Mirrored Entanglement Witnesses for Multipartite and High-Dimensional Quantum Systems

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Entanglement witnesses (EWs) are a versatile tool to detect entangled states and characterize related properties of entanglement in quantum information theory. A witness W corresponds to an observable satisfying $\mathrm{tr}[W\sigma_{\mathrm{sep}}] \geq 0$ for all separable states σ_{sep}; entangled states are detected once the inequality is violated. Recently, mirrored EWs have been introduced by showing that there exist non-trivial upper bounds to EWs,

$$u_W \geq \mathrm{tr}[W\sigma_{\mathrm{sep}}] \geq 0.$$

An upper bound to a witness W signifies the existence of the other one M, called a mirrored EW, such that $W + M = u_W \mathbb{I} \otimes \mathbb{I}$. The framework of mirrored EWs shows that a single EW can be even more useful, as it can detect a larger set of entangled states by lower and upper bounds.

In this work, we develop and investigate mirrored EWs for multipartite qubit states and also for high-dimensional systems, to find the efficiency and effectiveness of mirrored EWs in detecting entangled states. We provide mirrored EWs for n-partite GHZ states, graph states such as two-colorable states, and tripartite bound entangled states. We also show that optimal EWs can be reflected with each other. For bipartite systems, we present mirrored EWs for existing optimal EWs and also construct a mirrored pair of optimal EWs in dimension three. Finally, we generalize mirrored EWs such that a pair of EWs can be connected by another EW, i.e., $W + M = \mathbb{K}$ is also an EW. Our results enhance the capability of EWs to detect a larger set of entangled states in multipartite and high-dimensional quantum systems.

I. INTRODUCTION

In quantum information processing, each element of quantum theory is leveraged for various applications [1]. The fact that an unknown quantum state alone cannot be copied has been a cornerstone of quantum communication that achieves a higher level of security without relying on computational assumptions [2, 3]. Measurement-based quantum computing realizes quantum logic gates through quantum states and local measurements only [4]. Quantum dynamics corresponds to quantum logic gates that enable efficient computation, such as prime-number factoring or amplitude amplifications [5, 6]. Quantum measurements can also demonstrate probabilities that cannot be achieved by classical systems, such as contextuality [7, 8] and incompatibility [9], which are closely connected to Bell nonlocality [10–12]. All of these phenomena can be used to certify the quantum properties of systems.

Entanglement is a resource behind the quantum information applications. The monogamy of entanglement, or the shareability of entangled states, is another statement of the no-cloning theorem [13–15] and the precondition for secure quantum communication [16, 17]. Two-body interactions that can create entangled states are a key to universal quantum computation [18]. Nonclassical correlations such as Bell nonlocality and quantum steering certify the presence of entanglement [19, 20]; they do not occur without entanglement. Note also that quantum steering is isomorphic to the measurement incompatibility [21].

Therefore, the question lies in verifying entangled states in practice [22, 23]. Once entangled states are detected, they can be applied to various tasks in quantum information processing. However, verifying entangled states remains a challenging task in general. To describe the problem, let $\mathcal{B}(\mathcal{H})$ denote the set of bounded linear operators on a Hilbert space $\mathcal{H}$, and $S(\mathcal{H})$ the set of quantum states; $\rho \in S(\mathcal{H})$ is non-negative and of a unit trace, $\mathrm{tr}[\rho] = 1$ and $\rho \geq 0$.

On the one hand, let us consider a scenario where a quantum state $\rho \in S(\mathcal{H} \otimes \mathcal{H})$ may be provided after state verification, e.g., quantum tomography. The computational complexity of deciding whether it is entangled is known as *NP-Hard* [24]. As a theoretical tool, the so-called partial transpose was proposed, from which it follows that the state must be entangled if it is no longer a quantum state after the partial transpose, i.e., after taking the transpose on a subsystem only [25, 26]. However, there are entangled states which remain positive after

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partial transpose (PPT), called PPT entangled states [27]. There have been other theoretical tools, including the realignment criteria [28], moments of matrices [29], and symmetric extensions [14, 30, 31].

The precise characterization of entangled states can be achieved by referring to allowed and disallowed transformations on quantum states [26]. Quantum operations are generally described by positive (P) and completely positive (CP) maps on quantum states,

$$\begin{aligned}&(\mathrm{P}) : \Lambda \geq 0 \iff \Lambda[\rho] \geq 0,\ \forall \rho \in S(\mathcal{H})\\&(\mathrm{CP}) : \mathbb{I}\otimes\Lambda \geq 0 \iff \mathbb{I}\otimes\Lambda[\rho] \geq 0,\ \forall \rho \in S(\mathcal{H}\otimes\mathcal{H})\end{aligned}$$

Positive but not completely positive maps, which do not correspond to legitimate quantum operations, can define entangled states. That is, a state $\rho \in S(\mathcal{H}\otimes\mathcal{H})$ is entangled if and only if there exists a positive but not completely positive map such that $\mathbb{I}\otimes\Lambda[\rho] \ngeq 0$.

On the other hand, let us consider a scenario where one attempts to determine whether the state is entangled or not, even before a quantum state is verified. The scenario may share similarities with the Bell experiment, for instance the Clauser–Horne–Shimony–Holt inequality [11]; an expectation value larger than 2 certifies the existence of entanglement. That is, Bell tests demonstrate that it is possible to detect the presence of entanglement from measurements alone, even when these measurements are tomographically incomplete, i.e., before the quantum state is verified [32].

Entanglement witnesses (EWs) are exactly those observables that realize the detection of entanglement for unknown quantum states in general [32, 33]. An EW can be constructed as a dual to a positive but not completely positive map Λ,

$$W = (\mathbb{I}\otimes\Lambda)[Q],$$

for some $Q \geq 0$. Therefore, EWs characterize the set of separable states; equivalently, a state ρ is entangled if and only if there exists an observable $W = W^\dagger$ such that

$$\mathrm{tr}[W\rho] < 0 \text{ whereas } \mathrm{tr}\big[W\sigma_{\mathrm{sep}}\big] \geq 0\ \forall\sigma_{\mathrm{sep}} \in S_{\mathrm{sep}}, \quad (1)$$

where S_{sep} denotes the set of separable states. Note also that the detection scheme is given by the relation, $\mathrm{tr}[W\rho] = \mathrm{tr}\big[Q(\mathbb{I}\otimes\Lambda)^\dagger[\rho]\big]$ where Λ is not completely positive. Moreover, an EW can be factorized into local observables $\{A_i\}$ and $\{B_i\}$

$$W = \sum_i c_i A_i \otimes B_i,$$

for constants $\{c_i\}$ [34]. Thus, EWs are also feasible with experiments performing local measurements only.

We emphasize that the fundamental structure that enables EWs to characterize the set of separable states is the convexity. A convex mixture of separable states is also separable. An element outside the set, i.e., an entangled state, can be distinguished by a hyperplane, which corresponds to an EW. EWs for multipartite systems can be constructed by exploiting the convexity and can be used to find a rich structure of multipartite entangled states, such as genuine multipartite entangled states.

EWs can also be improved [33]. Suppose that for some $\epsilon > 0$ and $P \geq 0$, we have

$$W' = W - \epsilon P$$

is also an EW. Let D_W denote the set of states detected by an EW W

$$D_W = \{\rho \in S(\mathcal{H}\otimes\mathcal{H}) \ : \ \mathrm{tr}[W\rho] < 0\,\}. \quad (2)$$

It holds that $D_W \subset D_{W'}$. In this case, two EWs can be compared and we call W' is *finer* than W. EWs which cannot be improved anymore, that is, *finer* than any other, are called optimal EWs.

A shortcoming of EWs for detecting entangled states is that EWs are not robust against local unitaries. A straightforward example is two Bell states $|\phi^{\pm}\rangle = \frac{1}{\sqrt{2}}(|00\rangle \pm |11\rangle)$, which are equivalent to local unitaries. They are equally entangled as they are interconvertible by local unitaries. It holds that

$$\mathrm{tr}\big[W|\phi^+\rangle\langle\phi^+|\big] + \mathrm{tr}\big[W|\phi^-\rangle\langle\phi^-|\big] \geq 0$$

since

$$\mathrm{tr}\left[W\frac{1}{2}(|00\rangle\langle 00| + |11\rangle\langle 11|)\right] \geq 0.$$

One can conclude that no EW detects both of them: at best, an EW detects either of the Bell states. The shortcoming may also be rephrased as the limitation of the size D_W for an EW.

Recently, a non-trivial upper bound to an EW has been presented. For an EW, there exists $u_W > 0$ such that

$$u_W \geq \mathrm{tr}\big[W\sigma_{\mathrm{sep}}\big] \geq 0 \ \ \forall\sigma_{\mathrm{sep}} \in S_{\mathrm{sep}} \quad (3)$$

where the upper bound satisfied by all separable states may be obtained by $u_W = \max_{\sigma\in S_{\mathrm{sep}}} \mathrm{tr}[W\sigma]$. The upper bound may also be re-expressed by introducing an EW,

$$\mathrm{tr}\big[M\sigma_{\mathrm{sep}}\big] \geq 0 \ \ \forall\sigma_{\mathrm{sep}} \in S_{\mathrm{sep}} \quad (4)$$

where $M = u_W\mathbb{I} - W$. Entangled states detected by the upper bound in Eq. (3) can be identified by the detection by a standard EW in Eq. (4), and vice versa; for an entangled state ρ, it holds that

$$u_W < \mathrm{tr}[W\rho] \iff \mathrm{tr}[M\rho] < 0. \quad (5)$$

Then, since $W = u_W \mathbb{I} - M$ and the lower bound in Eq. (3), it holds that

$$u_W \mathbb{I} \geq \mathrm{tr}\left[M\sigma_{\mathrm{sep}}\right] \geq 0.$$

Similarly, we have for an entangled state ρ,

$$\mathrm{tr}[W\rho] < 0 \iff \mathrm{tr}[M\rho] > u_W. \tag{6}$$

We call W and M mirrored EWs.

Let $D_W^{(U)}$ denote the set of states detected by an upper bound of an EW W and $D_W^{(L)}$ by the lower bound. We introduce the set of states detected by mirrored EWs, denoted by $D_W^{(M)}$, which is equal to the union,

$$D_W^{(M)} = D_W^{(U)} \cup D_W^{(L)}. \tag{7}$$

Note that $D_W^{(U)} = D_M^{(L)}$ from Eq. (5) and $D_W^{(L)} = D_M^{(U)}$ from Eq. (6). Remarkably, mirrored EWs can detect two Bell states $|\phi^{\pm}\rangle$; one is by a lower bound, and the other by an upper bound [35]. Thus, we have from Eq. (2),

$$D_W = D_W^{(L)} \subsetneq D_W^{(M)}$$

i.e., a strictly larger set of entangled states can be detected by mirrored EWs.

We reiterate that implementing mirrored EWs does not require an additional experimental cost. The experimental setup and measurement data are used to estimate the expectation value of a single EW with respect to unknown states. Then, mirrored EWs offer opportunities to detect entangled states twice, by lower and upper bounds, whereas a standard one does so once with a lower bound. Hence, a larget set of entangled states can be verfied by mirrored EWs, without an extra experimental effort. Mirrored EWs are also of theoretical interest. An EW and its upper bound (W, u_W) produce its mirrored one as a non-trivial EW. Equivalently, a positive but not completely positive map can be generated.

The ultimate usefulness and significance of mirrored EWs lie in their ability to detect entangled states by upper and lower bounds, beyond the standard ones with a lower bound. To this end, there have been extensive efforts to find mirrored operators of optimal EWs. In fact, it is highly non-trivial to have optimal EWs after mirroring. For two-qubit states, mirroring an optimal EW does not result in an EW but a quantum state; hence, the conclusion is drawn that an EW must not be optimal to have an EW after mirroring [36]. Numerous examples in $3 \otimes 3$ and $4 \otimes 4$ systems have shown that mirroring optimal EWs, one cannot detect PPTES [36]. Non-decomposable EWs can be a mirrored pair of EWs while none of them is optimal. Remarkably, there is an instance of a mirrored pair of optimal EWs in $3 \otimes 3$.

In this work, we investigate mirrored EWs for multipartite and high-dimensional quantum systems. We provide a pedagogical review on mirrored EWs and present the structure of mirrored EWs via structural physical approximations and general observables. For multipartite systems, we show mirrored EWs for n-partite Greenberger–Horne–Zeilinger (GHZ) states [37], a class of graph states such as cluster states, and tripartite bound entangled states. In all of the cases, EWs in a mirrored pair are equivalent up to local unitaries, signifying that two EWs detect distinct sets of entangled states that are equivalent up to local unitaries. Remarkably, we also present a mirrored pair of optimal EWs for three-qubit states.

For bipartite systems, we provide a fairly comprehensive review on mirrored EWs, including a pair of optimal EWs in dimension three. We then present a generalization of mirrored EWs such that EWs are mirrored via another EW, not an identity operator. In this case, it is constructive to mirror optimal EWs with each other, and they may also detect a fraction of entangled states in common.

We remark that all of the mirrored pairs of optimal EWs obtained so far are local unitarily equivalent; that is, mirrored EWs are particularly useful to verify entangled states under rotations of local bases. The result resolves a drawback of standard EWs, which are robust against noise from interactions with an environment but not for rotations of local bases.

This work is structured as follows. In Sec. II, we introduce EWs and their properties. The general structure of mirrored EWs are provided, as well as their relations ot structural physical approximations. In Sec. III, we show mirrored EWs for multipartite states and investigate their properties, the separability windows and the equivalence of local unitaires of mirrored EWs. A pair of optimal EWs are also provided for three-qubit states. In Sec. IV, mirroring of optimal EWs is investigated. A mirrored pair of optimal EWs is shown. In Sec. V, generalized mirrored EWs are presented. Mirroring EWs with respect to another EW is shown. In Sec. VI, we summarize open problems for mirrored EWs, and in Sec. VII, we discuss and conclude the results.

II. GENERAL PROPERTIES

To begin with, we here summarize notations and terminologies to be used throughout. Let W denote a standard EW and M its mirrored one. We write S_{sep} as a set of separable states. Then, the set of states detected a witness W with its lower bound is denoted as D_W or $D_W^{(L)}$

$$D_W = D_W^{(L)} = \{\rho \;:\; \mathrm{tr}[W\rho] < 0\}$$

Then, $D_W^{(U)}$ denotes the set of states detected by an upper bound of W,

$$D_W^{(U)} = \{\rho \ : \ \mathrm{tr}[W\rho] > u_W\}$$

where an upper bound u_W relies on a given witness. Then, we also write by $D_W^{(M)} = D_W^{(U)} \cup D_W^{(L)}$, i.e., all of the states detected by both upper and lower bounds of a witness W.

For multipartite systems, Pauli matrices are denoted by $\mathbb{I}$, X, Y, and Z. We use the superscript for a label of a qubit. For instance, we may write a Pauli X gate on the second qubit among three qubits as $\mathbb{I}^{(1)}X^{(2)}\mathbb{I}^{(3)}$.

A. Entanglement witnesses

We here collect definitions, results, and properties of EWs. As mentioned above, with connections to positive but not completely positive maps, we consider bipartite systems.

Let us begin by describing a general optimality of EWs. Two EWs W_1 and W_2 can be compared by the sets of states D_{W_1} and D_{W_2}, respectively. W_1 is finer than W_2 if $D_{W_2} \subset D_{W_1}$, similarly to entanglement, which can be compared by local operations and classical communication. It follows that a witness

$$W^{'} = W - \epsilon P \tag{8}$$

for some $\epsilon > 0$ and $P \geq 0$ is finer than W. Once W cannot be optimized anymore and thus is finer than any other one, it is called an optimal EW.

The spanning property is useful for finding whether an EW is optimal [33]. We write by product states $|\psi_k \otimes \phi_k\rangle$ that vanish on a witness W: $\langle \psi_k \otimes \phi_k|W|\psi_k \otimes \phi_k\rangle = 0$. Then, we call a witness W has the spanning property if

$$\text{spanning property : span}\{|\psi_k \otimes \phi_k\rangle\} = \mathcal{H} \otimes \mathcal{H} \tag{9}$$

and W is optimal. However, the converse is not generally true. Several examples of EWs satisfying (9) [38–41] (cf. also review papers [42, 43]). Since the condition (9) is only sufficient, optimal EWs can be identified without the spanning property [44].

Then, the properties of EWs follow from the classification of positive maps. A positive and completely positive map is called decomposable if it can be written in terms of the transpose T such that $\Lambda = \Lambda_1 + T \circ \Lambda_2$ where Λ_1 and Λ_2 are completely positive. An EW $W \in \mathcal{B}(\mathcal{H} \otimes \mathcal{H})$ is also called decomposable if

$$W = P + Q^{\Gamma}, \tag{10}$$

where $P, Q \geq 0$ and Γ denotes the partial transposition. An optimal decomposable EW is given $W = Q^{\Gamma}$ for some $Q \geq 0$. It is clear from the definition that a decomposable EW is unable to detect PPT entangled states.

EWs detecting PPT entangled states are dual to non-decomposable (ND) maps; therefore, they are referred to as ND EWs. Consider an ND EW, denoted by W, and suppose that it remains an EW after subtracting a decomposable operator P_D, see Eq. (10)

$$W^{'} = W - \epsilon P_D \tag{11}$$

for some $\epsilon > 0$. We call $W^{'}$ ND-finer than W since it detects a larger set of PPT entangled states. An EW is ND-optimal when no decomposable operator can be subtracted anymore; it is ND-finer than any other.

NDEWs can also be described as those EWs which remain EWs after the partial transpose, i.e. both W and W^{Γ} are EWs. It turns out that W is an ND-optimal EW if and only if W and W^{Γ} are both optimal EWs.

From Eqs. (8) and (11), one can also consider an optimization with some other EWs, i.e.,

$$W^{'} = W - \epsilon W^{''}$$

for some $\epsilon > 0$ and and EW $W^{''}$. In other words, a witness W is a convex combination of other EWs $W^{'}$ and $W^{''}$. Once the subtraction is not possible, i.e., $W^{'}$ is no longer an EW, an EW is called extremal. Extremal EWs are optimal, but optimal EWs are generally not extremal.

B. Mirrored entanglement witnesses

EWs, denoted by W and M, are mirrored with each other if they are related as follows,

$$W + M = \mu \mathbb{I}_A \otimes \mathbb{I}_B \tag{12}$$

for some $\mu \geq 0$. Note that $\mu = 2/d^2$ for $\dim\mathcal{H} = d$ if EWs are normalized, i.e., $\mathrm{tr}[W] = \mathrm{tr}[M] = 1$. Note also that normalizing EWs has nothing to do with the ability to detect entangled states: for W and αW for $\alpha > 0$, it holds $D_W = D_{\alpha W}$.

Proposition 1. Mirrored EWs detect distinct sets of entangled states, i.e.,

$$D_W \cap D_M = \emptyset. \tag{13}$$

Proof. From Eq. (12), $\mathrm{tr}[W\rho] + \mathrm{tr}[M\rho] = 1$ for a state ρ. This means that if $\rho \in D_W$ we have $\rho \notin D_M$. Similarly, if $\rho \in D_M$ we have $\rho \notin D_W$. ■

From the relation in Eq. (12), non-trivial upper bounds to mirrored EWs can be found,

$$\mu \geq \mathrm{tr}\left[W\sigma_{\mathrm{sep}}\right] \geq 0 \ \text{ and } \ \mu \geq \mathrm{tr}\left[M\sigma_{\mathrm{sep}}\right] \geq 0 \tag{14}$$

for all separable states $\sigma_{\mathrm{sep}} \in S_{\mathrm{sep}}$. Note that entangled states detected by the upper bound of a witness W violate the lower bound of its mirrored one M. Similarly,

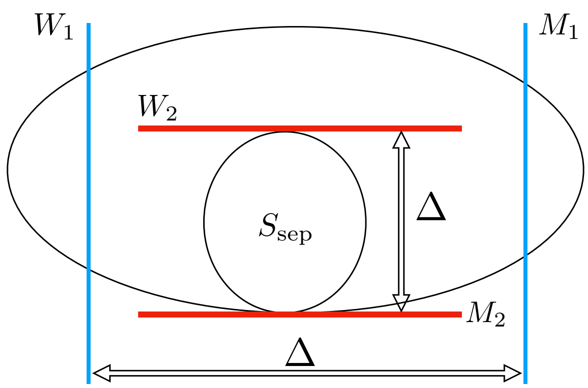

Figure 1. Mirrored EWs for two-qubit states from Examples 1 and 2 are depicted. (Blue) A pair of non-optimal EWs W_1 and M_2 are mirrored with each other, see Eqs. (15) and (16) in Example 1. They detect distinct sets of entangled states. (Red) A mirrored operator to an optimal EW is not an EW, see Eqs. (17) and (18) in Example 2. In both cases, the separability window is denoted by $\Delta = [0, 1/2]$.

entangled states detected by the lower bound of a witness W do not satisfy the upper bound of its mirrored one. Thus it holds that,

$$D_W^{(U)} = D_M^{(L)} \text{ and } D_W^{(L)} = D_M^{(U)}.$$

We also recall that all entangled states detected by upper and lower bounds of a witness W is denoted by $D_W^{(M)} = D_W^{(U)} \cup D_W^{(L)}$.

Example 1. An EW for detecting a Bell state $|\phi^+\rangle$ can be constructed as follows,

$$\begin{aligned} W &= \frac{1}{4}\mathbb{I} - \frac{1}{4}\left(X^{(1)}X^{(2)} + Z^{(1)}Z^{(2)}\right) \\ &= \frac{1}{4}\mathbb{I} - \frac{1}{2}\left(|\phi^+\rangle\langle\phi^+| - |\psi^-\rangle\langle\psi^-|\right) \\ &= \frac{1}{4}\begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 2 & -1 & 0 \\ 0 & -1 & 2 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}, \end{aligned} \tag{15}$$

where $|\psi^-\rangle = (|01\rangle - |10\rangle)/\sqrt{2}$. Note that W is normalized and thus $\mu = 1/2$ in Eq. (12) since $d = 2$. It follows that

$$\frac{1}{2} \geq \mathrm{tr}\left[W\sigma_{\rm sep}\right] \geq 0 \quad \text{for} \quad \sigma_{\rm sep} \in S_{\rm sep}.$$

It is straightforward to find its mirrored EW,

$$\begin{aligned} M &= \frac{1}{4}\mathbb{I} + \frac{1}{4}\left(X^{(1)}X^{(2)} + Z^{(1)}Z^{(2)}\right) \\ &= \frac{1}{4}\mathbb{I} + \frac{1}{2}\left(|\phi^+\rangle\langle\phi^+| - |\psi^-\rangle\langle\psi^-|\right) \\ &= \frac{1}{4}\begin{pmatrix} 2 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 2 \end{pmatrix}, \end{aligned} \tag{16}$$

which detects another Bell state $|\psi^-\rangle$. Note that EWs satisfy

$$W + M = \frac{1}{2}\mathbb{I} \otimes \mathbb{I}.$$

Similarly, mirrored EWs can be constructed for other pairs of Bell states.

Example 2. An illuminating example is an optimal EW

$$W = |\psi^-\rangle\langle\psi^-|^{\Gamma} = \frac{1}{2}\mathbb{I} \otimes \mathbb{I} - |\phi^+\rangle\langle\phi^+|. \tag{17}$$

The mirrored operator can be found from Eq. (12) with $\mu = 1/2$,

$$M = |\phi^+\rangle\langle\phi^+| \tag{18}$$

which is not an EW. For two-qubit states,

For mirrored EWs, the separability window is defined as a range between the lower and upper bounds of a normalized witness W. From Eq. (14), assuming that a witness W is normalized, the separability window is given as

$$\text{separability window} : \Delta = [0, \mu]. \tag{19}$$

The caveat when computing the separability window is that although a witness W is normalized, its mirrored one is not necessarily normalized. One can also rephrase the separability window as an upper bound to a normalized EW.

An optimization of mirrored EWs and the separability window are related as follows. For a non-optimal EW, let us apply an optimization,

$$W' = W - \epsilon P$$

for some $\epsilon \geq 0$ and non-negative operator $P \geq 0$. Let M denote the mirrored operator to W. From Eq. (12), it follows that $W' + \epsilon P + M = \mu\mathbb{I} \otimes \mathbb{I}$. This means that the mirrored operator to W' is given by

$$M' = M + \epsilon P$$

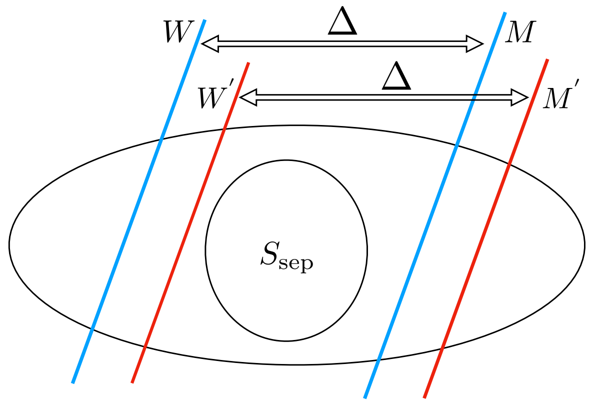

Figure 2. A witness W is optimized by subtracting a positive operator, and thus W' is finer than W. The consequence is that its mirror detects a smaller set of entangled states, M is finer than M', while the separability window is kept constant.

while the separabilty window is kept, i.e.,

$$W' + M' = \mu \mathbb{I} \otimes \mathbb{I}.$$

That is, W' is finer than W whereas M is finer than M', or vice versa. Hence, while the separability window is kept, optimization of an EW decreases the capability of its mirrored EW in detecting entangled states, see Fig. 2.

C. Structural physical approximation

The structural physical approximation (SPA) transforms positive maps into quantum operations. It can be equivalently formulated as a transformation of EWs to positive operators, which can be interpreted as quantum states. For convenience, we here omit the normalization of resulting positive operators, although EWs are normalized, and write the SPA as follows,

$$\text{SPA}: \ W \mapsto \widetilde{W} = W + p\mathbb{I} \otimes \mathbb{I}$$

with minimal p such that $\widetilde{W} \geq 0$. The SPA admixes an identity operator, which is of full rank, to wash out negative projections of an EW so that the resulting operator is non-negative for separable states. Since optimal EWs tightly characterize the set of separable states, SPA of optimal EWs are closely connected to separable states [45–47].

Note that negative projections are used to detect entangled states, while positive ones are used to maintain non-negative expectation values for separable states; for a decomposition $W = W_+ - W_-$ where $W_\pm \geq 0$, a witness W may detect entangled states with a negative projection W_-.

Let us consider another witness M and utilize its positive projections for detecting entangled states, i.e., $-M$. We introduce the mirrored SPA as follows,

$$\text{mSPA}: \ M \mapsto \widetilde{M} = -M + q\mathbb{I} \otimes \mathbb{I}$$

with a minimal q such that $\widetilde{M} \geq 0$ Note that SPA and mSPA can be applied to arbitrary EWs.

We derive interesting relations as follows.

- For an EW, i.e., $W = M$, one applies the SPA and the mSPA. It holds that
$$\widetilde{W} + \widetilde{M} = (q + p)\mathbb{I} \otimes \mathbb{I}.$$
- For two EWs, the SPA of one and the mSPA of the other coincide, i.e., $\widetilde{W} = \widetilde{M}$. Then, two EWs are mirrored with each other
$$W + M = (q - p)\mathbb{I} \otimes \mathbb{I}.$$

Note that $q > p$ in general, and thus the separability window is given by $\Delta = [0, q - p]$. Both W and M have an upper bound $\mu = q - p$ satisfied by all separable states.

D. Mirrored EWs as observables: POVM clouds

One of the lessons from mirrored EWs is that it is, in fact, handy to construct a scheme for verifying entangled states without referring to positive but not completely positive maps directly. Let us begin with an arbitrary observable $\mathbb{O} \in \mathcal{B}(\mathcal{H} \otimes \mathcal{H})$. That is, one can describe $\mathbb{O} = \sum_{ij} c_i \Pi_i \otimes \Pi_j$ with POVM elements $\{\Pi_i\}$, $\{\Pi_j\}$ and $\{c_i\}$ so that it can be estimated in an experiment.

For an operator $\mathbb{O}$, we compute,

$$u_{\mathbb{O}} = \max_{\sigma \in S_{\text{sep}}} \text{tr}[\mathbb{O}\sigma] \ \text{and} \ l_{\mathbb{O}} = \min_{\sigma \in S_{\text{sep}}} \text{tr}[\mathbb{O}\sigma] \quad (20)$$

where it suffices to run the optimization over pure states. With the bounds above, we construct a detection scheme with lower and upper bounds satisfied by all separable states,

$$u_{\mathbb{O}} \geq \text{tr}\left[\mathbb{O}\sigma_{\text{sep}}\right] \geq l_{\mathbb{O}} \quad \forall \sigma_{\text{sep}} \in S_{\text{sep}}.$$

The detection scheme above is equivalent to that of mirrored EWs in Eq. (12) by deriving EWs as follows,

$$W = \mathbb{O} - l_{\mathbb{O}}\mathbb{I} \otimes \mathbb{I} \ \text{and} \ M = u_{\mathbb{O}}\mathbb{I} \otimes \mathbb{I} - \mathbb{O}$$

which are mirrored with each other since it holds that

$$W + M = (u_{\mathbb{O}} - l_{\mathbb{O}})\mathbb{I} \otimes \mathbb{I} \quad (21)$$

where $\mu = u_{\mathbb{O}} - l_{\mathbb{O}} > 0$. Hence, mirrored EWs are obtained. We remark that EWs can be constructed with optimizations in Eq. (20).

Note that the construction of the detection scheme in Eq. (20) generally applies to resource theories in which free resources form a convex set [48]. In fact, the derived mirrored structure in Eq. (21) exploits the only fact that the set of separable states is convex.

E. EWs for graph states

In this subsection, we summarize graph states, an important class of multipartite entangled states.

1. *Graph states*

To introduce graph states, let $G = (V, E)$ denote a graph consisting of a set V of n vertices and a collection of edges E connecting pairs of these vertices. For a vertex i in the graph G, we write its neighbourhood $N(i)$ as the set of vertices directly connected to the vertex. For a vertex i, we introduce an operator g_i,

$$g_i = X^{(i)} \bigotimes_{j \in N(i)} Z^{(j)}$$

An n-qubit graph state $|G\rangle$ is defined as an eigenstate, $g_i |G\rangle = |G\rangle$ for $i = 1, \ldots, n$ with eigenvalue $+1$.

The stabilizer of the graph state is defined as,

$$\mathcal{S}(G) = \{s_j\} \quad \text{where} \quad s_j = \prod_{i \in I_j(G)} g_i, \qquad (22)$$

for a subset of the vertices $I_j(G)$. If a generator g_k appears in the product defining s_j, i.e., $k \in I_j(G)$, we say that s_j contains g_k. It is clear that $s_j |G\rangle = |G\rangle$.

An useful property of graph states and their stabilizers is that the projector onto $|G\rangle$ can be expressed as the sum of all stabilizer elements:

$$\frac{1}{2^n} \sum_{i=1}^{2^n} s_i = |G\rangle\langle G| . \qquad (23)$$

Note that the stabilizer $\mathcal{S}(G)$ forms a commutative group and has 2^n elements.

2. *Two-colorable graph states*

Two-coloring of a graph, or a bipartite coloring, is a way to color the vertices of a graph using two colors, which we write by red and blue, such that no two adjacent vertices share the same color. A graph is considered two-colorable if such a coloring exists. We now introduce stabilizer projectors, which are in turn employed in the construction of EWs for two-colorable graph states.

Examples of two-colorable states include one-dimensional cluster states, two-dimensional cluster states, n-partite GHZ states, see Fig. 3.

3. *Constructing EWs*

For graph states, we consider instances of EWs, called canonical, alternative, and two-measurement ones.

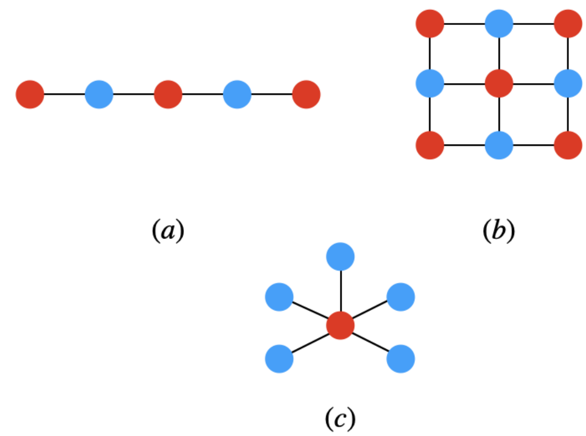

Figure 3. Examples of two-colorable graph states are shown: (a) a one-dimensional cluster state and (b) a two-dimensional cluster state (c) a GHZ state.

Suppose that one wants to construct an EW for detecting a particular n-partite entangled state $|\psi\rangle$. A straightforward construction may be found as follows,

$$W = \alpha\, \mathbb{I}^{\otimes n} - |\psi\rangle \langle\psi| ,$$

where α may be computed such that an EW is non-negative for all separable states. For instance, graph states $|G\rangle$, which are genuinely multipartite entangled, have $\alpha \geq 1/2$. An EW constructed in this manner is called a canonical EW. For an n-partite stabilizer state, we also have $\alpha \geq 1/2$. EWs can be expressed in terms of generators [49],

$$\text{canonical EW} : W_c = \frac{1}{2}\, \mathbb{I}^{\otimes n} - \prod_{i=1}^{n} \frac{\mathbb{I}^{\otimes n} + g_i}{2} \qquad (24)$$

Note that an EW above can be estimated by measurements on $2^n - 1$ stabilizers.

Measurement settings can be reduced in EWs in the following [49–51]:

$$\text{alternative EW} : W_a = \frac{n-1}{2}\, \mathbb{I}^{\otimes n} - \frac{1}{2} \sum_{i=1}^{n} g_i, \qquad (25)$$

which are called alternative EWs. These can detect genuinely multipartite entangled states. An alternative EW can be estimated by measurements on n generators.

For 2-colorable graph states, two-measurement EWs can be defined as follows [49],

$$\text{two} - \text{measurement EWs} :$$
$$W_{2m} = \frac{3}{2}\, \mathbb{I}^{\otimes n} - \prod_{\text{red } i} \frac{\mathbb{I}^{\otimes n} + g_i}{2} - \prod_{\text{blue } i} \frac{\mathbb{I}^{\otimes n} + g_i}{2}, \qquad (26)$$

where the vertices are colored in two different colors, red and blue, corresponding to two measurement settings. For example, two-measurement EWs for GHZ states can be computed by measuring X on each qubit and Z again on each qubit, i.e., $X^{(1)} \otimes X^{(2)} \otimes \cdots \otimes X^{(n)}$ and $Z^{(1)} \otimes Z^{(2)} \otimes \cdots \otimes Z^{(n)}$.

III. MULTIPARTITE SYSTEMS

In this section, we construct mirrored EWs for multipartite quantum systems and investigate their properties. We consider various mirrored EWs for graph states and compare their separability windows. We also present a mirrored pair of optimal EWs for three-qubit states.

A. n-partite GHZ states

Let us begin with n-partite GHZ states, denoted by

$$|GHZ_n\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle^{\otimes n} + |1\rangle^{\otimes n}\right). \tag{27}$$

which are also instances of two-colorable states. An n-partite GHZ state is stabilized by the following set of generators:

$$g_1 = X^{(1)}X^{(2)}\cdots X^{(n)} \text{ and } g_i = Z^{(i)}Z^{(i+1)}$$

for $i = 2, \cdots, n-1$. Note that $g\,|GHZ_n\rangle = |GHZ_n\rangle$ for all generators g. Thus, it also follows that

$$|GHZ_n\rangle\langle GHZ_n| = \prod_{i=1}^{n}\left(\frac{\mathbb{I}^{\otimes n} + g_i}{2}\right). \tag{28}$$

The projection onto a GHZ state is uniquely determined by generators. In what follows, we derive mirrored EWs for n-partite states and compare separability windows.

1. Mirrored EWs

Firstly, we derive a mirrored EW for the canonical one from Eq. (24),

$$\begin{aligned} W_c &= \frac{1}{2^{n-1}-1}\left(\frac{1}{2}\mathbb{I}^{\otimes n} - |GHZ_n\rangle\langle GHZ_n|\right), \\ M_c &= |GHZ_n\rangle\langle GHZ_n|, \end{aligned}$$

where the mirrored operator is not an EW. Note that a witness W is normalized. The separability window is computed as $\Delta = [0, \mu_c]$ where

$$\mu_c = \frac{1}{2^n - 2}, \tag{29}$$

which quickly converges to 0 as n tends to be large.

Secondly, let us consider alternative EWs from Eq. (25) and compute their mirrored EWs

$$\begin{aligned} W_a &= \frac{1}{2^n}\left(\mathbb{I}^{\otimes n} - \frac{1}{n-1}\sum_{i=1}^{n} g_i\right), \text{ and} \\ M_a &= \frac{1}{2^n}\left(\mathbb{I}^{\otimes n} + \frac{1}{n-1}\sum_{i=1}^{n} g_i\right), \end{aligned}$$

One can find that the mirrored one M detects GHZ states equivalent to the state in Eq. (27) up to local unitaries,

$$\left|GHZ_n^{(a)}\right\rangle = \frac{1}{\sqrt{2}}\left(|01010\cdots x\rangle - |10101\cdots(x\oplus 1)\rangle\right) \tag{30}$$

where $x = 1$ if n is even and $x = 0$ otherwise, and $\oplus$ denotes the bitwise addition. Note that two states $|GHZ_n\rangle$ and $|GHZ_n'\rangle$ are connected by local unitaries,

$$\begin{aligned} &\mathbb{I}^{(1)} \otimes Y^{(2)} \otimes \cdots \otimes Y^{(n-1)} \otimes \mathbb{I}^{(n)} \quad \text{for n odd} \\ \text{and} \quad &\mathbb{I}^{(1)} \otimes Y^{(2)} \otimes \cdots \otimes \mathbb{I}^{(n-1)} \otimes Y^{(n)} \quad \text{for n even.} \end{aligned}$$

Since a witness W is normalized, we have a separability window $\Delta_c = [0, \mu_a]$ where

$$\mu_a = \frac{1}{2^{n-1}} \tag{31}$$

which approaches zero rapidly as n increases.

Thirdly, we compute mirrored operators for two-measurement EWs, see Eq. (26)

$$\begin{aligned} W_{2m} &= \frac{1}{2^n-2}\left(\frac{3}{2}\mathbb{I}^{\otimes n} - \frac{\mathbb{I}^{\otimes n} + g_1}{2} - \prod_{i=2}^{n}\frac{\mathbb{I}^{\otimes n} + g_i}{2}\right), \text{ and} \\ M_{2m} &= \frac{1}{2^{n-1}+2}\left(\frac{\mathbb{I}^{\otimes n} + g_1}{2} + \prod_{i=2}^{n}\frac{\mathbb{I}^{\otimes n} + g_i}{2}\right) \end{aligned}$$

where the mirrored operator is positive semidefinite. Note that a witness W is normalized and thus the separabilty is computed as $\Delta_{2m} = [0, \mu_{2m}]$ where

$$\mu_{2m} = \frac{3}{2}\cdot\frac{1}{2^n-2} \tag{32}$$

which quickly converges to zero as n tends to be large.

2. Comparison of the separability window

Mirrored EWs with a smaller separability window may detect a larger set of entangled states. Three types of EWs above can be compared in terms of the separability window. From Eqs. (29), (31), and (32). Overall, the separability windows satisfy the hierarchy

$$\Delta_c \le \Delta_{2m} \le \Delta_a, \tag{33}$$

where the equality holds for $n = 2$, see Fig. 4.

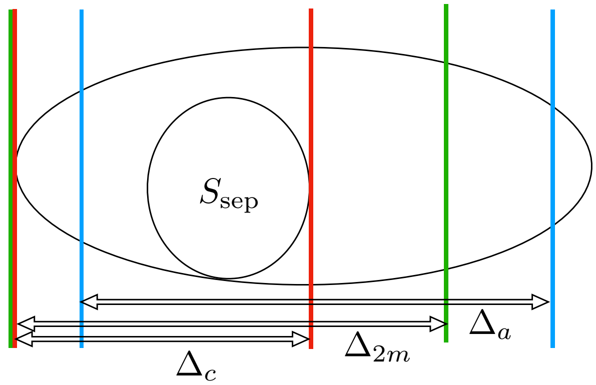

Figure 4. Separability windows of mirrored EWs are compared, see Eq. (33). An optimal EW having its mirror as a positive operator has the smallest separability window (red). Two-measurement (green) and alternative (blue) EWs, which are not optimal, have larger separability windows, $\Delta_{2m} < \Delta_a$. Note that a mirrored pair of EWs can be constructed for alternative EWs. Two alternative EWs in a mirrored pair are equivalent up to local unitaries.

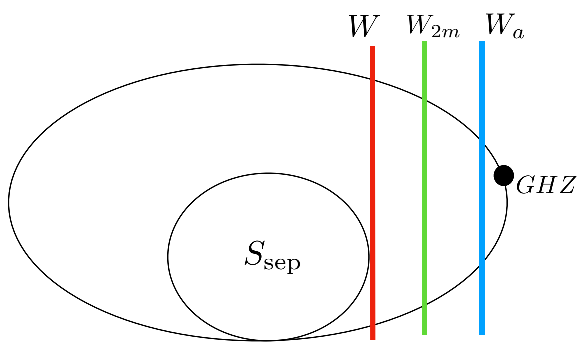

Figure 5. Negative expectation values show the robustness of EWs against noise on quantum systems, see the comparisons in Eqs. (34), (35), and (36).

3. *Mirrored EWs against local unitaries*

Noise on quantum systems generally decreases the entanglement existing in a quantum state. It can be classified into i) noise due to interaction with an environment and ii) unwanted changes of local basis. The former decreases the purity of quantum states, so does entanglement. The latter, however, keeps the entanglement. Nonetheless, EWs are robust to noise in the first type but not the latter one, to which mirrored EWs provide a partial solution.

The canonical witness W_c cannot detect a GHZ state in Eq. (30). Instead, one can take an alternative EW, W_a, in Eq. (25). Estimating an alternative EW also finds its mirrored EW, which can detect GHZ state in a different local basis in Eq. (30). That is, we have a limited capability with a canonical EW,

$$GHZ_n \in D_{W_c} \;\; \text{but} \;\; GHZ_n^{(a)} \notin D_{W_c}$$

whereas mirrored EWs exploiting both upper and lower bounds can detect a larger set of entangled states,

$$GHZ_n,\; GHZ_n^{(a)} \in D_{W_a}^{(U)} \cup D_{W_a}^{(L)}.$$

Therefore, mirrored EWs offer a strategy of detecting entangled states under rotations of local unitaries. The advantage makes them more suitable for practical entanglement detection in the presence of local unitary noise.

Note also that alternative and two-measurement EWs having non-trivial mirrored operators are less robust against noise due to unwanted interactions with the environment. For an n-partite GHZ state in Eq. (27), we have

$$\mathrm{tr}[W_c|GHZ_n\rangle\langle GHZ_n|] \;=\; \frac{-1}{2^n-2} \tag{34}$$

which means that W_c provides a negative expectation value up to a noise fraction less than $(2^n-1)^{-1}$. We also find that

$$\mathrm{tr}[W_a|GHZ_n\rangle\langle GHZ_n|] \;=\; \frac{-1}{(n-1)2^n} \tag{35}$$

$$\text{and} \;\; \mathrm{tr}[W_{2m}|GHZ_n\rangle\langle GHZ_n|] \;=\; \frac{-1}{2(2^n-2)} \tag{36}$$

which shows that the other EWs can tolerate smaller fractions of noise, see Fig. 5. It is also straightforward to find that

$$\mathrm{tr}\left[M_a|GHZ_n^{(a)}\rangle\langle GHZ_n^{(a)}|\right] \;=\; \frac{-1}{(n-1)2^n}$$

which is equal to Eq. (35).

B. EWs for graph states

So far, we have found that alternative EWs are useful to construct mirrored EWs. We further develop mirroring alternative EWs to detect graph states and, in particular, focus on alternative EWs for two-colorable graph states such as cluster states. Let $|G\rangle$ denote an n-qubit graph state $\{g_i\}_{i=1}^n$ generators, a product of Pauli operators X and Z. An EW for a graph state $|G\rangle$ is given as follows [52]

$$W = (n-1)\,\mathbb{I}^{\otimes n} - \sum_{i=1}^{n} g_i. \tag{37}$$

Note that an EW above can detect genuinely entangled multipartite states [52, 53].

We obtained its mirrored EW as follows,

$$M = (n-1)\,\mathbb{I}^{\otimes n} + \sum_{i=1}^{n} g_i. \quad (38)$$

The separability window is given by $\Delta = [0, 2^{1-n}]$. In what follows, we show that EWs in Eqs. (37) and (38) are connected by local unitaries. Therfore, entangled states detected by them are local unitarily equivalent.

Proposition 2. Mirrored alternative EWs in Eqs. (37) and (38) are equivalent up to local unitaries.

Proof. Let $G = (V, E)$ be a two-colorable graph on n vertices. We write by subsets of vertices

$$\begin{aligned} V_{\text{even}} &= \{i \in V \mid |N(i)| \text{ is even}\}, \\ V_{\text{odd}} &= \{i \in V \mid |N(i)| \text{ is odd}\} \end{aligned}$$

and also introduce local unitaries U as follows,

$$U = \left(\bigotimes_{i \in V_{\text{even}}} Y^{(i)}\right) \otimes \left(\bigotimes_{j \in V_{\text{odd}}} X^{(j)}\right) \quad (39)$$

A generator is given as

$$g_i = X^{(i)} \bigotimes_{j \in N(i)} Z^{(j)}.$$

Note that $YZY^\dagger = -Z$ and $XZX^\dagger = -Z$. It holds that

$$U g_i U^\dagger = -g_i,$$

and consequently we have $UWU^\dagger = M$. ∎

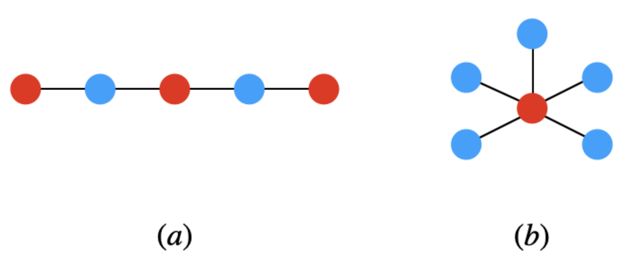

Figure 6. Instances of 2-colorable graph states are shown, (a) a linear cluster state and (b) a GHZ state.

Let us present mirrored EWs for instances of graph states. Firstly, we consider linear cluster states $|C\rangle$, for which generators are given by, is given by:

$$\begin{aligned} g_1 &= X^{(1)} Z^{(2)}, \\ g_n &= Z^{(n-1)} X^{(n)}, \\ g_i &= Z^{(i-1)} X^{(i)} Z^{(i+1)}, \quad \text{for } i = 2, \ldots, n-1. \end{aligned}$$

From Eq. (39), mirrored EWs are connected by a local unitary transform U_C,

$$U_C = X^{(1)} \otimes X^{(n)} \bigotimes_{k=2}^{n-1} Y^{(k)}.$$

Hence, an alternative EW detects a cluster state $|C\rangle$ and then its mirrored Ew does its local unitarily equivalent state, $U_C|C\rangle$.

For instance, for four qubits, generators are given by

$$\begin{aligned} g_1 &= X^{(1)} Z^{(2)}, \;\; g_2 = Z^{(1)} X^{(2)} Z^{(3)}, \\ g_3 &= Z^{(2)} X^{(3)} Z^{(4)}, \;\; \text{and} \;\; g_4 = Z^{(3)} X^{(4)}. \end{aligned}$$

from which mirrored EWs are constructed,

$$\begin{aligned} W &= 3\,\mathbb{I}^{\otimes 4} - (g_1 + g_2 + g_3 + g_4), \\ \text{and} \;\; M &= 3\,\mathbb{I}^{\otimes 4} + (g_1 + g_2 + g_3 + g_4) \end{aligned} \quad (40)$$

and they are connected by a local unitary transform, $X^{(1)} Y^{(2)} Y^{(3)} X^{(4)}$

For a four-qubit cluster state $|C_4\rangle$, which can be expressed as follows,

$$H^{(1)} H^{(4)} |C_4\rangle = \tfrac{1}{2}(|0000\rangle + |0011\rangle + |1100\rangle - |1111\rangle),$$

where H denotes a Hadamard gate, its mirrored EW detects a local unitarily equivalent one,

$$\begin{aligned} & H^{(1)} H^{(4)} \; X^{(1)} Y^{(2)} Y^{(3)} X^{(4)} |C_4\rangle \\ = \; & \frac{1}{2}(|1001\rangle - |0101\rangle - |1010\rangle - |0110\rangle). \end{aligned}$$

Hence, we have presented mirrored EWs in Eq. (40) detecting local unitarily equivalent cluster states.

Secondly, let us revisit alternative EWs for n-qubit GHZ states and show local unitaries explicitly. For instance, for $n = 3$, EWs are constructed as follows,

$$\begin{aligned} W &= 2\mathbb{I}^{\otimes 3} - (X^{(1)} X^{(2)} X^{(3)} + Z^{(1)} Z^{(2)} + Z^{(2)} Z^{(3)}), \\ M &= 2\mathbb{I}^{\otimes 3} + (X^{(1)} X^{(2)} X^{(3)} + Z^{(1)} Z^{(2)} + Z^{(2)} Z^{(3)}), \end{aligned}$$

where two EWs are related by a local unitary transform, $Z^{(1)} Y^{(2)} Z^{(3)}$.

We have shown that mirrored EWs connected by local unitaries detect entangled states which are local unitarily equivalent.

C. Mirrored pair of optimal EWs

In this section, we explore the existence of a pair of optimal EWs in multipartite systems. In particular, we present mirrored pairs of *optimal* EWs, each of which detects PPT entangled states.

1. Optimality of mirrored EWs

We begin by examining the optimality of mirrored EWs in a special class of operators known as *X-shaped* EWs. For n qubits, let $\mathbf{i}$ denote a bitstring of length n, indexing basis elements. A Hermitian operator W acting on n qubits is said to be *X-shaped* if its non-zero matrix entries $W_{\mathbf{i},\mathbf{j}}$ satisfy

$$W_{\mathbf{i},\mathbf{j}} \neq 0 \quad \text{only when} \quad \mathbf{i} = \mathbf{j} \quad \text{or} \quad \mathbf{i} = \bar{\mathbf{j}},$$

where $\bar{\mathbf{j}}$ is the bitwise complement of $\mathbf{j}$, i.e., $\bar{\mathbf{j}} = \mathbf{j} \oplus \mathbf{1}$. An X-shaped Hermitian operator can be typically put in the following matrix form

$$\begin{pmatrix} s_1 & & & & & & & u_1 \\ & s_2 & & & & & u_2 & \\ & & \ddots & & & \iddots & & \\ & & & s_{2^{n-1}} & u_{2^{n-1}} & & & \\ & & & \bar{u}_{2^{n-1}} & t_{2^{n-1}} & & & \\ & & \iddots & & & \ddots & & \\ & \bar{u}_2 & & & & & t_2 & \\ \bar{u}_1 & & & & & & & t_1 \end{pmatrix}.$$

Let us recall results from [54] for the optimality of X-shaped EWs.

Theorem 1. Let W be an X-shaped n-qubit genuine EW. The following statements are equivalent:

(i) W is an optimal genuine EW;

(ii) W satisfies the spanning property;

(iii) There exists a bitstring $\mathbf{i}$ and a real number $r > 0$ such that:

- $W_{\mathbf{i},\mathbf{i}} = W_{\bar{\mathbf{i}},\bar{\mathbf{i}}} = 0$ and $|W_{\mathbf{i},\bar{\mathbf{i}}}| = r$;
- For every $\mathbf{j} \neq \mathbf{i}$, one has $\sqrt{W_{\mathbf{j},\mathbf{j}} W_{\bar{\mathbf{j}},\bar{\mathbf{j}}}} = r$ and $W_{\mathbf{j},\bar{\mathbf{j}}} = 0$.

An example of an optimal genuine EW for a three-qubit system is given by the following matrix:

$$W_{opt} = \begin{pmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & e^{i\theta} \\ \cdot & s_2 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & s_3 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & s_4 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \frac{1}{s_4} & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \frac{1}{s_3} & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \frac{1}{s_2} & \cdot \\ e^{-i\theta} & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix}.$$

It can be readily verified that this matrix satisfies all the conditions stated in the theorem. Its mirror is given as

$$M_{opt} = \beta \mathbb{I} - W_{opt}$$

where $\beta \geq \max\{s_i, 1/s_i\}_{i=2}^4 \geq 1$ to ensure M_{opt} is non-negative for product states. Then we see that M_{opt} is actually positive. We can make generalize this observation in the following proposition:

Proposition 3. Let W be a multiqubit X-shaped genuine EW satisfying $W + M = \alpha\mathbb{I}$ for some $\alpha > 0$. If W is optimal, then the mirror operator M is positive semidefinite.

Proof. Let W be an X-shaped optimal genuine EW with $\mathbf{i}$ as specified in (iii). By definition, the only nonzero off-diagonal elements of W occur at positions $(\mathbf{i}, \bar{\mathbf{i}})$ and $(\bar{\mathbf{i}}, \mathbf{i})$. We define the corresponding mirror operator M by

$$M = \alpha\mathbb{I} - W.$$

This operator retains the X-shaped structure of W and has off-diagonal elements

$$M_{\mathbf{i},\bar{\mathbf{i}}} = -re^{i\theta}, \qquad M_{\bar{\mathbf{i}},\mathbf{i}} = -re^{-i\theta},$$

for some real number $r \in \mathbb{R}$ and angle $\theta \in [0, 2\pi)$.

To determine whether M is positive, we examine its submatrices. For any bitstring $\mathbf{j} \neq \mathbf{i}$, the corresponding off-diagonal entry vanishes, i.e., $M_{\mathbf{j},\bar{\mathbf{j}}} = 0$. The diagonal entries are given by

$$M_{\mathbf{j},\mathbf{j}} = \alpha - W_{\mathbf{j},\mathbf{j}}, \quad M_{\bar{\mathbf{j}},\bar{\mathbf{j}}} = \alpha - W_{\bar{\mathbf{j}},\bar{\mathbf{j}}}.$$

These are non-negative provided that α is greater than or equal to the largest diagonal entry of W. Due to condition (iii), we have $\sqrt{W_{\mathbf{j},\mathbf{j}} W_{\bar{\mathbf{j}},\bar{\mathbf{j}}}} = r$, meaning that at least one of the diagonal entries must be no less than r. Therefore, choosing $\alpha \geq r$ shows the non-negativity of these entries.

Now consider the 2×2 principal submatrix corresponding to indices $\mathbf{i}$ and $\bar{\mathbf{i}}$:

$$\begin{pmatrix} \alpha & -re^{i\theta} \\ -re^{-i\theta} & \alpha \end{pmatrix},$$

which has eigenvalues

$$\lambda_\pm = \alpha \pm r.$$

Both eigenvalues are non-negative for $\alpha \geq r$, implying that this submatrix is positive semi-definite. As a diagonal entry $M_{\mathbf{j},\mathbf{j}}$ is always positive for any bitstring $\mathbf{j} \neq \mathbf{i}$, the operator M itself is positive. This establishes that, for any optimal X-shaped genuine EW W, its mirror $M = \alpha\mathbb{I} - W$ is positive semi-definite. ∎

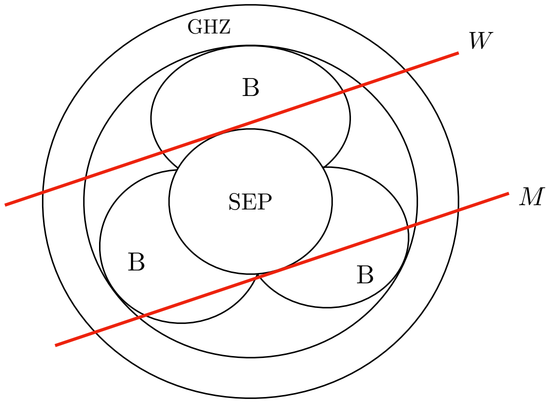

Figure 7. Three-qubit entangled states have an onion structure [55], where B denotes the set of bi-separable states. Three-qubit EWs in Eqs. (41) and (42)) are optimal and detect entangled states which are PPT in all bipartite splittings. Optimal three-qubit EWs can be mirrored with each other.

2. A pair of optimal mirrored witnesses detecting PPT states in three-qubit systems

We present a family of pairs of optimal mirrored EWs in three-qubit systems. We first consider the following class of three-qubit X-shaped density matrices:

$$\rho_{\mathrm{ppt}} = \frac{1}{\sum_{i=1}^{4}(s_i+t_i)} \begin{pmatrix} s_1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & u_1 \\ \cdot & s_2 & \cdot & \cdot & \cdot & \cdot & u_2 & \cdot \\ \cdot & \cdot & s_3 & \cdot & \cdot & u_3 & \cdot & \cdot \\ \cdot & \cdot & \cdot & s_4 & u_4 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \bar{u}_4 & t_4 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \bar{u}_3 & \cdot & \cdot & t_3 & \cdot & \cdot \\ \cdot & \bar{u}_2 & \cdot & \cdot & \cdot & \cdot & t_2 & \cdot \\ \bar{u}_1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & t_1 \end{pmatrix}$$

which is PPT in all bipartite splittings [55, 56] if

$$\begin{aligned} & s_i, t_i > 0 \quad \text{and} \quad s_i t_i = 1, \\ & |u_i| \leq 1 \qquad \text{for all } i = 1, \ldots, 4. \end{aligned}$$

Note that the state above reproduces a family of PPT states previously studied in [55, 57, 58].

Let us consider an EW that detects PPT states above,

$$\begin{aligned} W[i_1,i_2,i_3] \;=\; & \mathbb{I}^{\otimes 3} - Z^{(1)}Z^{(2)}Z^{(3)} - (-1)^{i_1}X^{(1)}X^{(2)}X^{(3)} \\ & -(-1)^{i_2}X^{(1)}Y^{(2)}Y^{(3)} - (-1)^{i_3}Y^{(1)}X^{(2)}Y^{(3)} \\ & -(-1)^{i_1+i_2+i_3+1}Y^{(1)}Y^{(2)}X^{(3)}, \end{aligned} \tag{41}$$

which has been studied in [56]. We compute its mirrored operator,

$$\begin{aligned} M[i_1,i_2,i_3] \;=\; & \mathbb{I}^{\otimes 3} + Z^{(1)}Z^{(2)}Z^{(3)} + (-1)^{i_1}X^{(1)}X^{(2)}X^{(3)} \\ & +(-1)^{i_2}X^{(1)}Y^{(2)}Y^{(3)} + (-1)^{i_3}Y^{(1)}X^{(2)}Y^{(3)} \\ & +(-1)^{i_1+i_2+i_3+1}Y^{(1)}Y^{(2)}X^{(3)}. \end{aligned} \tag{42}$$

In what follows, we summarize the properties of two EWs.

Firstly, two EWs are equivalent up to local unitaries $Y^{(123)} := Y^{(1)}Y^{(2)}Y^{(3)}$:

$$M[i_1,i_2,i_3] = Y^{(123)}W[i_1,i_2,i_3](Y^{(123)})^{\dagger}$$

More generally, it holds that

$$\begin{aligned} W[i_1',i_2',i_3'] &= UW[i_1,i_2,i_3]U^{\dagger}, \quad \text{and} \\ M[i_1',i_2',i_3'] &= UM[i_1,i_2,i_3]U^{\dagger}, \end{aligned}$$

for some local unitary U, e.g.,

$$\begin{aligned} W[1,1,1] &= (Z^{(1)}Z^{(2)}Z^{(3)})\, W[0,0,0]\, (Z^{(1)}Z^{(2)}Z^{(3)})^{\dagger}, \\ M[1,1,1] &= (Z^{(1)}Z^{(2)}Z^{(3)})\, M[0,0,0]\, (Z^{(1)}Z^{(2)}Z^{(3)})^{\dagger}. \end{aligned}$$

A complete characterization of the local equivalences between witness operators is detailed in the Appendix.

Secondly, both EWs are optimal from the spanning property [56]. For instance, $W[0,0,0]$ has the following eight product states, all of which yield zero expectation values:

$$\begin{aligned} & |000\rangle,\ |011\rangle,\ |101\rangle,\ |110\rangle, \\ & |+++\rangle,\ |+--\rangle,\ |-+-\rangle,\ |--+\rangle. \end{aligned}$$

That is, the spanning property is fulfilled. Since two EWs are equivalent up to local unitaries, the spanning property also holds.

Therefore, the EWs can detect entangled states that remain positive under partial transposition with respect to all bipartite splittings. We show that they detect PPT entangled states studied in [55, 57, 58].

- An EW $W[0,1,0]$ detects a known class of three-qubit bound entangled states in Refs. [55, 57],

$$\rho(x,y,z) = \frac{1}{\nu} \begin{pmatrix} 1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ \cdot & x & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & y & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & z & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & z^{-1} & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & y^{-1} & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & x^{-1} & \cdot \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 1 \end{pmatrix},$$

  with parameters $x, y, z > 0$ and $\nu = 2 + x + y + z + x^{-1} + y^{-1} + z^{-1}$ We can see that $\rho(x,y,z)$ above can be reproduced by ρ_{ppt} in Eq. (61). The state is thus positive under partial transposition with respect to all bipartitions whenever $x, y, z > 0$. We have

$$\mathrm{tr}\,[W[0,1,0]\,\rho] = \frac{2(x+y+z^{-1}-3)}{\nu},$$

which becomes negative when $0 < x, y < 1$ and $z > 1$. This shows that ρ is a PPT-entangled state.

d Note also that the locally Pauli-conjugated state

$$Y^{(123)} \rho(x, y, z) (Y^{(123)})^\dagger$$

can be detected by the mirrored one

$$M[0,1,0] = Y^{(123)} W[0,1,0] (Y^{(123)})^\dagger, \tag{43}$$

Both the witness $W[0,1,0]$ and its mirrored EW $M[0,1,0]$ detect bound entangled states in Ref. [55].

- An EW $W[1,1,0]$ detects another known class of three-qubit bound entangled states in Ref. [58]

$$\rho(b,c) = \frac{1}{6+b+c} \begin{pmatrix} 1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & -1 \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot & -1 & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & b & -1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & -1 & c & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & -1 & \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ -1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 1 \end{pmatrix},$$

with parameters $b, c > 0$ such that $bc \geq 1$. It is straightforward to check that $\rho(b,c)$ can be reproduced by ρ_{ppt} in Eq. (61). The state is thus positive under partial transposition with respect to all bipartitions whenever $bc = 1$.

The witness $W[1,1,0]$ detects this PPT entangled state for a range of parameters. Specifically, we compute

$$\operatorname{tr}\left[W[1,1,0]\,\rho(b,c)\right] = \frac{2(c-3)}{b+c+6},$$

which is negative for all $0 < c < 3$, thus confirming it is a PPT-entangled state. The calculation is detailed in the Appendix.

Furthermore, the locally Pauli-conjugated state is given,

$$(Y^{(123)}) \rho(b,c) (Y^{(123)})^\dagger = \frac{1}{6+b+c} \begin{pmatrix} 1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & -1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & c & 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 & b & \cdot & \cdot & \cdot \\ \cdot & \cdot & -1 & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 1 \end{pmatrix}.$$

Due to the equivalence by local unitaries, a state above is also PPT in all bipartite splittings. Note that

$$M[1,1,0] = (Y^{(123)}) W[1,1,0] (Y^{(123)})^\dagger,$$

and therefore, for $0 < c < 3$,

$$\begin{aligned} &\operatorname{tr}\left[M[1,1,0] (Y^{(123)}) \rho(b,c) (Y^{(123)})^\dagger\right] \\ = &\operatorname{tr}\left[W[1,1,0] \rho(b,c)\right] < 0, \end{aligned}$$

Hence, both EWs, $W[1,1,0]$ and $M[1,1,0]$, detect the PPT entangled states.

IV. BIPARTITE SYSTEMS: OPTIMALITY

In this section, we investigate mirrored EWs for bipartite systems $n \otimes n$ that contain symmetries, such as Bell diagonal and covariant with respect to a maximal commutative subgroup of the unitary group $U(n)$.

Let us summarize the construction of EWs, and then discuss the properties of their mirrored ones. A Weyl operator U_{mk} can be defined as [59, 60]

$$U_{mk} |\ell\rangle = \omega^{m\ell} |\ell + k\rangle \ (\text{mod } n), \tag{44}$$

with $\omega = e^{2\pi i/n}$. Weyl operators satisfy relations as follows

$$\begin{aligned} &U_{k\ell} U_{rs} = \omega^{ks} U_{k+r,\ell+s}, \quad U_{k\ell}^* = U_{-k\ell}, \\ &U_{k\ell}^\dagger = \omega^{k\ell} U_{-k,-\ell}, \quad \text{and} \quad \operatorname{tr}\Big[U_{k\ell} U_{rs}^\dagger\Big] = n\,\delta_{kr} \delta_{\ell s} \end{aligned}$$

where addition and subtraction are in modulo n. The generalized Bell states are denoted by

$$|\psi_{k\ell}\rangle = \mathbb{I} \otimes U_{k\ell} |\psi_{00}\rangle, \tag{45}$$

where $|\psi_{00}\rangle = 1/\sqrt{n} \sum_{k=0}^{n-1} |kk\rangle$. A Bell-diagonal operator can be written as $X = \sum_{k,\ell=0}^{n-1} x_{k\ell} P_{k\ell}$, with $P_{k\ell} = |\psi_{k\ell}\rangle\langle\psi_{k\ell}|$. Let us consider a maximal commutative subgroup of a unitary group $U(n)$

$$T(n) = \{\ U \in U(n) \,|\, U = \sum_{k=0}^{n-1} e^{i\phi_k} |k\rangle\langle k|\ \}.$$

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

$$U \otimes U^* X (U \otimes U^*)^\dagger = X, \tag{46}$$

for any $U \in T(n)$. Then, any covariant operator has the following structure

$$X = \sum_{k,\ell=0}^{n-1} A_{kl} |k\rangle\langle k| \otimes |\ell\rangle\langle\ell| + \sum_{k\neq\ell=0}^{n-1} B_{kl} |k\rangle\langle\ell| \otimes |k\rangle\langle\ell|, \tag{47}$$

with complex parameters $A_{k\ell}$ and $B_{k\ell}$. Note that for such operators the Hermitian matrix $A_{k\ell}$ is circulant, i.e. $A_{k\ell} = \alpha_{k-\ell}$ for some real vector $(\alpha_0, \alpha_1, \ldots, \alpha_{n-1})$ and B_{kl} is a constant, i.e. $B_{k\ell} = \beta \in \mathbb{R}$.

Proposition 1. *[61] A symmetric operator in the following is an EW,*

$$W = \sum_{k,\ell=0}^{n-1} \alpha_{k-l} |k\rangle\langle k| \otimes |\ell\rangle\langle\ell| - \sum_{k\neq\ell=0}^{n-1} |k\rangle\langle\ell| \otimes |k\rangle\langle\ell|, \quad (48)$$

when a circulant matrix $A_{k\ell}$ satisfies the following constraints

$$\alpha_0 + \alpha_1 + \ldots + \alpha_{n-1} = n-1, \quad (49)$$

and $AA^T = \mathbb{I} + (n-2)\mathbb{J}$ where $\mathbb{J}_{k\ell} = 1$.

A. EWs in $3 \otimes 3$

Let us consider a class of EWs that generalize the well-known Choi EWs [62]

$$\begin{aligned} W[a,b,c] &= \sum_{i=0}^{2} \Big[a\,|ii\rangle\langle ii| + b\,|i,i+1\rangle\langle i,i+1| \\ &+ c\,|i,i+2\rangle\langle i,i+2| \Big] - \sum_{i\neq j} |ii\rangle\langle jj| \end{aligned} \quad (50)$$

with parameters $a,b,c \geq 0$ satisfying

- $a+b+c \geq 2$, and
- if $a \leq 1$, then $bc \geq (1-a)^2$.

The well-known Choi EWs are intances, $W[1,1,0]$ or $W[1,0,1]$ [63–65]. Choi EWs are extremal [66, 67] and hence also optimal. Note, however, that though being optimal, Choi EWs do not satisfy the spanning property [38, 68]. Note that $W[a,b,c]$ are optimal when

$$a+b+c = 2 \;\text{ and }\; a^2+b^2+c^2 = 2,$$

if and only if $a \in [0,1]$, and extremal if and only if $a \in (0,1]$ [69, 70]). Note also that $W[a,b,c]$ is decomposable only if $b=c=1$.

Let us introduce parameterization as follows,

$$\begin{aligned} a &= \frac{2}{3}(1+\cos\phi), \quad b = \frac{1}{3}(2-\cos\phi-\sqrt{3}\sin\phi), \\ c &= \frac{1}{3}(2-\cos\phi+\sqrt{3}\sin\phi), \end{aligned} \quad (51)$$

that is, one has a 1-parameter family of EWs $W(\phi)$ for $\phi \in [0,2\pi)$. $W(\pi/3)$ and $W(5\pi/3)$ correspond to a pair of Choi witnesses and $W(\pi)$ corresponds to EW defined via the reduction map. $W(\phi)$ is optimal iff $\phi \in [\pi/3, 5\pi/3]$.

Then, mirrored operators are characterized as follows.

Proposition 2. *Mirrored operators to EWs in Eq. (50) are positive, i.e., which can be interpreted as quantum states, for $a \in [0,1/3]$ and decomposable EWs for $a \in (1/3,4/3]$.*

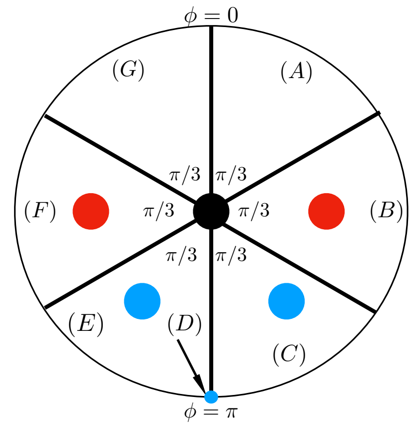

Figure 8. EWs in Eq. (50) are optimal for $\phi \in [\pi/3, 5\pi/3]$, see the parameterization in Eq. (51). For (A) and (G), EWs are not optimal. For (D), i.e., $\phi = \pi$, the EW is decomposable and not optimal, and its mirror is positive semidefinite. For (B) and (F), EWs are non-decomposable and optimal and their mirrored operators are decomposable EWs. For (C) and (E), EWs are non-decomposable and optimal, and their mirrored operators are positive definite.

B. EWs in $4 \otimes 4$

For $n=4$, we consider instances of EWs in Eq. (48) with four parameters [71]

$$\begin{aligned} W[a,b,c,d] &= \sum_{i=0}^{3} \Big[a\,|ii\rangle\langle ii| + b\,|i,i+1\rangle\langle i,i+1| \\ &+c\,|i,i+2\rangle\langle i,i+2| + d\,|i,i+3\rangle\langle i,i+3| \Big] \\ &- \sum_{i\neq j} |ii\rangle\langle jj| \end{aligned} \quad (52)$$

with $a,b,c,d \geq 0$ satisfying

$$\begin{aligned} a+b+c+d &= a^2+b^2+c^2+d^2 = 3, \\ ac+bd &= 1, \quad (a+c)(b+d) = 2. \end{aligned} \quad (53)$$

There are two solutions to the above set of equations [71]. From four parameters and four equations, we have two variables, called classes I and II:

$$\begin{aligned} \mathrm{I}: &\quad a+c = 2\,, \quad b+d = 1 \\ \mathrm{II}: &\quad a+c = 1\,, \quad b+d = 2 \end{aligned}$$

EWs from class I are not optimal, whereas those from class II are optimal [71].

1. Classs I: non-optimal non-decomposable EWs

EWs may expressed by a single parameter θ,

$$\begin{aligned} a &= \frac{1}{2}(2-\sin\theta)\,,\; b = \frac{1}{2}(1+\cos\theta)\,, \\ c &= 2-a\,,\; \text{and}\;\; d = 1-b, \end{aligned} \quad (54)$$

In particular, $W(0) = W[1,1,1,0]$ and $W(\pi) = W[1,0,1,1]$ are Choi-like EWs, and

$$W(\frac{\pi}{2}) = W[\frac{1}{2},\frac{1}{2},\frac{3}{2},\frac{1}{2}]$$

is the only decomposable EW in the class. The mirrored operator is computed for a witness $W(0) = W[1,1,1,0]$,

$$M[1,1,1,0] = \frac{4}{3}\mathbb{1}_4 \otimes \mathbb{1}_4 - W[1,1,1,0].$$

The mirrored operator can detect PPT entangled states in the following,

$$\begin{aligned} \rho_x \ \propto \ & \sum_{i=0}^{3} \Big[3\,|ii\rangle\langle ii| + x\,|i,i+1\rangle\langle i,i+1| + |i,i+2\rangle\langle i,i+2| \\ + \ & \frac{1}{x}\,|i,i+3\rangle\langle i,i+3| \Big] - \sum_{i\neq j} |ii\rangle\langle jj| \ , \end{aligned} \tag{55}$$

which is PPT for $x > 0$. It follows that

$$\mathrm{tr}[M[1,1,1,0]\rho_x] = \frac{4}{3x}(x^2 - 5x + 4),$$

which is negative for $x \in (1,4)$. Hence, the mirrored operator $M[1,1,1,0]$ is a non-decomposable EW.

We have shown that a pair of non-decomposable EWs can be mirrored with each other.

2. *Class II: optimal non-decomposable EWs*

We introduce a parameterization as follows:

$$\begin{aligned} a &= \frac{1}{2}(1+\cos\theta)\ ,\ b = \frac{1}{2}(2-\sin\theta)\ , \\ c &= 1-a\ ,\ d = 2-b, \end{aligned} \tag{56}$$

with $\theta \in [0,\pi]$. For $\theta = 0$ and $\theta = \pi$, EWs are decomposable. Otherwise, i.e., $\theta \in (0,\pi)$, they are non-decomposable and optimal.

It turns out that mirrored operators are positive semidefinite for EWs with $\theta \in (\pi/2,\pi)$ and decomposable EWs for $\theta \in\in (0,\pi/2)$. Hence, for optimal EWs in class II, their mirrored operators cannot be non-decomposable, i.e., either decomposable EWs or positive semidefinite [72].

C. Mirrored pair of optimal non-decomposable EWs

So far, we have considered mirrored operators of non-decomposable EWs and found that the mirrored ones are not EWs detecting PPT entangled states; they are either decomposable EWs or positive semidefinite operators. Recently, an intriguing instance of mirrored EWs has been presented in $3\otimes 3$ systems [72], where both EWs

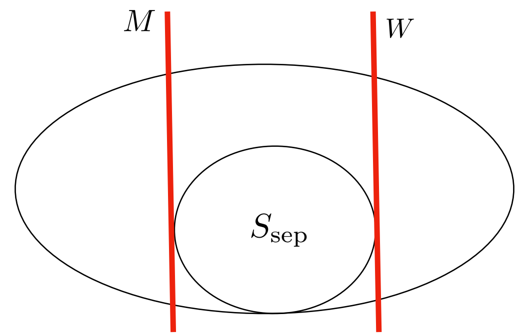

Figure 9. A pair of optimal EWs in Eqs. (57) can be mirrored with each other. Both are also non-decomposable. Two EWs are related by local unitaries.

are optimal, non-decomposable, and equivalent up to local unitaries. We here summarize the pair of optimal non-decomposable EWs.

Firstly, two EWs in the following are non-decomposable,

$$W = \left[\begin{array}{ccc|ccc|ccc} \cdot & \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot & 1 \\ \cdot & 3 & \cdot & \cdot & \cdot & -2 & -2 & \cdot & \cdot \\ \cdot & \cdot & 3 & -2 & \cdot & \cdot & \cdot & -2 & \cdot \\ \hline \cdot & \cdot & -2 & 3 & \cdot & \cdot & \cdot & -2 & \cdot \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ \cdot & -2 & \cdot & \cdot & \cdot & 3 & -2 & \cdot & \cdot \\ \hline \cdot & -2 & \cdot & \cdot & \cdot & -2 & 3 & \cdot & \cdot \\ \cdot & \cdot & -2 & -2 & \cdot & \cdot & \cdot & 3 & \cdot \\ 1 & \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot & \cdot \end{array}\right],$$

$$\text{and } M = \left[\begin{array}{ccc|ccc|ccc} 4 & \cdot & \cdot & \cdot & -1 & \cdot & \cdot & \cdot & -1 \\ \cdot & 1 & \cdot & \cdot & \cdot & 2 & 2 & \cdot & \cdot \\ \cdot & \cdot & 1 & 2 & \cdot & \cdot & \cdot & 2 & \cdot \\ \hline \cdot & \cdot & 2 & 1 & \cdot & \cdot & \cdot & 2 & \cdot \\ -1 & \cdot & \cdot & \cdot & 4 & \cdot & \cdot & \cdot & -1 \\ \cdot & 2 & \cdot & \cdot & \cdot & 1 & 2 & \cdot & \cdot \\ \hline \cdot & 2 & \cdot & \cdot & \cdot & 2 & 1 & \cdot & \cdot \\ \cdot & \cdot & 2 & 2 & \cdot & \cdot & \cdot & 1 & \cdot \\ -1 & \cdot & \cdot & \cdot & -1 & \cdot & \cdot & \cdot & 4 \end{array}\right] \tag{57}$$

as they detect PPT entangled states as follows,

$$\rho_W = \frac{1}{15}\left[\begin{array}{ccc|ccc|ccc} 3 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & 1 & 1 & \cdot & \cdot \\ \cdot & \cdot & 1 & 1 & \cdot & \cdot & \cdot & 1 & \cdot \\ \hline \cdot & \cdot & 1 & 1 & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & 3 & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & 1 & 1 & \cdot & \cdot \\ \hline \cdot & 1 & \cdot & \cdot & \cdot & 1 & 1 & \cdot & \cdot \\ \cdot & \cdot & 1 & 1 & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 3 \end{array}\right] \quad \text{and}$$

$$\rho_M = \frac{1}{15}\left[\begin{array}{ccc|ccc|ccc} 1 & \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot & 1 \\ \cdot & 2 & \cdot & \cdot & \cdot & -1 & -1 & \cdot & \cdot \\ \cdot & \cdot & 2 & -1 & \cdot & \cdot & \cdot & -1 & \cdot \\ \hline \cdot & \cdot & -1 & 2 & \cdot & \cdot & \cdot & -1 & \cdot \\ 1 & \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot & 1 \\ \cdot & -1 & \cdot & \cdot & \cdot & 2 & -1 & \cdot & \cdot \\ \hline \cdot & -1 & \cdot & \cdot & \cdot & -1 & 2 & \cdot & \cdot \\ \cdot & \cdot & -1 & -1 & \cdot & \cdot & \cdot & 2 & \cdot \\ 1 & \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot & 1 \end{array}\right],$$

such that

$$\mathrm{tr}[W\rho_W] = \mathrm{tr}[M\rho_M] = -\frac{2}{5}.$$

Note that EWs in Eq. (57) are constructed from positive maps via depolarization with mutually unbiased bases [72].

Both EWs in Eq. (57) are optimal as they fulfill the spanning property. In this case, it also holds that they are connected by local unitaries

$$M = U \otimes U^* W U^\dagger \otimes U^{*\dagger}$$

where

$$U = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 1 & \omega \\ 1 & \omega & 1 \\ \omega^* & \omega & \omega \end{pmatrix} \tag{58}$$

and $\omega = \exp[2\pi i/3]$.

V. BIPARTITE SYSTEMS: GENERALIZATION

We here generalize mirrored EWs in Eq. (12) such that they are connected by some other observable, not an identity,

$$W + M = \mathbb{K}, \tag{59}$$

where it follows that $\mathbb{K}$ block-positive, i.e., it is nonnegative for all separable states since W and M are EWs. Generalized mirrored EWs allow one to approach the following problems. Firstly, a pair of EWs may be constructed to detect a larger set of entangled states such

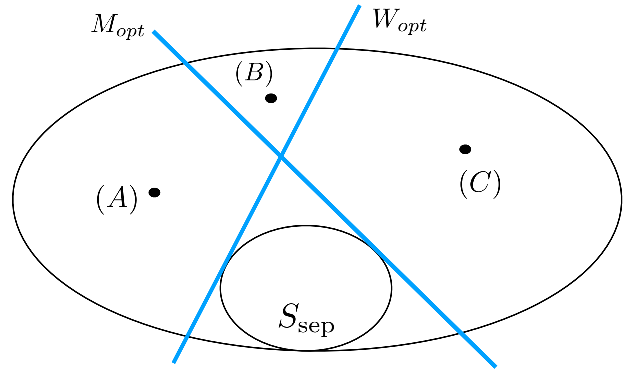

Figure 10. Entangled states (A) and (C) are detected by a witness W and its mirrored one M, respectively, where both EWs are non-decomposable and optimal. Both EWs detect an entangled state (B) in common, see Eq. (60), and $W + M$ also defines an EW, see Eq. (59).

that there may be entangled states detected by both EWs in common, i.e.,

$$D_W \cap D_M \neq \emptyset. \tag{60}$$

Secondly, one may attempt to characterize non-extremal EWs composed of optimal EWs and construct EWs that are efficient in the detection of entangled states.

Let us exploit EWs of class II in Eq. (52), which are optimal and non-decomposable EWs. We then apply a Weyl operator U_{jk} to construct its generalized mirrored one

$$M = (I \otimes U_{jk}) W (I \otimes U_{jk})^\dagger.$$

Note that two EWs, W and M, are unitarily equivalent; hence, both are optimal and non-decomposable, and the two sets D_W and D_M are unitarily equivalent.

A witness W detects a family of PPT entangled states ρ_x in Eq. (55) since,

$$\begin{aligned} \mathrm{tr}[W\rho_x] &= a + bx + c + \frac{d}{x} - 3 \\ &= b(x-1) + d\left(\frac{1}{x} - 1\right), \end{aligned}$$

which is negative for

$$\frac{1}{2b}\left(b + d - |b-d|\right) < x < \frac{1}{2b}\left(b + d + |b-d|\right).$$

We have $\mathrm{tr}[W\rho_x] < 0$ for $b \neq d$. Since W and M are unitarily equivalent, M detects entangled states$(I \otimes U_{jk})\rho_x(I \otimes U_{jk})^\dagger$, which are PPT; M is non-decomposable.

With two optimal EWs, we construct an operator

$$\mathbb{K} = W + (I \otimes U_{jk}) W (I \otimes U_{jk})^\dagger.$$

It is clear that $\mathbb{K}$ is non-negative for all separable states. Let us consider an entangled state

$$\tau = \frac{1}{2}(P_{00} + P_{j1})$$

where $P_{kl} = |\psi_{kl}\rangle\langle\psi_{kl}|$ in Eq. (45). Note that the state above does not remain positive after the partial transpose. From the parametrization of a, b, c, d in Eq. (56),

$$\begin{aligned} \mathrm{tr}[W\tau] &= \frac{1}{4}(\cos\theta - \sin\theta - 3), \\ \text{and} \quad \mathrm{tr}[M\tau] &= \frac{1}{4}(\cos\theta + \sin\theta - 3), \end{aligned}$$

both of which are negative. By construction, it follows that

$$\mathrm{tr}[\mathbb{K}\tau] = \mathrm{tr}[W\tau] + \mathrm{tr}[M\tau] < 0,$$

and each one W and M detects entangled states τ in common, see Fig. 10. Hence, we have shown that optimal and non-decomposable EWs can be mirrored with each other by another EW.

VI. OPEN PROBLEMS

Mirrored EWs pave the pathway to increasing the usefulness of an experimental realization of EWs. Once an EW is estimated, the estimation can be exploited to detect distinct types of entangled states. Our results open an avenue to develop EWs with intriguing questions in the following.

1. For bipartite systems, we have found that for two-qubit states, optimal EWs cannot be mirrored with each other. Then, a mirrored pair of optimal EWs have been obtained for systems $3 \otimes 3$. However, the result in systems $3 \otimes 3$ cannot be extended to higher-dimensional systems [72]. It remains open to find if a mirrored pair of optimal EWs exists for higher dimensions, in particular, the covariant Bell-diagonal EWs.

2. Optimal EWs can be mirrored via another EW, as shown in Eq. (59). Since optimal EWs are generally not extremal yet, it remains unanswered whether a pair of optimal EWs can be mirrored through another optimal EWs.

3. Mutually unbiased bases (MUBs) are a measurement setting for quantum state verification. They can also be used for constructing EWs [73, 74], in which extendible and unextendible MUBs, which are inequivalent, provide different efficiencies in detecting entangled states. For practical applications, it would be interesting to find mirrored EWs for EWs constructed from MUBs and investigate how efficient a subset of MUBs is in entanglement detection before a quantum state is fully verified.

4. Throughout, we have investigated mirrored linear EWs. In future directions, it is worth investigating the properties of mirrored nonlinear EWs.

5. All instances provided here about mirrored pairs of optimal EWs satisfy the equivalence up to local unitaries. That is, mirrored EWs detect distinct sets of entangled states in which states of one set can be transformed the others by local untaries. It remains open if there could be a mirrored pair of optimal EWs that cannot be transformed by local unitaries.

VII. CONCLUSION

In conclusion, we have developed mirrored EWs for multipartite and high-dimensional quantum systems. For multipartite systems, we have investigated mirrored EWs for n-partite GHZ states, graph states, and multipartite bound entangled states. A mirrored pair of optimal EWs is also shown for three-qubit systems. For bipartite systems, we have considered mirroring for existing optimal EWs and found that the resulting mirrored ones are either decomposable EWs or positive semidefinite. A mirrored pair of optimal EWs is then constructed in a three-dimensional bipartite system. Hence, we have shown that mirrored pairs of optimal EWs, which do not exist for two-qubit states, appear in higher dimensions and multipartite systems. The framework of mirrored EWs has been generalized by taking an EW, not an identity, to which two EWs are mirrored with each other. Our results shed new light on the theory of EWs and also on the efficient detection of entangled states in practical scenarios.

Our results are readily applied to realistic scenarios of quantum communication, e.g., fibre-optic communication, where rotations of local bases of qubit states are a critical source of errors. Entanglement is also a precondition in secure quantum communication [16, 17]. Mirrored pairs of EWs considered in the present work, when both are EWs, are connected by local unitaries. Consequently, entangled states detected by each EW of a pair are local unitarily equivalent. Therefore, mirrored EWs are robust against the noise from rotations of local bases. We envisage that mirrored EWs can enhance the detection of entangled states in realistic entanglement-based quantum communication protocols.

APPENDIX

A. Local equivalences of $W[i_1, i_2, i_3]$

As stated earlier, two different EWs $W[i_1, i_2, i_3]$ and $W[i'_1, i'_2, i'_3]$ from Eq. (41) are locally equivalent. More precisely, one $W[i'_1, i'_2, i'_3]$ is given by the Pauli-conjugated operator:

$$W[i'_1, i'_2, i'_3] = UW[i_1, i_2, i_3]U^\dagger,$$

where U is a local unitary, a product of Pauli matrices. Specifically,

$$\begin{aligned}
W[1,1,1] &= (Z^{(1)}Z^{(2)}Z^{(3)})\, W[0,0,0]\, (Z^{(1)}Z^{(2)}Z^{(3)})^\dagger \\
W[1,1,0] &= (Z^{(1)}X^{(2)}X^{(3)})\, W[0,0,0]\, (Z^{(1)}X^{(2)}X^{(3)})^\dagger \\
W[1,0,1] &= (X^{(1)}Z^{(2)}X^{(3)})\, W[0,0,0]\, (X^{(1)}Z^{(2)}X^{(3)})^\dagger \\
W[1,0,0] &= (X^{(1)}X^{(2)}Z^{(3)})\, W[0,0,0]\, (X^{(1)}X^{(2)}Z^{(3)})^\dagger \\
W[0,1,1] &= (Y^{(1)}Y^{(2)}\mathbb{I}^{(3)})\, W[0,0,0]\, (Y^{(1)}Y^{(2)}\mathbb{I}^{(3)})^\dagger \\
W[0,1,0] &= (Y^{(1)}\mathbb{I}^{(2)}Y^{(3)})\, W[0,0,0]\, (Y^{(1)}\mathbb{I}^{(2)}Y^{(3)})^\dagger \\
W[0,0,1] &= (\mathbb{I}^{(1)}Y^{(2)}Y^{(3)})\, W[0,0,0]\, (\mathbb{I}^{(1)}Y^{(2)}Y^{(3)})^\dagger
\end{aligned}$$

The same applies to $M[i_1, i_2, i_3]$.

B. Calculations for detecting $\rho_{\rm ppt}$

We provide details of coefficients of ρ, introduced in (61),

$$\rho_{\rm ppt} = \frac{1}{\sum_{i=1}^4 (s_i + t_i)} \begin{pmatrix}
s_1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & u_1 \\
\cdot & s_2 & \cdot & \cdot & \cdot & \cdot & u_2 & \cdot \\
\cdot & \cdot & s_3 & \cdot & \cdot & u_3 & \cdot & \cdot \\
\cdot & \cdot & \cdot & s_4 & u_4 & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \bar{u}_4 & t_4 & \cdot & \cdot & \cdot \\
\cdot & \cdot & \bar{u}_3 & \cdot & \cdot & t_3 & \cdot & \cdot \\
\cdot & \bar{u}_2 & \cdot & \cdot & \cdot & \cdot & t_2 & \cdot \\
\bar{u}_1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & t_1
\end{pmatrix},$$

when expanded in the Pauli basis. We first denote

$$r_{ijk} := 8\,\mathrm{tr}[\rho_{\rm ppt}(\sigma_i \otimes \sigma_j \otimes \sigma_k)],$$
$$\sigma_0 = \mathbb{I}, \sigma_1 = X, \sigma_2 = Y, \sigma_3 = Z.$$

Then we can rewrite $\rho_{\rm ppt}$ in the Pauli basis as [56]:

$$\begin{aligned}
\rho_{\rm ppt} = \frac{1}{8}\Big[& \mathbb{I}^{(1)}\mathbb{I}^{(2)}\mathbb{I}^{(3)} + r_{300}\, Z^{(1)}\mathbb{I}^{(2)}\mathbb{I}^{(3)} + r_{030}\, \mathbb{I}^{(1)}Z^{(2)}\mathbb{I}^{(3)} \\
& + r_{003}\, \mathbb{I}^{(1)}\mathbb{I}^{(2)}Z^{(3)} + r_{330}\, Z^{(1)}Z^{(2)}\mathbb{I}^{(3)} + r_{303}\, Z^{(1)}\mathbb{I}^{(2)}Z^{(3)} \\
& + r_{033}\, \mathbb{I}^{(1)}Z^{(2)}Z^{(3)} + r_{333}\, Z^{(1)}Z^{(2)}Z^{(3)} + r_{111}\, X^{(1)}X^{(2)}X^{(3)} \\
& + r_{112}\, X^{(1)}X^{(2)}Y^{(3)} + r_{121}\, X^{(1)}Y^{(2)}X^{(3)} + r_{211}\, Y^{(1)}X^{(2)}X^{(3)} \\
& + r_{122}\, X^{(1)}Y^{(2)}Y^{(3)} + r_{212} Y^{(1)}\, X^{(2)}Y^{(3)} + r_{221} Y^{(1)}\, Y^{(2)}X^{(3)} \\
& + r_{222}\, Y^{(1)}Y^{(2)}Y^{(3)}\Big].
\end{aligned}$$

The coefficients r_{ijk} are given by

$$\begin{aligned}
r_{111} &= \frac{2}{\nu}(\mathrm{Re}\, u_1 + \mathrm{Re}\, u_2 + \mathrm{Re}\, u_3 + \mathrm{Re}\, u_4), \\
r_{112} &= \frac{2}{\nu}(\mathrm{Im}\, u_1 - \mathrm{Im}\, u_2 + \mathrm{Im}\, u_3 - \mathrm{Im}\, u_4), \\
r_{121} &= \frac{2}{\nu}(\mathrm{Im}\, u_1 + \mathrm{Im}\, u_2 - \mathrm{Im}\, u_3 - \mathrm{Im}\, u_4), \\
r_{211} &= \frac{2}{\nu}(-\mathrm{Im}\, u_1 - \mathrm{Im}\, u_2 - \mathrm{Im}\, u_3 - \mathrm{Im}\, u_4), \\
r_{122} &= \frac{2}{\nu}(-\mathrm{Re}\, u_1 + \mathrm{Re}\, u_2 + \mathrm{Re}\, u_3 - \mathrm{Re}\, u_4), \\
r_{212} &= \frac{2}{\nu}(\mathrm{Re}\, u_1 - \mathrm{Re}\, u_2 + \mathrm{Re}\, u_3 - \mathrm{Re}\, u_4), \\
r_{221} &= \frac{2}{\nu}(\mathrm{Re}\, u_1 + \mathrm{Re}\, u_2 - \mathrm{Re}\, u_3 - \mathrm{Re}\, u_4), \\
r_{222} &= \frac{2}{\nu}(\mathrm{Im}\, u_1 - \mathrm{Im}\, u_2 - \mathrm{Im}\, u_3 + \mathrm{Im}\, u_4), \\
r_{300} &= \frac{1}{\nu}(s_1 + s_2 + s_3 + s_4 - t_1 - t_2 - t_3 - t_4), \\
r_{030} &= \frac{1}{\nu}(s_1 + s_2 - s_3 - s_4 - t_1 - t_2 + t_3 + t_4), \\
r_{330} &= \frac{1}{\nu}(s_1 + s_2 - s_3 - s_4 + t_1 + t_2 - t_3 - t_4), \\
r_{303} &= \frac{1}{\nu}(s_1 - s_2 + s_3 - s_4 + t_1 - t_2 + t_3 - t_4), \\
r_{033} &= \frac{1}{\nu}(s_1 - s_2 - s_3 + s_4 + t_1 - t_2 - t_3 + t_4), \\
r_{333} &= \frac{1}{\nu}(s_1 - s_2 - s_3 + s_4 - t_1 + t_2 + t_3 - t_4),
\end{aligned}$$

where ν is the normalization factor, $\nu = \sum_{i=1}^4 (s_i + t_i)$. For $W[i_1, i_2, i_3]$ presented in Eq. (41),

$$\begin{aligned}
W[i_1, i_2, i_3] \;=\; & \mathbb{I}^{\otimes 3} - Z^{(1)}Z^{(2)}Z^{(3)} - (-1)^{i_1} X^{(1)}X^{(2)}X^{(3)} \\
& -(-1)^{i_2} X^{(1)}Y^{(2)}Y^{(3)} - (-1)^{i_3} Y^{(1)}X^{(2)}Y^{(3)} \\
& -(-1)^{i_1+i_2+i_3+1} Y^{(1)}Y^{(2)}X^{(3)},
\end{aligned} \tag{61}$$

we compute the following expectation value:

$$\begin{aligned}
\mathrm{tr}\big[W[i_1, i_2, i_3]\rho_{\rm ppt}\big] = & \; 1 - r_{333} - (-1)^{i_1} r_{111} - (-1)^{i_2} r_{122} \\
& - (-1)^{i_3} r_{212} - (-1)^{i_1+i_2+i_3+1} r_{221},
\end{aligned} \tag{62}$$

To evaluate the expectation value of 3-qubit PPT state $\rho(b, c)$ in Eq. (44) with respect to $W[i_1, i_2, i_3]$, we expand it in the Pauli basis and compute selected correlation coefficients. The nonzero off-diagonal entries of $\rho(b, c)$ appear as $u_1 = u_2 = u_4 = -1$ and $u_3 = 1$. The diagonal elements yield $s_1 = s_2 = s_3 = 1$, $s_4 = b$ and $t_1 = t_2 = t_3 = 1$, $t_4 = c$. Substituting these into the general expressions for the Pauli coefficients, we obtain:

$$r_{333} = \frac{b-c}{b+c+6},$$
$$r_{111} = -\frac{4}{b+c+6},$$
$$r_{122} = 0,$$
$$r_{212} = \frac{4}{b+c+6},$$
$$r_{221} = -\frac{4}{b+c+6},$$

where $\nu = \sum_{i=1}^{4}(s_i + t_i) = b + c + 6$ is the normalization factor. Plugging all coefficients $r_{333}, r_{111}, r_{122}, r_{212}$ and r_{221} into Eq. (62) gives

$$\mathrm{tr}[W[i_1,i_2,i_3]\,\rho(b,c)] = \frac{2c+6+4\left((-1)^{i_1} - (-1)^{i_3} + (-1)^{i_1+i_2+i_3+1}\right)}{b+c+6}$$

Plugging $i_1 = i_2 = 1$ and $i_3 = 0$ gives

$$\mathrm{tr}[W[1,1,0]\,\rho(b,c)] = \frac{2(c-3)}{b+c+6}.$$

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