\phi + (2 + \sin\theta)\cos(2\phi - \theta)]$$

$$\times \min\left\{\frac{x_{1+}^2}{\sin^2\phi}, \frac{x_{0+}^2}{\cos^2\phi}\right\}$$

$$\leqslant 2(x_{0+} + x_{1+})^2 - \sin(2\phi - \theta)(x_{0+}^2 - x_{1+}^2). \tag{A22}$$

First, we consider the scenario when $\frac{x_{1+}^2}{\sin^2\phi} \leqslant \frac{x_{0+}^2}{\cos^2\phi}$. Therefore,

$$\cos(2\phi - \theta)[\sin 2\phi + (2 + \sin\theta)\cos(2\phi - \theta)]x_{1+}^2$$

$$\leqslant \sin^2\phi[2(x_{0+} + x_{1+})^2 - \sin(2\phi - \theta)(x_{0+}^2 - x_{1+}^2)]. \tag{A23}$$

Ordering the terms, we get

$$
x_{0+}^2 \sin^2 \phi [2 - \sin(2\phi - \theta)] + 4\sin^2 \phi \, x_{0+} x_{1+}
$$
$$
+ x_{1+}^2 [\sin^2 \phi (2 + \sin(2\phi - \theta)) - \cos(2\phi - \theta)\sin 2\phi
$$
$$
- (2 + \sin \theta) \cos^2(2\phi - \theta)] \geqslant 0. \tag{A24}
$$

It is equivalent to say that the quadratic function

$$
\frac{x_{0+}}{x_{1+}} \mapsto \sin^2 \phi [2 - \sin(2\phi - \theta)] \left(\frac{x_{0+}}{x_{1+}} \right)^2
$$
$$
+ 4\sin^2 \phi \frac{x_{0+}}{x_{1+}} + \{ \sin^2 \phi [2 + \sin(2\phi - \theta)]
$$
$$
- \cos(2\phi - \theta)\sin 2\phi - (2 + \sin \theta)\cos^2(2\phi - \theta) \},
$$
$$
\tag{A25}
$$

has to be positive in the range $[|\cot \phi|, \infty)$. As the function is increasing for positive arguments, it is equivalent to check its positivity at the end point, i.e., at the point $|\cot \phi|$

$$
[2 - \sin(2\phi - \theta)]\cos^2 \phi + 4|\sin \phi \cos \phi|
$$
$$
+ \sin^2 \phi [2 + \sin(2\phi - \theta)] - \cos(2\phi - \theta)\sin 2\phi
$$
$$
- (2 + \sin \theta)\cos^2(2\phi - \theta) \geqslant 0. \tag{A26}
$$

After simplification, we arrive at

$$
2 + 2|\sin 2\phi| - \sin(4\phi - \theta) - (2 + \sin \theta)\cos^2(2\phi - \theta)
$$
$$
\geqslant 0. \tag{A27}
$$

To show that this inequality holds, it suffices to consider $\phi \in [0, \pi/2]$ due to the periodicity of the left-hand side. And therefore one can remove the modulus from the above inequality. Decomposing the coefficients of the above inequality in the following way:

$$
\sin(4\phi - \theta) = \sin(2\phi)\cos(2\phi - \theta) + \cos(2\phi)\sin(2\phi - \theta), \tag{A28}
$$

$$
\sin(\theta) = \sin(2\phi)\cos(2\phi - \theta) - \cos(2\phi)\sin(2\phi - \theta), \tag{A29}
$$

and organizing terms, one can rewrite the above inequality (A27) as

$$
\sin^2(2\phi - \theta)[2 - \cos(2\phi)\sin(2\phi - \theta)]
$$
$$
+ \sin 2\phi [2 - \cos(2\phi - \theta) - \cos^3(2\phi - \theta)] \geqslant 0. \tag{A30}
$$

This inequality obviously holds, as all factors in both summands are nonnegative. One can clearly see that the inequality is saturated iff $2\phi = \theta$, hence it is saturated for four values of ϕ if $\theta \in [0, \pi]$ due to periodicity. Additionally, this inequality will never be saturated if $\theta \in (\pi, 2\pi)$ because, in this range of θ, $\phi > \pi/2$ which implies we are already out of our domain.

Now, we consider the other scenario, i.e., $\frac{x_{1+}^2}{\sin^2 \phi} \geqslant \frac{x_{0+}^2}{\cos^2 \phi}$. Then

$$
\cos(2\phi - \theta)[\sin 2\phi + (2 + \sin \theta)\cos(2\phi - \theta)x_{0+}^2
$$
$$
\leqslant \cos^2 \phi [2(x_{0+} + x_{1+})^2 - \sin(2\phi - \theta)(x_{0+}^2 - x_{1+}^2)]. \tag{A31}
$$

By ordering the terms, we obtain

$$
\cos^2 \phi [2 + \sin(2\phi - \theta)]x_{1+}^2 + 4\cos^2 \phi \, x_{0+} x_{1+}
$$
$$
+ \{ \cos^2 \phi [2 - \sin(2\phi - \theta)] - \cos(2\phi - \theta)\sin 2\phi
$$
$$
- (2 + \sin \theta)\cos^2(2\phi - \theta)x_{0+}^2 \geqslant 0. \tag{A32}
$$

It is equivalent to say that the quadratic function

$$
\frac{x_{1+}}{x_{0+}} \mapsto \cos^2 \phi [2 + \sin(2\phi - \theta)] \left(\frac{x_{1+}}{x_{0+}} \right)^2
$$
$$
+ 4\cos^2 \phi \frac{x_{1+}}{x_{0+}} + \{ \cos^2 \phi [2 - \sin(2\phi - \theta)]
$$
$$
- \cos(2\phi - \theta)\sin 2\phi - (2 + \sin \theta)\cos^2(2\phi - \theta) \},
$$
$$
\tag{A33}
$$

has to be positive in the range $[|\tan \phi|, \infty)$. As the function is increasing for positive arguments, it is equivalent to check its positivity at the point $|\tan \phi|$:

$$
\sin^2 \phi [2 + \sin(2\phi - \theta)] + 4|\cos \phi||\sin \phi|
$$
$$
+ \cos^2 \phi [2 - \sin(2\phi - \theta)] - \cos(2\phi - \theta)\sin 2\phi
$$
$$
- (2 + \sin \theta)\cos^2(2\phi - \theta) \geqslant 0. \tag{A34}
$$

Simplifying the above inequality, we obtain again the same inequality (A27), which has been proven already.

The inequality (A30) is saturated if $\theta \in [0, \pi]$ and $\phi = \frac{\theta}{2} + k\frac{\pi}{2}$. We obtained Eq. (A30) putting $x_{0+} = |\sin \phi|$, $x_{1+} = |\cos \phi|$, and hence $R = 1$. The inequality (A20) is satisfied in the following four points:

$$
x_{0+} = \cos \frac{\theta}{2}, \qquad x_{1+} = \sin \frac{\theta}{2}, \qquad x_{0-} = \cos \frac{\theta}{2}, \qquad x_{1-} = \sin \frac{\theta}{2}, \tag{A35}
$$

$$
x_{0+} = \sin \frac{\theta}{2} \qquad x_{1+}, = \cos \frac{\theta}{2}, \qquad x_{0-} = -\sin \frac{\theta}{2}, \qquad x_{1-} = \cos \frac{\theta}{2}, \tag{A36}
$$

$$
x_{0+} = \cos \frac{\theta}{2}, \qquad x_{1+} = \sin \frac{\theta}{2}, \qquad x_{0-} = -\cos \frac{\theta}{2}, \qquad x_{1-} = -\sin \frac{\theta}{2}, \tag{A37}
$$

$$
x_{0+} = \sin \frac{\theta}{2}, \qquad x_{1+} = \cos \frac{\theta}{2}, \qquad x_{0-} = \sin \frac{\theta}{2}, \qquad x_{1-} = -\cos \frac{\theta}{2}. \tag{A38}
$$

Additional solutions are for $R = 0$. Then $x_{0-} = x_{1-} = 0$ and x_{0+}, x_{1+} are arbitrary. The additional solution exists for the whole range of θ. It corresponds to

$$
|\psi_0|^2 = \cos \frac{\theta}{2}, \quad |\psi_1|^2 = \sin \frac{\theta}{2}, \quad |\psi_2|^2 = 0, \quad |\psi_3|^2 = 0, \tag{A39}
$$

$$|\psi_0|^2 = 0, \quad |\psi_1|^2 = \cos\frac{\theta}{2}, \quad |\psi_2|^2 = \sin\frac{\theta}{2}, \quad |\psi_3|^2 = 0, \tag{A40}$$

$$|\psi_0|^2 = 0, \quad |\psi_1|^2 = 0, \quad |\psi_2|^2 = \cos\frac{\theta}{2}, \quad |\psi_3|^2 = \sin\frac{\theta}{2}, \tag{A41}$$

$$|\psi_0|^2 = \sin\frac{\theta}{2}, \quad |\psi_1|^2 = 0, \quad |\psi_2|^2 = 0, \quad |\psi_3|^2 = \cos\frac{\theta}{2}, \tag{A42}$$

$$|\psi_0|^2 = t, \quad |\psi_1|^2 = 1 - t, \quad |\psi_2|^2 = t, \quad |\psi_3|^2 = 1 - t. \tag{A43}$$

For such vectors $|\psi\rangle$ with the arbitrary choice of phases, the determinant of $\Phi(|\psi\rangle\langle\psi|)$ is zero. Therefore, the kernel of $\Phi(|\psi\rangle\langle\psi|)$ is spanned by, respectively,

$$\ker\Phi\left(\begin{bmatrix}\sqrt{\cos\frac{\theta}{2}}\\\sqrt{\sin\frac{\theta}{2}}e^{i\phi}\\0\\0\end{bmatrix}\begin{bmatrix}\sqrt{\cos\frac{\theta}{2}} & \sqrt{\sin\frac{\theta}{2}}e^{-i\phi} & 0 & 0\end{bmatrix}\right) = \mathrm{span}\begin{bmatrix}\sqrt{\sin\frac{\theta}{2}}e^{i\phi}\\\sqrt{\cos\frac{\theta}{2}}\\0\\0\end{bmatrix}, \tag{A44}$$

$$\ker\Phi\left(\begin{bmatrix}0\\\sqrt{\cos\frac{\theta}{2}}\\\sqrt{\sin\frac{\theta}{2}}e^{i\phi}\\0\end{bmatrix}\begin{bmatrix}0 & \sqrt{\cos\frac{\theta}{2}} & \sqrt{\sin\frac{\theta}{2}}e^{-i\phi} & 0\end{bmatrix}\right) = \mathrm{span}\begin{bmatrix}0\\\sqrt{\sin\frac{\theta}{2}}e^{i\phi}\\\sqrt{\cos\frac{\theta}{2}}\\0\end{bmatrix}, \tag{A45}$$

$$\ker\Phi\left(\begin{bmatrix}0\\0\\\sqrt{\cos\frac{\theta}{2}}\\\sqrt{\sin\frac{\theta}{2}}e^{i\phi}\end{bmatrix}\begin{bmatrix}0 & 0 & \sqrt{\cos\frac{\theta}{2}} & \sqrt{\sin\frac{\theta}{2}}e^{-i\phi}\end{bmatrix}\right) = \mathrm{span}\begin{bmatrix}0\\0\\\sqrt{\sin\frac{\theta}{2}}e^{i\phi}\\\sqrt{\cos\frac{\theta}{2}}\end{bmatrix}, \tag{A46}$$

$$\ker\Phi\left(\begin{bmatrix}\sqrt{\sin\frac{\theta}{2}}e^{i\phi}\\0\\0\\\sqrt{\cos\frac{\theta}{2}}\end{bmatrix}\begin{bmatrix}\sqrt{\sin\frac{\theta}{2}}e^{-i\phi} & 0 & 0 & \sqrt{\cos\frac{\theta}{2}}\end{bmatrix}\right) = \mathrm{span}\begin{bmatrix}\sqrt{\cos\frac{\theta}{2}}\\0\\0\\\sqrt{\sin\frac{\theta}{2}}e^{i\phi}\end{bmatrix}, \tag{A47}$$

$$\ker\Phi\left(\begin{bmatrix}\sqrt{t}\\\sqrt{1-t}e^{i\alpha}\\\sqrt{t}e^{i\beta}\\\sqrt{1-t}e^{i\gamma}\end{bmatrix}\begin{bmatrix}\sqrt{t} & \sqrt{1-t}e^{-i\alpha} & \sqrt{t}e^{-i\beta} & \sqrt{1-t}e^{-i\gamma}\end{bmatrix}\right) = \mathrm{span}\begin{bmatrix}\sqrt{t}\\\sqrt{1-t}e^{i\alpha}\\\sqrt{t}e^{i\beta}\\\sqrt{1-t}e^{i\gamma}\end{bmatrix}. \tag{A48}$$

Therefore we can say that for $\theta < \pi$, the last family (A43) along with arbitrary phases spans the 14-dimensional subspace and the additional solutions (A39), (A40), (A41), and (A42) spans the whole 16-dimensional space. Hence our entanglement witness $W_I'(\theta)$ is optimal. It completes the proof.

APPENDIX B: PROOF OF PROPOSITION 3

In this section, we will prove Eq. (52). For that purpose, let us consider the local contraction of the witness $W_{II}(\theta)$ of the second class satisfying Eq. (45) with the projector $|\psi\rangle\langle\psi|$ in the second subsystem, and we get

$$\begin{aligned}W_\psi(\theta) &= \mathrm{Tr}_2(\mathbb{I} \otimes |\psi\rangle\langle\psi| W_{II}(\theta)) \\ &= \mathrm{diag}\{y_0, y_1, y_2, y_3\} - |\psi^*\rangle\langle\psi^*|, \quad \text{(B1)}\end{aligned}$$

where

$$y_0 = \frac{3+c}{2}|\psi_0|^2 + \frac{2-s}{2}|\psi_1|^2 + \frac{1-c}{2}|\psi_2|^2 + \frac{2+s}{2}|\psi_3|^2, \tag{B2}$$

$$y_1 = \frac{3+c}{2}|\psi_1|^2 + \frac{2-s}{2}|\psi_2|^2 + \frac{1-c}{2}|\psi_3|^2 + \frac{2+s}{2}|\psi_0|^2, \tag{B3}$$

$$y_2 = \frac{3+c}{2}|\psi_2|^2 + \frac{2-s}{2}|\psi_3|^2 + \frac{1-c}{2}|\psi_0|^2 + \frac{2+s}{2}|\psi_1|^2, \tag{B4}$$

$$y_3 = \frac{3+c}{2}|\psi_3|^2 + \frac{2-s}{2}|\psi_0|^2 + \frac{1-c}{2}|\psi_1|^2 + \frac{2+s}{2}|\psi_2|^2, \tag{B5}$$

with $s := \sin\theta$ and $c := \cos\theta$. The determinant of $W_\psi(\theta)$ is given by

$$\det[W_\psi(\theta)] = y_0 y_1 y_2 y_3 - |\psi_0| y_1 y_2 y_3 - |\psi_1| y_2 y_3 y_0 - |\psi_2| y_3 y_0 y_1 - |\psi_3| y_0 y_1 y_2$$

$$= \left[(X_0 + X_1 + X_2 + X_3)^2 - \left(\frac{1+c}{2}(X_0 - X_2) - \frac{s}{2}(X_1 - X_3) \right)^2 \right]\left[(X_0 + X_1 + X_2 + X_3)^2 \right.$$

$$- \left(\frac{1+c}{2}(X_1 - X_3) + \frac{s}{2}(X_0 - X_2) \right)^2 \left. \right] - \left[(X_0 + X_1 + X_2 + X_3)^2 - \left(\frac{1+c}{2}(X_0 - X_2) \right. \right.$$

$$\left. \left. - \frac{s}{2}(X_1 - X_3) \right)^2 \right]\left[(X_1 + X_3)^2 - \frac{1+c}{2}(X_1 - X_3)^2 + (X_1 + X_3)(X_0 + X_2) \right.$$

$$\left. - \frac{s}{2}(X_1 - X_3)(X_0 - X_2) \right] - \left[(X_0 + X_1 + X_2 + X_3)^2 - \left(\frac{1+c}{2}(X_1 - X_3) + \frac{s}{2}(X_0 - X_2) \right)^2 \right].$$

$$\times \left[(X_0 + X_2)^2 - \frac{1+c}{2}(X_0 - X_2)^2 + (X_1 + X_3)(X_0 + X_2) + \frac{s}{2}(X_1 - X_3)(X_0 - X_2) \right]$$

$$= S_1 + S_2 + S_3, \tag{B6}$$

where

$$S_1 = \left(\frac{1+c}{2} \right)^2 \left(\frac{s}{2}(X_0 - X_2)^2 - \frac{s}{2}(X_1 - X_3)^2 + c(X_0 - X_2)(X_1 - X_3) \right)^2,$$

$$S_2 = \left(\frac{1+c}{2}(X_0 - X_2) - \frac{s}{2}(X_1 - X_3) \right)^2 \left[(X_1 + X_3)(X_0 + X_1 + X_2 + X_3) \right.$$

$$\left. - (X_1 - X_3)\left(\frac{1+c}{2}(X_1 - X_3) + \frac{s}{2}(X_0 - X_2) \right) \right],$$

$$S_3 = \left(\frac{1+c}{2}(X_1 - X_3) - \frac{s}{2}(X_0 - X_2) \right)^2 \left[(X_0 + X_2)(X_0 + X_1 + X_2 + X_3) - (X_0 - X_2)\left(\frac{1+c}{2}(X_0 - X_2) - \frac{s}{2}(X_1 - X_3) \right) \right]. \tag{B7}$$

We introduce the following notation $X_i := |\psi_i|^2$, for $i = 0, 1, 2, 3$. We observe that $S_1 \geqslant 0$. Moreover,

$$\left| (X_1 - X_3)\left(\frac{1+c}{2}(X_1 - X_3) + \frac{s}{2}(X_0 - X_2) \right) \right|$$

$$\leqslant (X_1 + X_3)(X_0 + X_1 + X_2 + X_3), \tag{B8}$$

hence $S_2 \geqslant 0$. Similarly, we show that $S_3 \geqslant 0$.

If $\theta = \pi$, then $\frac{1+c}{2} = \frac{s}{2} = 0$, and the contraction is always singular because then the witness corresponds to the reduction map. In another case, i.e., $\theta \in [0, \pi)$, the inequality (B8) is never saturated, and the only way to have zero determinant is $X_0 = X_2$ and $X_1 = X_3$. For such $|\psi\rangle$, we have $W_\psi(\theta) = \mathbb{I}|\psi|^2 - |\psi^*\rangle\langle\psi^*|$ and its kernel is spanned by $\{|\psi^*\rangle\}$. Hence the vectors $|\psi^* \otimes \psi\rangle$ are the only product vectors for which the expectation value of $W_{II}(\theta)$ vanishes.

One can observe that the vectors in Eqs. (50) and (51) are orthogonal to all $|\psi^* \otimes \psi\rangle$ satisfying Eq. (52). Hence

$$\dim\{\psi^* \otimes \psi : \langle\psi^* \otimes \psi|W_{II}(\theta)|\psi^* \otimes \psi\rangle = 0$$

$$\wedge |\psi_0| = |\psi_2| \wedge |\psi_1| = |\psi_3|\} \leqslant 14. \tag{B9}$$

Taking 14 random vectors from the above subspace, one easily checks that the above inequality is saturated.

APPENDIX C: PROOF OF THEOREM 2

To show optimality of the entanglement witness $W_{II}(\theta)$ in class II we show that for any vector $|\Psi_{x,y}\rangle = x|\Psi_1\rangle + y|\Psi_2\rangle$, with $|\Psi_1\rangle$ and $|\Psi_2\rangle$ defined in Eqs. (50) and (51), respectively, the following operator

$$W_{II}(\theta) - \lambda|\Psi_{x,y}\rangle\langle\Psi_{x,y}|, \tag{C1}$$

is not an EW whenever $\lambda > 0$. Consider the corresponding linear map defined in Eq. (A3), that is,

$$\Phi_{\theta,\lambda,x,y}(X) := \Phi_\theta(X) - \lambda D_{x,y} \circ X, \tag{C2}$$

where

$$D_{x,y} = \begin{pmatrix} |x|^2 & xy^* & -|x|^2 & -xy^* \\ yx^* & |y|^2 & -yx^* & -|y|^2 \\ -|x|^2 & -xy^* & |x|^2 & xy^* \\ -yx^* & -|y|^2 & yx^* & |y|^2 \end{pmatrix}. \tag{C3}$$

Now, our idea is to show that the determinant of $\Phi_{\theta,\lambda,x,y}(|\psi\rangle\langle\psi|)$ is negative for appropriately chosen $|\psi\rangle$, if $\lambda > 0$ and x, y are arbitrary. Hence we claim that no rank-1 projector (hence no positive operators) can be subtracted from the EW $W_{II}(\theta)$ in this class and this witness is optimal without having the spanning property for $\theta \in (0, \pi)$.

For this purpose, let us consider the following vector:

$$|\psi_{\lambda,k}\rangle = \begin{pmatrix} 0 \\ 1 \\ \sqrt{2k\sin\frac{\theta}{2}\lambda} \\ 1 + k\cos\frac{\theta}{2}\lambda \end{pmatrix}, \qquad \text{(C4)}$$

with the correction λ and arbitrary small parameter $k > 0$. The action of the positive map on the projector onto this vector is

$$\Phi_\theta(|\psi_{\lambda,k}\rangle\langle\psi_{\lambda,k}|) - \lambda D_{x,y} \circ |\psi_{\lambda,k}\rangle\langle\psi_{\lambda,k}|. \qquad \text{(C5)}$$

Now, we show that the determinant of the above operator is negative. To do so, we consider its determinant as a series of powers of λ. The leading power is 3 and the corresponding coefficient reads

$$8k^2\left(k\sin\frac{\theta}{2}\cos^2\frac{\theta}{2} - |x|^2\sin^2\frac{\theta}{2}\right). \qquad \text{(C6)}$$

Now it is clear that for any value of θ and for any nonzero value of x one can choose k small enough to make the leading coefficient negative, hence the determinant is negative for small enough λ. Clearly here we cannot exclude the correction for $x = 0$, $y = 1$ in this way. However, in this case the correction can be excluded by considering the same vector (C4), but with permuted entries. This ends the proof.

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