Quantum entanglement estimation via symmetric-measurement-based positive maps

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We provide a class of positive and trace-preserving maps based on symmetric measurements. From these positive maps we present separability criteria, entanglement witnesses, and the lower bounds of concurrence. We show by detailed examples that our separability criteria, entanglement witnesses, and lower bounds can detect and estimate the quantum entanglement better than existing related results.

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I. INTRODUCTION

Quantum entanglement is the key resource in quantum information processing and plays an important role in quantum communication, quantum computing, and other modern quantum technologies [1]. Therefore, it is of significance to distinguish the entangled states from the separable ones and estimate the degree of entanglement for the entangled states. However, generally the separability problem and the estimation of entanglement are very difficult and even NP-hard [2]. For low-dimensional systems such as $\mathbb{C}^2 \otimes \mathbb{C}^2$ (qubit-qubit) and $\mathbb{C}^2 \otimes \mathbb{C}^3$ (qubit-qutrit) systems, the celebrated positive partial transposition criterion is both necessary and sufficient for separability [3,4]. For higher-dimensional systems, more sophisticated methods are needed to detect the entanglement.

One separability criterion to detect entanglement is given by positive maps. A bipartite state ρ is separable if and only if $(\mathbb{I} \otimes \Phi)(\rho) \ge 0$ for any positive map Φ [5], where \mathbb{I} is the identity operator. More specifically, ρ is entangled if $(\mathbb{I} \otimes \Phi)(\rho)$ has negative eigenvalues for some positive map Φ .

Entanglement can be also detected by entanglement witnesses. A Hermitian operator *W* is called an entanglement witness if $Tr(W\rho_{sep}) \ge 0$ for all separable states ρ_{sep} and $Tr(W\rho) < 0$ for some entangled states ρ [6,7]. By Choi-Jamiołkowski isomorphism, an entanglement witness is related to a positive but not completely positive map Φ . One kind of entanglement witnesses is the decomposable one, for which an entanglement witness can be written as $W = A + B^{\Gamma}$, where $A, B \ge 0$ and $B^{\Gamma} = (\mathbb{I} \otimes T)B$, with *T* denoting the transpose. However, the decomposable witness cannot detect the positive partial transpose (PPT) entangled states that are positive under a partial transpose. The indecomposable witnesses can detect the PPT states [5,8–11], which can be constructed by using the realignment separability criterion [12–14] and covariance matrix criterion [15–17]. In [18] the

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authors constructed a class of indecomposable witnesses by using mutually unbiased bases. This method was extended to the one using mutually unbiased measurements (MUMs) and symmetric informationally complete (SIC) positive-operatorvalued measures (POVMs). New entanglement witnesses have been also obtained [19–21]. Recently, a new kind of measurement, called symmetric measurement, was proposed in [22]. Based on the symmetric measurements, a class of positive maps and entanglement witnesses was constructed in [23].

To quantify the entanglement, many measures have been presented such as the entanglement of formation (EOF) [24,25] and concurrence [26–28]. However, it is a challenge to evaluate the entanglement measures for general quantum states. Instead of analytic formulas, progress has been made toward the lower bounds of EOF and concurrence. Based on a positive map, a new lower bound of concurrence for arbitrary-dimensional bipartite systems was derived in [29], which detects the entanglement that is not detected by the previous lower bounds [30,31].

In this paper we first present a family of positive and tracepreserving maps based on symmetric measurements. Then we present separability criteria and show that these separability criteria detect better entanglement of quantum states with an exact example. We then construct a series of entanglement witnesses which includes some existing ones as special cases. These entanglement witnesses are shown to detect better entanglement including bound entanglements. Finally, we give a family of lower bounds of concurrence and demonstrate that the bounds better estimate the quantum entanglement than the existing ones.

II. POSITIVE MAPS AND SEPARABILITY CRITERIA

A POVM is given by a set of positive operators $\{E_{\alpha} \mid E_{\alpha} \ge 0, \sum_{\alpha} E_{\alpha} = \mathbb{I}\}$. For a given state ρ , the probability of the measurement outcome with respect to E_{α} is $p_{\alpha} = \text{Tr}(E_{\alpha}\rho)$. Recall that a new POVM called symmetric measurement was provided in [22]. A set of *N d*-dimensional POVMs $\{E_{\alpha,k} \mid E_{\alpha,k} \ge 0, \sum_{k=1}^{M} E_{\alpha,k} = \mathbb{I}_d\}$ ($\alpha = 1, \ldots, N$) is called an

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(N, M) POVM, which satisfies the symmetry properties

$$Tr(E_{\alpha,k}) = \frac{d}{M},$$

$$Tr(E_{\alpha,k}^{2}) = x,$$

$$Tr(E_{\alpha,k}E_{\alpha,\ell}) = \frac{d - Mx}{M(M - 1)}, \quad \ell \neq k$$

$$Tr(E_{\alpha,k}E_{\beta,\ell}) = \frac{d}{M^{2}}, \quad \beta \neq \alpha,$$
(1)

where

$$\frac{d}{M^2} < x \leqslant \min\left\{\frac{d^2}{M^2}, \frac{d}{M}\right\}.$$
(2)

For any fixed dimension $d < \infty$, there are at least four different types of informationally complete (N, M)POVMs: (i) $M = d^2$ and N = 1 (a general SIC POVM) [32], (ii) M = d and N = d + 1 (a MUM) [33], (iii) M =2 and $N = d^2 - 1$, and (iv) M = d + 2 and N = d - 1. A general construction of informationally complete (N, M)POVMs is presented by using orthonormal Hermitian operator bases { $G_0 = \mathbb{I}_d / \sqrt{d}, G_{\alpha,k}; \alpha = 1, ..., N; k = 1, ..., M - 1$ } with $\text{Tr}(G_{\alpha,k}) = 0$,

$$E_{\alpha,k} = \frac{1}{M} \mathbb{I}_d + t H_{\alpha,k}, \qquad (3)$$

where

$$H_{\alpha,k} = \begin{cases} G_{\alpha} - \sqrt{M}(\sqrt{M} + 1)G_{\alpha,k}, & k = 1, \dots, M - 1\\ (\sqrt{M} + 1)G_{\alpha}, & k = M, \end{cases}$$
(4)

and $G_{\alpha} = \sum_{k=1}^{M-1} G_{\alpha,k}$. The parameters t and x satisfy the relation

$$x = \frac{d}{M^2} + t^2 (M - 1)(\sqrt{M} + 1)^2.$$
 (5)

The optimal value x_{opt} , which is the greatest x such that $E_{\alpha,k} \ge 0$, depends on the operator bases. There always exist informationally complete (N, M) POVMs for any integer d.

Reference [23] presented the class of positive maps

$$\Phi(X) = \frac{1}{b} \left(a \Phi_0(X) + \sum_{\alpha=L+1}^N \Phi_\alpha(X) - \sum_{\alpha=1}^L \Phi_\alpha(X) \right), \quad (6)$$

where a = b - N + 2L, $b = \frac{(d-1)M(x-y)}{d}$, $\Phi_0(X) = \frac{\text{Tr}(X)}{d} \mathbb{I}_d$, and

$$\Phi_{\alpha}(X) = \frac{M}{d} \sum_{k,l=1}^{M} \mathcal{O}_{k\ell}^{(\alpha)} E_{\alpha,k} \operatorname{Tr}(X E_{\alpha,l})$$
(7)

are *N* trace-preserving maps given by (N, M) POVMs $\{E_{\alpha,k}\}$ with $\{\mathcal{O}^{(\alpha)}|\mathcal{O}^{(\alpha)} = (\mathcal{O}^{(\alpha)}_{k\ell}), \alpha = 1, \ldots, N\}$ a set of $M \times M$ orthogonal rotation operators that preserve the vector $\mathbf{n}_* = (1, \ldots, 1)/\sqrt{d}$. Using the maps (6), we have the following theorem.

Theorem 1. A bipartite state ρ is entangled if $(\mathbb{I} \otimes \Phi_z)(\rho) \geq 0$, where

$$\Phi_z(X) = (1 - z)\Phi_0(X) + z\Phi(X) \,\forall X \in \mathbb{M}_d \tag{8}$$

are positive and trace-preserving linear maps with $z \in [-1, 1]$.

Proof. In order to prove the positivity of Φ_z , we only need to prove [34]

$$\operatorname{Tr}\{[\Phi_{z}(P)]^{2}\} \leqslant \frac{1}{d-1}$$
(9)

for every rank-1 projector $P = |\psi\rangle\langle\psi|$. By straightforward calculation we have

$$\operatorname{Tr}\{[\Phi_{z}(P)]^{2}\} = \operatorname{Tr}\{(1-z)^{2}\Phi_{0}(P)^{2} + z^{2}\Phi(P)^{2} + z(1-z)[\Phi_{0}(P)\Phi(P) + \Phi(P)\Phi_{0}(P)]\}$$

$$= \frac{(1-z)^{2}}{d}[\operatorname{Tr}(P)]^{2} + \frac{2z}{d}[\operatorname{Tr}(P)]^{2}(1-z) + z^{2}\operatorname{Tr}[\Phi(P)^{2}]$$

$$\leqslant \frac{(1-z)^{2}}{d} + \frac{2z(1-z)}{d} + \frac{z^{2}}{d-1}$$

$$= \frac{(z^{2}-1)+d}{d(d-1)} \leqslant \frac{1}{d-1}, \quad (10)$$

which completes the proof of positivity. The proof of trace preservation is obvious. The theorem follows from the separability criterion based on positive maps.

The map (8) is a linear but not convex combination of the map Φ and the completely depolarizing channel Φ_0 for $z \in [-1, 0)$, namely, it is truly a new positive but not completely positive map. To illustrate the theorem, let us consider the state [35]

$$\rho = \frac{1}{4} \operatorname{diag}(q_1, q_4, q_3, q_2, q_2, q_1, q_4, q_3, q_3, q_2,$$

$$q_1, q_4, q_4, q_3, q_2, q_1) + \frac{q_1}{4} \sum_{i,j=1,6,11,16}^{i \neq j} F_{i,j}, \quad (11)$$

where $F_{i,j}$ is a matrix with the (i, j) entry 1 and the rest of the entries 0, $q_m \ge 0$, and $\sum q_m = 1$, with m = 1, 2, 3, 4. We set d = 4, N = L = 5, M = 4, and $\mathcal{O}^{(\alpha)} = I_4$ for any $\alpha \in [N]$. The (5,4) POVMs are constructed from the Gell-Mann matrices (see Appendix A). From Theorem 1 we obtain that ρ is entangled for 0.25 $< q_1 < 1$ by straightforward calculation (see Appendix C). The criterion given in [29] detects the entanglement when $q_1 > q_4$. Our criterion shows that when $0.25 < q_1 < 1, \rho$ is entangled even if $q_1 < q_4$.

III. CONSTRUCTION OF ENTANGLEMENT WITNESSES FROM POSITIVE MAPS

By entanglement witnesses we can detect the entanglement of unknown quantum states experimentally. An entanglement witness W can be obtained based on the positive but not completely positive map Φ through Choi-Jamiołkowski isomorphism [36]

$$W = \sum_{k,\ell=1}^{d} |k\rangle \langle \ell| \otimes \Phi(|k\rangle \langle \ell|), \qquad (12)$$

where $\{|k\rangle\}_{k=1}^d$ is an orthonormal basis in \mathbb{C}^d . Therefore, by using the positive maps in Theorem 1, we get the

entanglement witnesses

$$W = \frac{1}{b} \left(\frac{aw}{d} \mathbb{I}_{d^2} + \sum_{\alpha=L+1}^N K_\alpha - \sum_{\alpha=1}^L K_\alpha \right), \quad (13)$$

where

$$K_{\alpha} = \frac{Mz}{d} \sum_{k,\ell=1}^{M} \mathcal{O}_{k\ell}^{(\alpha)} \bar{E}_{\alpha,\ell} \otimes E_{\alpha,k}, \qquad (14)$$

with $\bar{E}_{\alpha,\ell}$ the conjugation of $E_{\alpha,l}$. In particular, when z = 1 our witnesses include the one given in [23] as a special case.

As the informationally complete (N, M) POVMs can be constructed by using an orthogonal basis { $\mathbb{I}_d/\sqrt{d}, G_{\alpha,k}$ } of traceless Hermitian operators $G_{\alpha,k}$ for any dimension *d*, we have the entanglement witnesses

$$\tilde{W} = \frac{b}{t^2} W = \frac{d-1}{d^2} M^2 (\sqrt{M} + 1)^2 \mathbb{I}_{d^2} + \sum_{\alpha = L+1}^N J_\alpha - \sum_{\alpha = 1}^L J_\alpha,$$
(15)

where

$$J_{\alpha} = \frac{Mz}{d} \sum_{k,\ell=1}^{M} \mathcal{O}_{kl}^{(\alpha)} \bar{H}_{\alpha,\ell} \otimes H_{\alpha,k}, \qquad (16)$$

with $\bar{H}_{\alpha,\ell}$ the conjugation of $H_{\alpha,l}$. Note that these witnesses do not depend on the parameter *x* that characterizes the

symmetric measurements, but \tilde{W} are related to the number M of operators in a single POVM. The larger the value of M is, the larger the L can be.

Note that J_{α} in (16) can be directly represented by the operator basis $\{G_0 = \mathbb{I}_d / \sqrt{d}, G_{\alpha,k}; \alpha = 1, \dots, N; k = 1, \dots, M - 1\}$, since $H_{\alpha,k}$ are directly given by $G_{\alpha,k}$. By using (4) we further obtain

$$J_{\alpha} = \frac{Mz}{d} \sum_{k,\ell=1}^{M-1} \mathcal{Q}_{kl}^{(\alpha)} \bar{G}_{\alpha,\ell} \otimes G_{\alpha,k},$$

where

$$\mathcal{Q}_{k\ell}^{(\alpha)} = M \big(\mathcal{O}_{MM}^{(\alpha)} - 1 \big) + M (\sqrt{M} + 1)^2 \mathcal{O}_{k\ell}^{(\alpha)} - M (\sqrt{M} + 1) \big(\mathcal{O}_{M\ell}^{(\alpha)} + \mathcal{O}_{kM}^{(\alpha)} \big).$$
(17)

Since

$$\mathcal{Q}^{(\alpha)T}\mathcal{Q}^{(\alpha)} = \mathcal{Q}^{(\alpha)}\mathcal{Q}^{(\alpha)T} = M^2(\sqrt{M}+1)^4\mathbb{I}_{M-1},$$

 $Q^{(\alpha)} = (Q^{(\alpha)}_{k\ell}) \ (\alpha = 1, ..., N)$ are $M \times M$ rescaled orthogonal matrices. When $\mathcal{O}^{(\alpha)} = \mathbb{I}_M$, Eq. (17) can be rewritten as

$$\mathcal{Q}_{k\ell}^{(\alpha)} = M(\sqrt{M}+1)^2 \delta_{k\ell}.$$
 (18)

Next we illustrate that \tilde{W} (15) are related to a well-known class of entanglement witnesses. Suppose the (N, M) POVM is informationally complete and L = N. The corresponding witnesses is

$$\tilde{W} = \frac{M^2}{d} (\sqrt{M} + 1)^2 \left(\mathbb{I}_{d^2} - G_0 \otimes G_0 - \frac{d}{M^2 (\sqrt{M} + 1)^2} \sum_{\alpha = 1}^N J_\alpha \right),\tag{19}$$

where $G_0 = \mathbb{I}_d / \sqrt{d}$. By a simple relabeling of the indices $(\alpha, k) \mapsto \mu$, we have

$$\widetilde{W}' = \frac{d\widetilde{W}}{M^2(\sqrt{M}+1)^2} = \mathbb{I}_{d^2} - \sum_{\mu,\nu=0}^{d^2-1} \mathcal{Q}_{\mu\nu} G^T_{\mu} \otimes G_{\nu},$$
(20)

where $Q_{\mu\nu}$ are the entries of the block-diagonal orthogonal matrix

$$Q = \frac{1}{M(\sqrt{M}+1)^2} \begin{bmatrix} M(\sqrt{M}+1)^2 & & & \\ & zQ^{(1)T} & & \\ & & zQ^{(2)T} & & \\ & & & \ddots & \\ & & & & zQ^{(N)T} \end{bmatrix}.$$
 (21)

Therefore, the entanglement witnesses \tilde{W} constructed from symmetric measurements belong to a larger category of witnesses

$$W' = \mathbb{I}_{d^2} - \sum_{\mu,\nu=0}^{d^2 - 1} Q_{\mu\nu} G_{\mu}^T \otimes G_{\nu}, \qquad (22)$$

which are related to the computable cross norm or realignment criterion [37]. The G_{μ} (22) are the elements of an arbitrary orthonormal Hermitian basis and $Q = Q_{\mu\nu}$ is an arbitrary $d^2 \times d^2$ orthogonal matrix with $Q^T Q = \mathbb{I}_{d^2}$ (in fact, $Q^T Q \leq \mathbb{I}_{d^2}$ is sufficient).

For any informationally complete (N, M) POVM, assume that $\mathcal{O}^{(\alpha)} = \mathbb{I}_M$ and L = N. According to (18) we have $Q = \text{diag}(1, z, z, \dots, z)$. The associated entanglement witnesses are written

$$\tilde{W}' = \mathbb{I}_{d^2} - G_0 \otimes G_0 - z \sum_{\mu=1}^{d^2 - 1} G_{\mu}^T \otimes G_{\mu}.$$
 (23)

Therefore, it is possible to use different (N, M) POVMs to generate the same witnesses \tilde{W}' , provided the same Hermitian orthonormal basis is used.

$$\tilde{W}' = \mathbb{I}_{d^2} - G_0 \otimes G_0 + z \left(\sum_{\alpha=L+1}^N G_\alpha^T \otimes G_\alpha - \sum_{\alpha=1}^L G_\alpha^T \otimes G_\alpha \right),$$
(24)

where $N \leq d^2 - 1$.

To show the advantages of our entanglement witnesses in detecting quantum entanglement, we compare our entanglement witnesses with the ones presented in [23] using three examples, which show that our entanglement witnesses can detect more entangled quantum states (see Appendix D).

IV. LOWER BOUND OF CONCURRENCE

Let H_1 and H_2 be *d*-dimensional vector spaces. A bipartite quantum pure state $|\psi\rangle$ in $H_1 \otimes H_2$ has a Schmidt form

$$|\psi\rangle = \sum_{i} \alpha_{i} |e_{i}^{1}\rangle \otimes |e_{i}^{2}\rangle, \qquad (25)$$

where $|e_i^1\rangle$ and $|e_i^2\rangle$ are the orthonormal bases in H_1 and H_2 , respectively, and α_i are the Schmidt coefficients satisfying $\sum_i \alpha_i^2 = 1$. The concurrence $C(|\psi\rangle)$ of the state $|\psi\rangle$ is given by

$$C(|\psi\rangle) = \sqrt{2\left(1 - \mathrm{Tr}\rho_1^2\right)} = 2\sqrt{\sum_{i < j} \alpha_i^2 \alpha_j^2}, \qquad (26)$$

where $\rho_1 = \text{Tr}_2(|\psi\rangle\langle\psi|)$ is the reduced state obtained by tracing over the second space [27].

The concurrence is extended to mixed states ρ by the convex roof,

$$C(\rho) = \min \sum_{i} p_i C(|\psi_i\rangle), \qquad (27)$$

where the minimum is taken over all possible pure state decompositions of $\rho = \sum_i p_i |\psi_i\rangle \langle \psi_i|$, where $p_i \ge 0$ and $\sum_i p_i = 1$. Generally, it is extremely difficult to calculate

 $C(\rho)$. Instead, one considers the lower bound of $C(\rho)$.

In [31] the authors presented a lower bound of $C(\rho)$,

$$C(\rho) \geqslant \sqrt{\frac{2}{d(d-1)}} f(\rho), \tag{28}$$

where $f(\rho)$ is a real-valued and convex function satisfying

$$f(|\psi\rangle\langle\psi|) \leqslant 2\sum_{i< j} \alpha_i \alpha_j \tag{29}$$

for all pure states $|\psi\rangle$ given by (25). A lower bound (28) of concurrence can be obtained from a function *f* satisfying (29) for arbitrary pure states. Nevertheless, it is still a problem to find such a function *f*. In fact, there are positive maps which can be used as separability criteria, but there are difficulties using them to obtain lower bounds of concurrence by finding such functions *f*. Based on the positive map defined in (8), we construct below new functions *f* to obtain new lower bounds of concurrence $C(\rho)$. Setting M = d and L = N = d + 1 and using the (N, M) POVM constructed from the Gell-Mann matrices [33] in Φ , we have the following theorem (the proof is given in Appendix E).

Theorem 2. For any bipartite quantum state $\rho \in H_1 \otimes H_2$, the concurrence $C(\rho)$ satisfies

$$C(\rho) \ge \sqrt{\frac{2}{d(d-1)}} [\|(\mathbb{I}_d \otimes \Phi_z)\rho\| - 1], \qquad (30)$$

where \mathbb{I}_d is the identity operator, Φ_z is given in (8), and $\|\cdot\|$ stands for the trace norm.

It has been always a challenging problem to find new separability criteria which detect better entanglement and new lower bounds of entanglement which are larger than the existing ones, at least for some quantum states. We have presented such separability criteria and lower bounds. We illustrate our results below with a detailed example.

Example 1. Let us consider the state (11). From (30) we have

$$C(\rho) \ge \sqrt{\frac{1}{6}} [\|(\mathbb{I}_4 \otimes \Phi_z)(\rho)\| - 1] = \frac{1}{2\sqrt{6}} (\frac{2}{3}q_1z - \frac{1}{24}z - \frac{1}{8} + |\frac{2}{3}q_1z - \frac{1}{24}z - \frac{1}{8}|).$$
(31)

In [29] a lower bound of the concurrence was given by

$$C(\rho) \ge \sqrt{\frac{1}{6}} [\|(\mathbb{I}_4 \otimes \Phi')(\rho)\| - 3] = \frac{1}{4\sqrt{6}} (q_1 - q_4 + |q_1 - q_4|).$$
(32)

Figure 1 shows the lower bounds of concurrence given in (31) for the state (11) versus parameters z and q_1 . We see that the lower bounds of concurrence are greater than 0 when $0.2 < z \le 1$, namely, the entanglement of states (11) are detected in this case. When z = 1 and $0.25 < q_1 < 1$, the lower bound of concurrence is greater than 0. When z < 1, from Fig. 1 we see the detected entanglement range of ρ and the lower bound of concurrence decreases with z. When $z \le 0.2$, it can be seen

from Fig. 1 that the lower bounds of concurrence become 0. The lower bound of (31) reaches the maximum at z = 1.

Our lower bounds of concurrence in (31) are better than the lower bounds of concurrence in (32) given in [29] at least for some states. Let us take z = 1 and $q_4 = -\frac{1}{3}q_1 + \frac{1}{2}$. Then (31) can be written as $C(\rho) \ge \frac{1}{2\sqrt{6}} (\frac{2}{3}q_1 - \frac{1}{6} + |\frac{2}{3}q_1 - \frac{1}{6}|)$, while (32) can be written as $C(\rho) \ge \frac{1}{4\sqrt{6}} (\frac{4}{3}q_1 - \frac{1}{2} + |\frac{4}{3}q_1 - \frac{1}{2}|)$.



FIG. 1. Lower bounds with respect to the parameters z and q_1 .

From Fig. 2 it can be seen that our bound of concurrence (31) detects the entanglement for $q_1 > 0.25$, while the bound of concurrence in (32) detects entanglement for $q_1 > 0.375$.

V. CONCLUSION

Based on symmetric measurements, we have presented a family of positive and trace-preserving maps. From these maps we have obtained separability criteria which better detect the entanglement of quantum states. We have also constructed a series of entanglement witnesses which includes some existing ones as special cases and detects even the entanglement of bound entangled states. We have derived a family of lower bounds of concurrence which are tighter than the related existing ones. Since our approach is based on the symmetric measurements, the entanglement of



FIG. 2. Lower bound given in (31) (solid line) and in (32) (dashed line) as a function of q_1 .

any known quantum states can be experimentally estimated. Moreover, our results may be applied also to the investigation on multipartite entanglement and highlight the detection of entanglement in optimal entanglement manipulations [38].

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APPENDIX A: GELL-MANN MATRICES

For d = 4, the Hermitian orthonormal basis is given by the Gell-Mann matrices

and $G_0 = \mathbb{I}_4/\sqrt{4}$. For the entanglement estimation with respect to the state (11), we set the indices of $G_{\alpha,k}$ as

$$G_{1,1} = g_{01}, \quad G_{1,2} = g_{02}, \quad G_{1,3} = g_{03},$$

$$G_{2,1} = g_{10}, \quad G_{2,2} = g_{12}, \quad G_{2,3} = g_{13},$$

$$G_{3,1} = g_{20}, \quad G_{3,2} = g_{21}, \quad G_{3,3} = g_{23},$$

$$G_{4,1} = g_{30}, \quad G_{4,2} = g_{31}, \quad G_{4,3} = g_{32},$$

$$G_{5,1} = g_{11}, \quad G_{5,2} = g_{22}, \quad G_{5,3} = g_{33}.$$
(A1)

For d = 3, the Hermitian orthonormal basis is given by the Gell-Mann matrices

$$g_{01} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad g_{10} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix},$$
$$g_{02} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \quad g_{20} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix},$$
$$g_{12} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad g_{21} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix},$$
$$g_{11} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad g_{22} = \frac{1}{\sqrt{6}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix},$$

and $G_0 = \mathbb{I}_3/\sqrt{3}$. For the entanglement witnesses in Example 2, we set the indices of $G_{\alpha,k}$ as

$$G_{1,1} = g_{01}, \quad G_{1,2} = g_{10}, \quad G_{2,1} = g_{02}, \quad G_{2,2} = g_{20},$$

$$G_{3,1} = g_{12}, \quad G_{3,2} = g_{21}, \quad G_{4,1} = g_{11}, \quad G_{4,2} = g_{22}.$$
(A2)

In Example 4 we set

$$G_{1,1} = g_{01}, \quad G_{1,2} = g_{02}, \quad G_{1,3} = g_{10}, \quad G_{1,4} = g_{20},$$

$$G_{2,1} = g_{12}, \quad G_{2,2} = g_{21}, \quad G_{2,3} = g_{11}, \quad G_{2,4} = g_{22}.$$
(A3)

APPENDIX B: HERMITIAN ORTHONORMAL BASIS FROM MUTUALLY UNBIASED BASES

Using the complete set of four mutually unbiased bases in d = 3 and the corresponding projectors

$$E_{1,1} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad E_{2,1} = \frac{1}{3} \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix}, \quad E_{3,1} = \frac{1}{3} \begin{pmatrix} 1 & \omega^2 & \omega^2 \\ \omega & 1 & 1 \\ \omega & 1 & 1 \end{pmatrix}, \quad E_{4,1} = \frac{1}{3} \begin{pmatrix} 1 & \omega & \omega \\ \omega^2 & 1 & 1 \\ \omega^2 & 1 & 1 \end{pmatrix}, \quad E_{1,2} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad E_{2,2} = \frac{1}{3} \begin{pmatrix} 1 & \omega^2 & \omega \\ \omega & 1 & \omega^2 \\ \omega^2 & \omega & 1 \end{pmatrix}, \quad E_{3,2} = \frac{1}{3} \begin{pmatrix} 1 & \omega & 1 \\ \omega^2 & 1 & \omega^2 \\ 1 & \omega & 1 \end{pmatrix}, \quad E_{4,2} = \frac{1}{3} \begin{pmatrix} 1 & \omega^2 & 1 \\ \omega & 1 & \omega \\ 1 & \omega^2 & 1 \end{pmatrix}, \quad (B1)$$
$$E_{1,3} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad E_{2,3} = \frac{1}{3} \begin{pmatrix} 1 & \omega & \omega^2 \\ \omega^2 & 1 & \omega \\ \omega & \omega^2 & 1 \end{pmatrix}, \quad E_{3,3} = \frac{1}{3} \begin{pmatrix} 1 & 1 & \omega \\ 1 & 1 & \omega \\ \omega^2 & \omega^2 & 1 \end{pmatrix}, \quad E_{4,3} = \frac{1}{3} \begin{pmatrix} 1 & 1 & \omega^2 \\ 1 & 1 & \omega^2 \\ \omega & \omega & 1 \end{pmatrix},$$

where $\omega = \exp(2\pi i/3)$, we find the corresponding Hermitian orthonormal basis

$$G_{1,1} = \frac{1}{\sqrt{3}(1+\sqrt{3})} \begin{pmatrix} -2-\sqrt{3} & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & 1+\sqrt{3} \end{pmatrix}, \quad G_{1,2} = \frac{1}{\sqrt{3}(1+\sqrt{3})} \begin{pmatrix} 1 & 0 & 0\\ 0 & -2-\sqrt{3} & 0\\ 0 & 0 & 1+\sqrt{3} \end{pmatrix},$$

$$\begin{aligned} G_{2,1} &= \frac{1}{2\sqrt{3}(1+\sqrt{3})} \begin{pmatrix} 0 & -v^* & -v \\ -v & 0 & -v^* \\ -v^* & -v & 0 \end{pmatrix}, \quad G_{2,2} &= \frac{1}{\sqrt{3}(1+\sqrt{3})} \begin{pmatrix} 0 & iv^* & -iv \\ -iv & 0 & iv^* \\ iv^* & -iv & 0 \end{pmatrix}, \\ G_{3,1} &= \frac{1}{2\sqrt{3}(1+\sqrt{3})} \begin{pmatrix} 0 & u^* & iv^* \\ u & 0 & -v^* \\ -iv & -v & 0 \end{pmatrix}, \quad G_{3,2} &= \frac{1}{\sqrt{3}(1+\sqrt{3})} \begin{pmatrix} 0 & u & -v^* \\ u^* & 0 & iv^* \\ -v & -iv & 0 \end{pmatrix}, \\ G_{4,1} &= \frac{1}{2\sqrt{3}(1+\sqrt{3})} \begin{pmatrix} 0 & u & -iv \\ u^* & 0 & -v \\ iv^* & -v^* & 0 \end{pmatrix}, \quad G_{4,2} &= \frac{1}{\sqrt{3}(1+\sqrt{3})} \begin{pmatrix} 0 & u^* & -v \\ u & 0 & -iv \\ -v^* & iv^* & 0 \end{pmatrix}, \end{aligned}$$

and $G_0 = \mathbb{I}/\sqrt{3}$, where $u = (1 - i)(1 + \sqrt{3})$ and $v = 2 + \sqrt{3} + i$. The entanglement witnesses in Example 3 are given by (24) with G_{μ} grouped in the following way: $\{G_1, G_2, G_3\} = \{G_{1,2}, G_{2,1}, G_{2,2}\}$ and $\{G_4, G_5, G_6, G_7, G_8\} = \{G_{1,1}, G_{3,1}, G_{3,2}, G_{4,1}, G_{4,2}\}$.

APPENDIX C: CALCULATION PROCESS OF SEC. II

By direct computation,

where

$$A = -z \left(\frac{3}{8}q_1 + \frac{5}{24}q_4 + \frac{5}{24}q_3 + \frac{5}{24}q_2 + 1\right) + \frac{1}{8} + \frac{5}{4}z,$$

$$B = -z \left(\frac{5}{24}q_1 + \frac{3}{8}q_4 + \frac{5}{24}q_3 + \frac{5}{24}q_2 + 1\right) + \frac{1}{8} + \frac{5}{4}z,$$

$$C = -z \left(\frac{5}{24}q_1 + \frac{5}{24}q_4 + \frac{3}{8}q_3 + \frac{5}{24}q_2 + 1\right) + \frac{1}{8} + \frac{5}{4}z,$$

$$D = -z \left(\frac{5}{24}q_1 + \frac{5}{24}q_4 + \frac{5}{24}q_3 + \frac{3}{8}q_2 + 1\right) + \frac{1}{8} + \frac{5}{4}z.$$

We have the following set of eigenvalues of $(\mathbb{I}_4 \otimes \Phi_z)(\rho)$: $\{\frac{1}{2}(A - \frac{1}{2}q_1z), \frac{1}{2}(A + \frac{1}{6}q_1z), \frac{$

APPENDIX D: EXAMPLES OF ENTANGLEMENT WITNESSES

Example 2. Let us take N = 4 and M = 3 and fix the operator basis $G_{\alpha,k}$ to be the Gell-Mann matrices (see Appendix A). For L = 1 we take

$$\mathcal{O}^{(\alpha)} = \begin{pmatrix} 1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & 1 \end{pmatrix} \quad \text{for any } \alpha \in [N].$$
(D1)

The corresponding entanglement witnesses have the form

$$\tilde{W}_{1} = (\sqrt{3}+1)^{2} \begin{bmatrix} 2z+2 & \cdot & \cdot & \cdot & -3z & \cdot & \cdot & \cdot & 3z \\ \cdot & -z+2 & \cdot \\ \cdot & \cdot & -z+2 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ -3z & \cdot & \cdot & -z+2 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & -z+2 & \cdot & \cdot & \cdot & 3z \\ \cdot & \cdot & \cdot & \cdot & -z+2 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & -z+2 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & -z+2 & \cdot & \cdot \\ 3z & \cdot & \cdot & 3z & \cdot & \cdot & -z+2 & \cdot \\ 3z & \cdot & \cdot & 3z & \cdot & \cdot & 2z+2 \end{bmatrix}.$$
(D2)

When z = -1, it is verified that the entanglement of the following state can be detected:

$$\rho_{1} = \frac{1}{27} \begin{bmatrix}
7 & \cdot & \cdot & \cdot & 6 & \cdot & \cdot & \cdot & 6 \\
\cdot & 1 & \cdot \\
\cdot & \cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\
6 & \cdot & \cdot & \cdot & 7 & \cdot & \cdot & 6 \\
\cdot & \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\
6 & \cdot & \cdot & \cdot & 6 & \cdot & \cdot & 7
\end{bmatrix}.$$
(D3)

When z = 1, it is the witness constructed in [23] that cannot detect the entanglement of the state ρ_1 .

Example 3. Let M = 2. Instead of the Gell-Mann matrices, we take the (N, 2) POVM constructed from the orthonormal Hermitian basis presented in Appendix B. For N = 7 and L = 4, the corresponding witnesses \tilde{W}_2 are given by

$$\tilde{W}_{2} = \frac{1}{6} \begin{bmatrix} 4(1-z) & \cdot & \cdot & \cdot & 4 & z & Az & 4 & A^{*}z & z \\ \cdot & 2(2+z) & \cdot & Bz & 4 & Cz & Ez & 4 & Fz \\ \cdot & 2(2+z) & C^{*}z & Dz & 4 & Gz & -7z & 4 \\ \hline 4 & B^{*}z & Cz & 2(2+z) & \cdot & \cdot & 4 & C^{*}z & Hz \\ \hline 2 & 4 & D^{*}z & \cdot & 4(1-z) & \cdot & Dz & 4 & zi \\ \hline A^{*}z & C^{*}z & 4 & \cdot & 2(2+z) & Mz & Nz & 4 \\ \hline 4 & E^{*}z & G^{*}z & 4 & D^{*}z & M^{*}z & 2(2+z) & \cdot & \cdot \\ \hline Az & 4 & -7z & Cz & 4 & N^{*}z & \cdot & 2(2+z) & \cdot \\ z & F^{*}z & 4 & H^{*}z & -zi & 4 & \cdot & \cdot & 4(1-z) \end{bmatrix},$$
(D4)

where

$$A = \frac{1}{2}(\sqrt{3} - i), \quad B = \frac{1}{2}(3\sqrt{3} - 5i), \quad C = -(8 - 2\sqrt{3}i),$$

$$D = \frac{1}{2}(5\sqrt{3} - i), \quad E = -(8 + 2\sqrt{3})i, \quad F = -\frac{1}{2}(5\sqrt{3} + 3i),$$

$$G = \frac{1}{2}(7\sqrt{3} + 3i), \quad H = \frac{1}{2}(3\sqrt{3} + 11i), \quad M = -(7 - \sqrt{3}i),$$

$$N = -\frac{1}{2}(\sqrt{3} + 3i).$$

When z = -1, it can detect the entanglement of the state

For z = 1, these witnesses reduce to the one given in [23], which cannot detect the entanglement of the state ρ_2 .

It is well known that indecomposable witness is a very important kind of entanglement witnesses, but it is difficult to construct. A witness *W* is decomposable if it can be written as $W = A + B^{\Gamma}$, with *A* and *B* being positive operators and $\Gamma = \mathbb{I} \otimes T$ denoting a partial transpose. Otherwise the *W* is indecomposable. Next we give an example of indecomposable witnesses obtained from symmetric measurements.

$$\mathcal{O}^{(1)} = \begin{pmatrix} 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix}.$$
 (D6)

From (20) we get the entanglement witnesses

$$\tilde{W}_{3}^{\prime} = \frac{1}{6} \begin{bmatrix} 4 & \cdot & \cdot & \cdot & B^{*}z & C^{*}z & \cdot & D^{*}z & B^{*}z \\ \cdot & 4 & \cdot & A^{*}z & \cdot & \cdot & -30zi & \cdot & \cdot \\ \cdot & \cdot & 4 & 30zi & \cdot & \cdot & -A^{*}z & \cdot & \cdot \\ \cdot & Az & -30zi & 4 & \cdot & \cdot & -A^{*}z & \cdot & \cdot \\ Bz & \cdot & \cdot & 4 & \cdot & \cdot & \cdot & \cdot \\ Cz & \cdot & \cdot & 4 & \cdot & \cdot & \cdot & \cdot \\ 0z & \cdot & \cdot & Az & -A^{*}z & \cdot & \cdot & A & \cdot \\ Bz & \cdot & \cdot & Az & -A^{*}z & \cdot & \cdot & A & \cdot \\ Bz & \cdot & \cdot & Az & -A^{*}z & \cdot & A & -A & -A \\ \hline \end{array} \right],$$
(D7)

where

$$A = 15(1 - i)(2 - i + \sqrt{5}),$$

$$B = 15(1 - i)(2 + i + \sqrt{5}),$$

$$C = -30\sqrt{5}(2 + \sqrt{5}),$$

$$D = 30(1 - 2i)(2 + \sqrt{5}).$$

Consider the state

It is directly verified that ρ_3 is a PPT state. Take z = -1. From (D7) we have that the state ρ_3 is entanglement. Hence the entanglement witness (D7) is an indecomposable witness when z = -1. For z = 1, these witnesses reduce to the one given in [23] and we have Tr($\tilde{W}'_3 \rho_2 \ge 0$, i.e., it cannot detect the entanglement of ρ_3 .

From the above examples, we see that the entanglement witnesses we presented cover the ones in [23] and can detect more entangled states including bound entangled ones.

APPENDIX E: PROOF OF THEOREM 2

Let $f(|\psi\rangle\langle\psi|) = ||(\mathbb{I}_d \otimes \Phi_z)|\psi\rangle\langle\psi|| - 1$. Obviously $f(|\psi\rangle\langle\psi|)$ is convex as the trace norm is convex. What we need to prove is that for any pure state in the Schmidt form (25), the inequality (29) holds.

Since the trace norm does change under local coordinate transformation, we take $|\psi\rangle = (\alpha_1, 0, \dots, 0, 0, \alpha_2, \dots, 0, 0, 0, \alpha_3, \dots, 0, \dots, 0, \alpha_d)^T$, where *T* denotes transpose and the Schmidt coefficients satisfy $0 \le \alpha_1, \alpha_2, \alpha_3, \dots, \alpha_d \le 1$, $\sum_{i=1}^{d} \alpha_i^2 = 1$. By direct computation, we have

$$(\mathbb{I}_d \otimes \Phi_z)(|\psi\rangle\langle\psi|) = \frac{1}{d(d-1)} \begin{bmatrix} (d-1+z)\alpha_1^2 & -dz\alpha_1\alpha_2 & \cdots & -dz\alpha_1\alpha_d \\ -dz\alpha_1\alpha_2 & (d-1+z)\alpha_2^2 & \cdots & -dz\alpha_2\alpha_d \\ \vdots & \vdots & \ddots & \vdots \\ -dz\alpha_1\alpha_d & -dz\alpha_2\alpha_d & \cdots & (d-1+z)\alpha_d^2 \end{bmatrix}$$
$$\oplus (d-1+z)\alpha_1^2 I_{d-1} \oplus \cdots \oplus (d-1+z)\alpha_d^2 I_{d-1}.$$

)

The matrix $(\mathbb{I}_d \otimes \Phi_z)(|\psi\rangle\langle\psi|)$ has *d* singular values with the multiplicity d-1, $\frac{1}{d(d-1)}(d-1+z)\alpha_1^2$, $\frac{1}{d(d-1)}(d-1+z)\alpha_2^2$, \dots , $\frac{1}{d(d-1)}(d-1+z)\alpha_d^2$, and the remaining *d* values are the singular values of the matrix *P*,

$$P = \frac{1}{d(d-1)} \begin{bmatrix} (d-1)(1-z)\alpha_1^2 & -dz\alpha_1\alpha_2 & \cdots & -dz\alpha_1\alpha_d \\ -dz\alpha_1\alpha_2 & (d-1)(1-z)\alpha_2^2 & \cdots & -dz\alpha_2\alpha_d \\ \vdots & \vdots & \ddots & \vdots \\ -dz\alpha_1\alpha_d & -dz\alpha_2\alpha_d & \cdots & (d-1)(1-z)\alpha_d^2 \end{bmatrix}$$
$$= \frac{dz}{d(d-1)} \begin{bmatrix} t\alpha_1^2 & -\alpha_1\alpha_2 & \cdots & -\alpha_1\alpha_d \\ -\alpha_1\alpha_2 & t\alpha_2^2 & \cdots & -\alpha_2\alpha_d \\ \vdots & \vdots & \ddots & \vdots \\ -\alpha_1\alpha_d & -\alpha_2\alpha_d & \cdots & t\alpha_d^2 \end{bmatrix} \triangleq \frac{dz}{d(d-1)}H,$$

where $t = \frac{(d-1)(1-z)}{dz}$. As *P* is Hermitian and real, its singular values are simply given by the square roots of the eigenvalues of P^2 . In fact, we need to consider only the absolute values of the eigenvalues of *P*. The eigenpolynomial equation of *H* is

$$h(x) = |xI_d - H| = x^d - tx^{d-1} + (t-1)(t+1) \left(\sum_{i < j} \alpha_i^2 \alpha_j^2 \right) x^{d-2} - (t-2)(t+1)^2 \left(\sum_{i < j < k} \alpha_i^2 \alpha_j^2 \alpha_k^2 \right) x^{d-3} + (t-3)(t+1)^3 \left(\sum_{i_1 < i_2 < i_3 < i_4} \alpha_{i_1}^2 \alpha_{i_2}^2 \alpha_{i_3}^2 \alpha_{i_4}^2 \right) x^{d-4} + \cdots + (-1)^{d-2}(t-d+3)(t+1)^{d-3} \left(\sum_{i_1 < i_2 < \cdots < i_{d-2}} \alpha_{i_1}^2 \alpha_{i_2}^2 \cdots \alpha_{i_{d-2}}^2 \right) x^2 + (-1)^{d-1}(t-d+2)(t+1)^{d-2} \left(\sum_{i_1 < i_2 < \cdots < i_{d-1}} \alpha_{i_1}^2 \alpha_{i_2}^2 \cdots \alpha_{i_{d-1}}^2 \right) x^4 + (-1)^d (t-d+1)(t+1)^{d-1} \left(\alpha_1^2 \alpha_2^2 \cdots \alpha_d^2 \right) = 0.$$
(E1)

Let $x_1, x_2, x_3, \ldots, x_d$ denote the *d* roots of (E1). By using the relations between the roots and the coefficients of the polynomial equation, we have

$$\sum_{i=1}^{d} x_i = t, \quad \prod_{i=1}^{d} x_i = (t - d + 1)(t + 1)^{d-1} \left(\alpha_1^2 \alpha_2^2 \cdots \alpha_d^2 \right).$$
(E2)

From (E1) and that $\sum_{i=1}^{d} \alpha_i^2 = 1$, the inequality (29) that needs to be proved now has the form

$$f(|\psi\rangle\langle\psi|) = \|(I_d \otimes \Phi_z)|\psi\rangle\langle\psi|\| - 1 = \frac{dz}{d(d-1)} \sum_{i=1}^d |x_i| + \frac{d-1}{d(d-1)}(d-1+z) - 1 \leqslant 2\left(\sum_{i< j} \alpha_i \alpha_j\right).$$
(E3)

Next we consider the eigenpolynomial equation (E1). We set $\beta = \prod_{i=1}^{d} \alpha_i^2$. Since $t = \frac{(d-1)(1-z)}{dz}$, when $z \in (0, 1]$, we get $t \in [0, +\infty)$, and when $z \in (-1, 0]$, we have $t \in (-\infty, -(2 - \frac{2}{d}))$. (i) When $t \ge d - 2$ the following conditions hold.

(a) If $\beta = 0$, then h(0) = 0, where 0 is an eigenvalue of H. From the derivative of h(x) with respect to x,

$$h'(x) = dx^{d-1} - t(d-1)x^{d-2} + (d-2)(t-1)(t+1)\left(\sum_{i(E4)$$

we have that if *d* is even, h'(x) < 0 when x < 0. Therefore, h(x) is a monotonically decreasing function for x < 0. Taking into account that h(0) = 0, we see that there exist no negative roots of (E1) in this case. When *d* is odd, h(x) is a monotonically increasing function for x < 0. There are also no negative roots of (E1).

The inequality (E3) that needs to be proved now has the form

$$\frac{dz}{d(d-1)} \sum_{i=1}^{d} x_i + \frac{d-1}{d(d-1)}(d-1+z) - 1$$
$$\leqslant 2\left(\sum_{i< j} \alpha_i \alpha_j\right). \tag{E5}$$

According to the relations in (E2) and $t = \frac{(d-1)(1-z)}{dz}$, the lefthand side of the inequality (E5) is zero. Hence the inequality (E3) holds.

(b) If $\beta \neq 0$, we have $h(0) = (-1)^d (t - d + 1)(t + 1)^{d-1} (\alpha_1^2 \alpha_2^2 \cdots \alpha_d^2)$. When $t \in (d - 1, +\infty)$, we have h(0) > 0. If *d* is even, since h(x) is a monotonically decreasing function for x < 0, there exist no negative roots of (E1) in this case. If *d* is odd, $\prod_{i=1}^d x_i = (t - d + 1)(t + 1)^{d-1} (\alpha_1^2 \alpha_2^2 \cdots \alpha_d^2) > 0$. Then (E1) has no negative roots or even-number negative roots. Since h(x) is monotonically increasing when x < 0, it has at most one negative roots. This case is similar to (a) and can be shown to satisfy (E3).

When $t \in [d-2, d-1)$, we have $\prod_{i=1}^{d} x_i = (t-d+1)(t+1)^{d-1}(\alpha_1^2\alpha_2^2\cdots\alpha_d^2) < 0$. Therefore, there exists at least one negative root, say, $x_1 < 0$, such that $h(x_1) = 0$.

If *d* is even, then h(0) < 0 and h(x) is a monotonically decreasing function when x < 0. Thus, $x_1 < 0$ is the only negative root. Hence the inequality (E3) needing to be proved becomes

$$\frac{dz}{d(d-1)} \left(\sum_{i=2}^{d} x_i - x_1 \right) + \frac{d-1}{d(d-1)} (d-1+z) - 1$$
$$\leqslant 2 \left(\sum_{i < j} \alpha_i \alpha_j \right). \tag{E6}$$

From (E2) we only need to prove that $x_1 \ge -\frac{d-1}{z} (\sum_{i < j} \alpha_i \alpha_j)$. From the definition of h(x) we have $h(-\frac{d-1}{z} (\sum_{i < j} \alpha_i \alpha_j)) = |-\frac{d-1}{z} (\sum_{i < j} \alpha_i \alpha_j) I_d - H| = |\frac{d-1}{z} (\sum_{i < j} \alpha_i \alpha_j) I_d + H| \ge 0$, where in the last step the property of the diagonally dominant matrix $\frac{d-1}{z} (\sum_{i < j} \alpha_i \alpha_j) I_d + H$ is used. Since $h(x_1) = 0 \le h(-\frac{d-1}{z} (\sum_{i < j} \alpha_i \alpha_j))$ and h(x) is a monotonically decreasing function when x < 0, we have that $x_1 \ge -\frac{d-1}{z} (\sum_{i < j} \alpha_i \alpha_j)$. If *d* is odd, then h(0) > 0 and h(x) is a monotonically

If *d* is odd, then h(0) > 0 and h(x) is a monotonically increasing function when x < 0. Similarly, h(x) only has one negative root. Hence, we still only need to prove the inequality (E6). From (E2) we need to prove that $x_1 \ge -\frac{d-1}{z} (\sum_{i < j} \alpha_i \alpha_j)$. From the definition of h(x), we have $h(-\frac{d-1}{z} (\sum_{i < j} \alpha_i \alpha_j)) = |-\frac{d-1}{z} (\sum_{i < j} \alpha_i \alpha_i)I_d - H| = -|\frac{d-1}{z} (\sum_{i < j} \alpha_i \alpha_i)I_d + H| \le 0$, where in the last step the property of the diagonally dominant matrix $\frac{d-1}{z}(\sum_{i < j} \alpha_i \alpha_j)I_d + H$ is used. Since $h(x_1) = 0 \ge h(-\frac{d-1}{z}(\sum_{i < j} \alpha_i \alpha_j))$ and h(x) is a monotonically increasing function when x < 0, we have that $x_1 \ge -\frac{d-1}{z}(\sum_{i < j} \alpha_i \alpha_j)$. (ii) When $t \in [d-3, d-2)$ we have the following. Set

$$p_{0} = 1,$$

$$p_{1} = -t,$$

$$p_{2} = (t-1)(t+1)\left(\sum_{i < j} \alpha_{i}^{2} \alpha_{j}^{2}\right),$$

$$p_{3} = -(t-2)(t+1)^{2}\left(\sum_{i < j < k} \alpha_{i}^{2} \alpha_{j}^{2} \alpha_{k}^{2}\right),$$

$$p_{4} = (t-3)(t+1)^{3}\left(\sum_{i_{1} < i_{2} < i_{3} < i_{4}} \alpha_{i_{1}}^{2} \alpha_{i_{2}}^{2} \alpha_{i_{3}}^{2} \alpha_{i_{4}}^{2}\right),$$

$$\vdots$$

$$p_{d-2} = (-1)^{d-2}(t-d+3)(t+1)^{d-3}$$

$$\times \left(\sum_{i_{1} < i_{2} < \cdots < i_{d-2}} \alpha_{i_{1}}^{2} \alpha_{i_{2}}^{2} \cdots \alpha_{i_{d-2}}^{2}\right),$$

$$p_{d-1} = (-1)^{d-1}(t-d+2)(t+1)^{d-2}$$

$$\times \left(\sum_{i_{1} < i_{2} < \cdots < i_{d-1}} \alpha_{i_{1}}^{2} \alpha_{i_{2}}^{2} \cdots \alpha_{i_{d-1}}^{2}\right),$$

$$p_{d} = (-1)^{d}(t-d+1)(t+1)^{d-1} (\alpha_{1}^{2} \alpha_{2}^{2} \cdots \alpha_{d}^{2}).$$
(E7)

If $\rho = |\psi\rangle\langle\psi|$ is an entangled pure state, there are at most d-2 Schmidt coefficients that are zero. We can assume the following.

(a) If $\beta \neq 0$, except that p_{d-2} has the same sign as p_{d-1} , we have $p_0 > 0$, $p_1 < 0$, $p_2 > 0$, $p_3 < 0$, etc. The sign of the polynomial coefficients $\{p_i\}_{i=0}^d$ changes $V(\{p_i\}_{i=0}^d) = d - 1$ times. By the Descartes rule of signs for the polynomial which has only real roots [39], there are $V(\{p_i\}_{i=0}^d) = d - 1$ positive roots of h(x). Since there is no zero root of h(x), we have that there is only one negative root of h(x), say, $x_1 < 0$, such that $h(x_1) = 0$. Therefore, we still only need to prove the inequality $x_1 \ge -\frac{d-1}{2}(\sum_{i < i} \alpha_i \alpha_i)$.

Infat $h(\alpha_1) = 0$. Infection, we sum only have 1inequality $x_1 \ge -\frac{d-1}{z} (\sum_{i < j} \alpha_i \alpha_j)$. When d is even, $h(-\frac{d-1}{z} (\sum_{i < j} \alpha_i \alpha_j)) = |-\frac{d-1}{z} (\sum_{i < j} \alpha_i \alpha_j) I_d - H| = |\frac{d-1}{z} (\sum_{i < j} \alpha_i \alpha_j) I_d + H| \ge 0$. If $h(-\frac{d-1}{z} (\sum_{i < j} \alpha_i \alpha_j)) = 0$, $x_1 = -\frac{d-1}{z} (\sum_{i < j} \alpha_i \alpha_j)$ since h(x) has only one negative root. If $h(-\frac{d-1}{z} (\sum_{i < j} \alpha_i \alpha_j)) > 0$, let us suppose $x_1 < -\frac{d-1}{z} (\sum_{i < j} \alpha_i \alpha_j) < 0$. Because h(0) < 0and h(x) is continuous, by the zero-point theorem, there exists another root between $-\frac{d-1}{z} (\sum_{i < j} \alpha_i \alpha_j)$ and 0, which is contradicted by the fact that h(x) has only one negative root. Hence, $x_1 \ge -\frac{d-1}{z} (\sum_{i < j} \alpha_i \alpha_j)$.

Contradicted by the fact that h(x) has only one negative root. Hence, $x_1 \ge -\frac{d-1}{z} (\sum_{i < j} \alpha_i \alpha_j)$. When d is odd, $h(-\frac{d-1}{z} (\sum_{i < j} \alpha_i \alpha_j)) = |-\frac{d-1}{z} (\sum_{i < j} \alpha_i \alpha_j) I_d - H| = -|\frac{d-1}{z} (\sum_{i < j} \alpha_i \alpha_j) I_d + H| \le 0$. If $h(-\frac{d-1}{z} (\sum_{i < j} \alpha_i \alpha_j)) = 0$, $x_1 = -\frac{d-1}{z} (\sum_{i < j} \alpha_i \alpha_j)$ since h(x) has only one negative root. If $h(-\frac{d-1}{z}(\sum_{i< j}\alpha_i\alpha_j)) < 0$, suppose $x_1 < -\frac{d-1}{z} (\sum_{i < j} \alpha_i \alpha_j) < 0$. Because h(0) > 0 and h(x) is continuous, by the zero-point theorem there exists another root between $-\frac{d-1}{z}(\sum_{i < j} \alpha_i \alpha_j)$ and 0, which is contradicted by the fact that h(x) has only one negative root. Hence, $x_1 \ge -\frac{d-1}{z} (\sum_{i < j} \alpha_i \alpha_j)$.

(b) If $\beta = 0$, we set $\alpha_1 = \cdots = \alpha_K = 0$ and $\alpha_{K+1}, \ldots, \alpha_d \neq 0$, where $1 \leq K \leq d-2$. Then $p_{d-K+1} =$ $\cdots = p_d = 0$ and there exist K zero roots of h(x). The sign of the polynomial coefficients $V(\{p_i\}_{i=0}^d)$ changes $V(\{p_i\}_{i=0}^d) = d - K$ or d - K - 1 times. Then either there are no negative roots or there is only one negative root of h(x). The case that h(x) has no negative roots can be proved as the case (i a). When h(x) has only one negative root, say, $x_1 < 0$, such that $h(x_1) = 0$, we still only need to prove $x_1 \ge -\frac{d-1}{z} (\sum_{i < j} \alpha_i \alpha_j).$

When d is even, $h(-\frac{d-1}{2}(\sum_{i < j} \alpha_i \alpha_j)) = | \frac{d-1}{z} (\sum_{i < j} \alpha_i \alpha_j) I_d - H | = |\frac{d-1}{z} (\sum_{i < j} \alpha_i \alpha_j) I_d + H| \ge 0.$ If $h(-\frac{d-1}{z} (\sum_{i < j} \alpha_i \alpha_i)) = 0, \ x_1 = -\frac{d-1}{z} (\sum_{i < j} \alpha_i \alpha_i)$ since h(x) has only one negative root. If $h(-\frac{d-1}{z}(\sum_{i< j}\alpha_i\alpha_j)) > 0$, from the derivative of h(x) with respect to x,

$$h'(x) = dp_0 x^{d-1} + (d-1)p_1 x^{d-2} + (d-2)p_2 x^{d-3} + \cdots + k p_{d-k} x^{k-1},$$
(E8)

the sign of the polynomial coefficients of h'(x) changes d - Kor d - K - 1 times and there are K zero roots of h'(x). Hence, h'(x) has no negative roots or only one negative root. Since $h(x_1) = h(0) = 0$ and h(x) is continuous, according to Rolle's mean value theorem, there exists a $\xi \in (x_1, 0)$ such that $h'(\xi) = 0$. Thus, h'(x) must have only one negative root. Since $h'(x) \to -\infty$ when $x \to -\infty$, h'(x) < 0 when $x < \xi$. According to $h(-\frac{d-1}{z}(\sum_{i< j}\alpha_i\alpha_j)) > 0, -\frac{d-1}{z}(\sum_{i< j}\alpha_i\alpha_j) \in$ $(-\infty, x_1) \cup (\xi, 0)$. Suppose $-\frac{d-1}{z} (\sum_{i < i} \alpha_i \alpha_i) \in (\xi, 0)$ and

thus that $h(\xi) < 0$ and h(x) is continuous. By the zero-point theorem we have that there exists another negative root between ξ and $-\frac{d-1}{z}(\sum_{i < j} \alpha_i \alpha_j)$, which is contradicted by the fact that h(x) has only one negative root. Therefore, $-\frac{d-1}{z}(\sum_{i < j} \alpha_i \alpha_j) \in (-\infty, x_1)$, i.e., $x_1 \ge -\frac{d-1}{z}(\sum_{i < j} \alpha_i \alpha_j)$. When d is odd, $h(-\frac{d-1}{z}(\sum_{i < j} \alpha_i \alpha_j)) = | \frac{d-1}{z} \left(\sum_{i < j} \alpha_i \alpha_j \right) I_d - H | = -|\frac{d-1}{z} \left(\sum_{i < j} \alpha_i \alpha_j \right) I_d + H | \leq 0.$ If $h\left(-\frac{d-1}{z} \left(\sum_{i < j} \alpha_i \alpha_j \right) \right) = 0, \ x_1 = -\frac{d-1}{z} \left(\sum_{i < j} \alpha_i \alpha_j \right)$ since h(x) has only one negative root. If $h(-\frac{\tilde{d}-1}{z}(\sum_{i< j}\alpha_i\alpha_j)) < 0$, from (E8) the sign of the polynomial coefficients of h'(x) changes d - K or d - K - 1 times and there are K zero roots of h'(x). Hence, h'(x) has no negative roots or only one negative root. Since $h(x_1) = h(0) = 0$ and h(x) is continuous, according to Rolle's mean value theorem, we get that there exists a $\xi \in (x_1, 0)$ such that $h'(\xi) = 0$. Thus, h'(x) must have only one negative root. Since $h'(x) \to +\infty$ when $x \to -\infty$, h'(x) > 0when $x < \xi$. According to $h(-\frac{d-1}{z}(\sum_{i < j} \alpha_i \alpha_j)) < 0$, we have $-\frac{d-1}{z}(\sum_{i < j} \alpha_i \alpha_j) \in (-\infty, x_1) \cup (\xi, 0)$. Suppose $-\frac{d-1}{z}(\sum_{i< j} \alpha_i \alpha_j) \in (\xi, 0)$. Taking into account that $h(\xi) > 0$ and h(x) is continuous, by the zero-point theorem we get that there exists another negative root between ξ and $-\frac{d-1}{z}(\sum_{i < j} \alpha_i \alpha_j)$, which is contradicted by the fact that h(x) has only one negative root. Hence, $-\frac{d-1}{z}(\sum_{i < j} \alpha_i \alpha_j) \in (-\infty, x_1)$, i.e., $x_1 \ge -\frac{d-1}{z}(\sum_{i < j} \alpha_i \alpha_j)$. Similarly, we can prove that Theorem 2 holds when $t \in$

 $[d-4, d-3), [d-5, d-4), \dots, [0, 1).$

(iii) When $t \in (-\infty, -(2 - \frac{2}{d}))$ we have the following. We have $h(0) = (-1)^d (t - d + 1)(t + 1)^{d-1} (\alpha_1^2 \alpha_2^2 \cdots \alpha_d^2) \ge$ 0. From (E4) we have h'(x) > 0 when x > 0. Taking into account that $h(0) \ge 0$, we see that there exist no positive roots of (E1) in this case. The inequality (29) that we need to prove also has the same form as (E5) and holds as well.

(iv) When z = 0, $f(|\psi\rangle\langle\psi|) = ||(\mathbb{I}_d \otimes \Phi_z)|\psi\rangle\langle\psi|| - 1 =$ 0. The inequality (29) also holds.

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