A family of nonlocal bound entangled states

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Bound entanglement, being entangled yet not distillable, is essential to our understandings of the relations between nonlocality and entanglement besides its applications in certain quantum information tasks. Recently, bound entangled states that violate a Bell inequality have been constructed for a two-qutrit system, disproving a conjecture by Peres that bound entanglement is local. Here we shall construct such kind of nonlocal bound entangled states for all finite dimensions larger than two, making possible their experimental demonstrations on most general systems. We propose a Bell inequality, based on a Hardy-type argument for nonlocality, and a steering inequality to identify their nonlocality. We also provide a family of entanglement witnesses to detect their entanglement beyond the Bell inequality and the steering inequality.

Introduction — Quantum nonlocality \cite{1,2} and entanglement \cite{3,4} are two intricately entwined quantum features that are essential in most quantum information processes in addition to shedding light on our understandings of reality. On the one hand, every entangled pure state is nonlocal \cite{5–7}, which can be signaled by the violation of a single Bell inequality \cite{8}. On the other hand, we are dealing with mixed states in most cases due to ubiquitous noises and there are entangled mixed states, e.g., Werner’s states \cite{9}, that admit a local realistic model, i.e., cannot violate any Bell inequality. Fortunately, by using distillation protocols \cite{9} that involve only local operations and classical communications one can extract pure entanglement from many copies of entangled mixed states, showing therefore the nonlocality of entangled states that are distillable.

However there are entangled states, namely bound entangled states \cite{10}, that are not distillable. This delicate entanglement does not exist in two-qubit and qubit-qutrit systems and the only examples known so far are entangled states with positive partial transpose (PPT) \cite{11,12}. This mystical invention of nature, as called by its founder \cite{13}, is useful in certain quantum communication tasks not achievable by local means, e.g., distilling a secure quantum key \cite{13} and reducing the communication complexity \cite{14}. Peres \cite{15} conjectured that bound entangled states were local, i.e., cannot violate any Bell inequality, and this conjecture was disproved at first in the multipartite case \cite{16,17} and most recently for a two-qutrit system by the discovery of a family of bound entangled states \cite{18} that violate a Bell inequality \cite{19}. A stronger version of Peres conjecture \cite{20} on the steerability \cite{21} was also disproved by the same family of states \cite{18}.

In this Letter we generalize this family of nonlocal bound entangled states to all finite dimensions greater than two. We propose a Bell inequality, which comes from a Hardy-type argument, and a steering inequality and identify non-empty sets of nonlocal bound entangled states that give rise to small but finite violations. Our analytical approach also enables us to find the asymptotic violations in the limit of large local dimension. Moreover we present a family of entanglement witnesses to detect their entanglement.

Nonlocality, steerability, and entanglement — Let Alice and Bob be two space-like separated observers, each performing some local measurements on the compound system they share. If the correlation $P(a, b | A, B)$ of every pairs of local measurements $A$ and $B$ with outcomes $a, b$ assumes the following local form

$$P(a, b | A, B) = \sum_{\lambda} P(\lambda) P_a(a | A, \lambda) P_b(b | B, \lambda)$$

with $\alpha, \beta \in \{q, c\}$, then the state of the compound system is separable \cite{9} in the case of $(\alpha, \beta) = (q, q)$, unsteerable by $A$ or $B$ \cite{22} if $(\alpha, \beta) = (c, q)$ or $(\alpha, \beta) = (q, c)$, which is also called as a local hidden state model, and local if $(\alpha, \beta) = (c, c)$, which is known as a local hidden variable model. Here for a given hidden variable $\lambda$ distributed according to $P(\lambda)$, we denote $P_q(a | A, \lambda) = \text{Tr}(\sigma_\lambda A)$ for some quantum state $\sigma_\lambda$ and a quantum measurement $\{A\}$ and by $P_c(a | A, \lambda)$ a most general probability distribution, including quantum statistics as a special case. If such a local model does not exist, then the state is called as entangled (not $qq$), $A(B)$-steerable (not $qc$ or not $cq$), and Bell nonlocal (not $cc$), respectively. Entanglement is necessary for steerability and steerability is necessary for the nonlocality. Various kinds of entanglement witnesses \cite{23}, e.g., via local orthogonal observables \cite{24}, steering inequalities \cite{22}, and Bell inequalities have been proposed to detect the entanglement and nonlocality.

The nonlocal bound entangled states — Consider a bipartite system of two qudits with each qudit having $d \geq 3$ distinguishable states $\{|i\}_{i=0}^{d-1}$ and denote by $\{|i, j\} = |i\rangle \otimes |j\rangle$ the computational basis of the whole system. Essential to our construction is a set $\Theta_d = \{\theta_p\}_{p=0}^{d-1}$ of $d$ normalized pure states of a single qudit in the $d - 1$ dimensional subspace spanned by $\{|i\}_{i=1}^{d-1}$ satisfying

$$\langle \theta_p | \theta_q \rangle = -\frac{1}{d-1}, \quad (\forall \, p \neq q).$$
A recursive construction and basic properties of these highly symmetric states $\Theta_d$ are provided in the supplementary material. Our state reads

$$\varrho_{xy} = \frac{xy}{R} |\Psi\rangle\langle\Psi| + \frac{\Delta}{R} \sum_{i<j=1}^{d-1} |\psi_{ij}\rangle\langle\psi_{ij}| + \frac{1}{R} \sum_{k=1}^{d-1} |\psi_k\rangle\langle\psi_k|$$

where $x, y > 0$ satisfy $\Delta := z^2/(d-2) - xy > 0$ with $z = \sqrt{1 - x^2 - y^2}$ and $R = dxy + (d-1)(d-2)\Delta + d-1$ is the normalization constant, and

$$|\Psi\rangle = \sum_{i=0}^{d-1} |i, i\rangle, \quad |\psi_{ij}\rangle = |i, j\rangle - |j, i\rangle,$$

$$|\psi_k\rangle = x|0, k\rangle + y|k, 0\rangle + z|\phi_k\rangle,$$

$$|\phi_k\rangle = \frac{(d-1)^2}{d\sqrt{d-2}} \sum_{p=0}^{d-1} \sum_{p'=0}^{d-1} |\theta_p\rangle \otimes |\theta_{p'}\rangle |k\rangle.$$

We denote by $D = \{(x, y)|x, y, \Delta > 0\}$ and for each $(x, y) \in D$ the state $\varrho_{xy}$ is well defined, with the pure states appearing in its definition as eigenstates, and has positive partial transpose because $\varrho_{xy}^{\text{PT}} = \varrho_{xy}$ as shown in supplementary material. If $d = 3$ our states are equivalent to those nonlocal bound states given in [18] under a local unitary transformation $\{|1\rangle \rightarrow |2\rangle, |2\rangle \rightarrow |1\rangle\}$ on the first qutrit together with $\{|1\rangle \leftrightarrow |2\rangle\}$ on the second qutrit, with $\{0\}$ unchanged. Our main result reads:

**Theorem** The state $\varrho_{xy}$ is Bell nonlocal if $(x, y) \in D_N^y \cup D_N^y$, $B(A)$-steerable if $(x, y) \in D_S^y (D_S^y)$, respectively, and entangled if $(x, y) \in D_E$, where $D_N^y \subset D$ denotes the open set defined by

$$\frac{(y\bar{z} + y^2 - \bar{x}^2)}{x^2 + (d-1)y^2} < \frac{(x - d_x y)(x + d_y y)}{(d-1)^2}$$

with $\bar{z} = z\sqrt{d-2}$ and $d_x = d\sqrt{(d-1)(d-2)} \pm (d-1)^2$ and $D_S^y \subset D$ denotes the open set defined by conditions i) $x > y > 0$ and ii)

$$\frac{(d-1)x + y}{2} \left(1 + \sqrt{\frac{y}{x}}\right) < \bar{z} + 2y$$

while $D_E \subset D$ denotes the open set defined by

$$\frac{z}{\sqrt{d-2}} > \begin{cases} \frac{(d-1)^2 x + (d-2)^2 y}{2(d-1)(d-2)}, & \sqrt{\frac{z}{d-2}} \leq \frac{d-1}{2d-2}, \\ \frac{(d-1)^2 y + (d-2)^2 x}{2(d-1)(d-2)}, & \sqrt{\frac{z}{d-2}} > \frac{d-1}{2d-2}. \end{cases}$$

The open sets $D_N^y$ and $D_S^y$ are obtained by exchanging $x, y$ in the definitions of $D_N^y$ and $D_S^y$ respectively and it holds $D_N^y(x) \subset D_S^y(x) \subset D_E$.

Open sets $D_N^{x,y}$ and $D_S^{x,y}$ defined above are nonempty for all dimensions since $D_N^y$ is nonempty. This is because the curve defined by $y\bar{z} + y^2 = \frac{1}{d^2-1}x^2$ with $0 < y < x/d_+$, which is shown as the blue curve in the inset of Fig.1, lies inside $D_N^y$ because the left hand side of Eq.(4) vanishes identically while its right hand side is positive as long as $x \neq d+y$. Moreover the open set $D_N^y$ is contained in the triangle formed by $y = 0$, $x = x_N := \sqrt{d-2}/(d^2-d-1)$, and $x = d_y w$ while $D_S^y$ is contained in the triangle formed by $y = 0$, $x = y$, and $x = x_S := 2\sqrt{d-2}/(d^2+2d-7)$ (see supplementary material). In Fig.1 we have illustrated these open sets, together with $x_N < x_S < x_E := 2(d-1)/\sqrt{d^2-2d+4d-4}$ in the case of $d = 3, 4$ and in the general case of $d \geq 5$. 

**Bell nonlocality** — We consider the Bell scenario in which Alice performs $d$ 2-outcome measurements $A_p = \{A_p, A\}$ with $p = 0, 1, \ldots, d-1$ while Bob performs one
d-outcome measurement $B = \{B_0, B_1, \ldots, B_{d-1}\}$ and one 2-outcome measurement $B' = \{B'_0, B'_1\}$. We shall denote by, e.g., $P(A_pB_y)$ (or $P(A_pB'_y)$) the probability of the event in which Alice measures $A_p$ obtaining outcome 0 (or 1) and Bob measures $B$ (or $B'$) obtaining outcome $q$ (or 0). In any local realistic model the following 2d conditions cannot be satisfied simultaneously

$$P(A_pB_y) = 0, \quad (\forall p), \quad (8a)$$

$$P(A_pB'_y) = 0, \quad (p \neq 0), \quad (8b)$$

$$P(A_0B'_0) > 0. \quad (8c)$$

In fact, any hidden variable triggering the event $A_0B'_0$, i.e., Alice obtain outcome 0 when measuring $A_0$ and Bob obtains outcome 0 when measuring $B'$, will either cause the measurement $A_p$ to have outcome 1 for some $p \neq 0$, i.e., conditions Eq.(8b) cannot be satisfied, or cause the measurement $A_p$ to have outcome 0 for all $p$, i.e., conditions Eq.(8a) cannot be satisfied since any hidden variable has to trigger one of the event $\{B'_p\}$. This Hardy-type of nonlocality test also gives rise to a Bell inequality

$$P(A_0B'_0) - \sum_{p=1}^{d-1} P(A_pB'_0) - \sum_{p=0}^{d-1} P(A_0B_p) \leq 0. \quad (9)$$

In the case of $d = 3$ our Bell inequality is equivalent to the one in [1] up to some nonsignaling conditions. Although we fail to detect the nonlocality of our states by using the Hardy-type of argument Eq.(8) we manage to identify a nonempty set of our states that do violate the corresponding Bell inequality Eq.(9).

To this aim we have to properly choose the measurement settings for each party. We consider the following family of basis (which may not be orthogonal)

$$\{|A_p\} = \{a(0) + b|\theta_p\rangle \mid |\theta_p\rangle \in \Theta_d\} \quad (10)$$

for a single qudit with $a, b$ being two arbitrary real numbers satisfying $a^2 + b^2 = 1$. The 2-outcome measurements for Alice are taken to be $\{A_p = |A_p\rangle\langle A_p|, A_p = I - A_p\}$ with $p = 0, 1, \ldots, d - 1$. The orthonormal basis

$$\{|B_p\} = \{|0\rangle + \frac{\sqrt{d-1}|\theta_p\rangle}{\sqrt{d}} \mid |\theta_p\rangle \in \Theta_d\} \quad (11)$$

is taken to be the $d$-outcome measurement for Bob. The 2-outcome measurement $B'$ for Bob is simply $\{B_0 = |0\rangle\langle 0|, B_0 = I - P_0\}$. Given these measurement settings, we can express the quantum mechanical version of the left hand side of the Bell inequality Eq.(9) as the expectation value of

$$W_N = A_0 \otimes P_0 - \sum_{p=1}^{d-1} A_p \otimes P_0 - \sum_{p=0}^{d-1} A_0 \otimes B_p \quad (12)$$

in the given state $\varrho_{xy}$, which turns out to be, as shown in supplementary material,

$$\text{Tr}(\varrho_{xy} W_N) = -\frac{d-1}{R} (a,b) M_N \left( \begin{array}{c} a \\ b \end{array} \right) \quad (13)$$

with

$$M_N = \begin{pmatrix} x^2 + (d-1)y^2 & x(2y+\bar{z}) \sqrt{d-1} \\ x(2y+\bar{z}) \sqrt{d-1} & 2y^2 + z^2 + 2xy + (d-2)y^2 \end{pmatrix}. \quad (14)$$

In order to violate the Bell inequality Eq.(5) it suffices to demand $\det M_N < 0$ which turns out to be exactly the condition $\varrho_{xy} \in D_N^x$ determined by Eq.(3). By exchanging the roles of Alice and Bob we can obtain a similar Bell inequality from Eq.(3) and similar violations by the state $\varrho_{xy}$ can be obtained if $(x, y) \in D_N^x$, since the state $\varrho_{xy}$ is changed into $\varrho_{yx}$ if two qudits are exchanged.

In the cases of $3 \leq d \leq 9$ the maximal violations over all possible nonlocal bound entangled states in $D_N^x$, together with the optimal $a$ determining the measurements $\{A_p\}$, are documented in Table I. The maximization is taken over all the measurements parametrized by some $(a, b)$ as specified above. Larger violations might be possible by choosing different kind of measurements. In the case of $d = 3$ the analytical counterexample presented in [19] corresponds to $a = \sqrt{24}/5$ while $x = 3/10$ and $y = 1/60$. Actually, the violation can be obtained analytically for every single state in $D_N^x$ for all dimensions and in the large $d$ limit the maximal violation can also be obtained analytically as shown in supplementary material.

**Steerability beyond nonlocality —** Bell nonlocal states are also steerable. Next we consider the steerability of our states, e.g., the possibility of Bob steering Alice, i.e., $B$-steerability. For Bob we assume the same measurement settings as in the Bell scenario, i.e., $\mathcal{B} = \{B_p\}_{p=0}^{d-1}$ and $\mathcal{B}' = \{B'_0, B'_1\}$. For Alice, since quantum theory is applicable, we consider a set of $d+3$ positive semidefinite operators $\{Z_{dd}, Z_{dp}, Z_{dt}\}_{p=0}^{d-1}$ satisfying

$$Z_{dd} - Z_{dt} - Z_{pd} \leq 0, \quad (\forall p, \tau). \quad (15)$$

If the bipartite state is unsteerable from Bob to Alice, it holds the following inequality

$$P_A(Z_{dd}) - \sum_{\tau=0}^{1} P(Z_{dt}B'_\tau) - \sum_{p=0}^{d-1} P(Z_{pd}B_p) \leq 0. \quad (16)$$

TABLE I: The maximum violation of Bell inequality by the bound entangled state $\varrho_{xy}$ with measurement settings determined by $a$ in the case of $3 \leq d \leq 9$ and in the large $d$ limit.
In [18] an additional constraint \( Z_{dd} = Z_{0d} \) has been imposed. A slightly larger violation to the above inequality can be expected by a more general choice. We consider the following family of operators

\[
Z_{d1} = Z_{dd} = (1 - s) a^2 p_0,
\]

\[
Z_{d0} = (s^{-1} - 1)b^2 \tilde{p}_0,
\]

\[
Z_{pd} = |A_p \rangle \langle A_p| \tag{17}
\]

that are parametrized by \((a, b)\) and \(0 < s < 1\). For any \( p, a, b, \) and \( 1 > s > 0 \) we have the following inequality, as shown in supplementary material,

\[
|A_p \rangle \langle A_p| - (1 - s) a^2 p_0 + (s^{-1} - 1)b^2 \tilde{p}_0 \geq 0 \tag{18}
\]

so that the conditions Eq. (15) for \( Z \) operators are satisfied. By choosing the same measurement settings for Bob as in the Bell scenario, i.e., \( \{ B_p = |B_p \rangle \langle B_p| \} \) and \( \{ B'_0 = P_0, B'_1 = \tilde{P}_0 \} \), the quantum mechanical version of the left hand side of the steering inequality is given by the expectation value of

\[
W_S = Z_{dd} \otimes P_0 - Z_{d0} \otimes P_0 - \sum_{p=0}^{d-1} Z_{pd} \otimes B_p \tag{19}
\]

in the given state \( \varrho_{xy} \) which assumes the same form as Eq. (13) with \( M_N \) replaced by

\[
M_S = \left( x^2 + \frac{xy}{d-1} \left( \frac{x(2y+1)}{d-1} + \frac{(y+1)^2}{d-1} \right) + xy + \frac{1-s}{s} y^2 \right). \tag{20}
\]

In order to violate the steering inequality Eq. (16) it suffices to demand \( M_S < 0 \) for some \( 0 < s < 1 \). A straightforward calculation yields the conditions \( x > y \) and Eq. (6), i.e., \((x, y) \in D_S^x \) (see supplementary material). By minimizing the negative eigenvalue of \( M_S \) over all possible \( s \) with \((a, b)\) taken to be the eigenstate of \( M_S \) corresponding to the negative eigenvalue, we obtain the maximal violation for a given state. The maximal violation over all possible states in \( D_S^x \) for each \( 3 \leq d \leq 9 \) are documented in Table II, as well as the asymptotical maximal violation (see supplementary material). As expected, in the case of \( d = 3 \) there is a larger violation to the steering inequality Eq. (16) than that found in [18] with a restricted measurement setting, which identifies only a subset of steerable states \( \varrho_{xy} \) in \( D_S \).

**Entanglement beyond steerability and nonlocality—**

The violation to the steering inequality as well as the Bell inequality provides naturally an entanglement witness, namely \( W_N \) and \( W_S \), for the nonlocal bound entangled states \( \varrho_{xy} \). These witnesses are however relatively weak with respect to entanglement detection because the quantum nature of none or only one party is taken into account. It turns out that these two witnesses belong to the following family of entanglement witnesses

\[
W_E = (1 - \alpha) a^2 P_0 \otimes P_0 - \beta b^2 \tilde{P}_0 \otimes P_0 - \sum_{p=0}^{d-1} A_p \otimes B_p \tag{21}
\]

where \( \alpha \) and \( \beta \) are two real numbers and \( P_0, |B_p \rangle \langle B_p| \) and \( |A_p \rangle \langle A_p| \) are defined as before with \( a^2 + b^2 = 1 \). In fact \( W_S \) corresponds to the choice \( \alpha_S = s \) and \( \beta_S = s^{-1} - 1 \) with \( 0 < s < 1 \) while \( W_N \) corresponds to the choice \( \alpha_N = (d - 1)b^2/a^2 \) and \( \beta_N = (d - 1)/b^2 - \frac{d}{a^2} \).

For \( W_E \) to be an entanglement witness it should hold

\[
Tr(\rho_{sep} W_E) \leq 0 \text{ for all separable states } \rho_{sep} \text{ or equivalently, } Tr_A[|\psi \rangle \langle \psi| \otimes I] W_E \leq 0 \text{ for all single qudit pure state } |\psi \rangle \text{ with the partial trace taken over the first qudit.}
\]

As shown in supplementary material \( W_E \) is an entanglement witness if and only if \( 1 > \alpha \geq 0 \) and

\[
\alpha t^2 + \beta \geq \gamma(t) := \frac{3\gamma(t)}{2} - \frac{2d-2}{d-1} - \frac{1}{d-1} \tag{22}
\]

for \( 1 \leq t \leq 1 + \frac{d}{(d-1)(d-2)} \). Let \( J \) denote the set of all pairs \((\alpha, \beta)\) satisfying the conditions above, as illustrated in Fig. 2, and its boundaries are \( \alpha = 0, 1 \) and the envelope of the straight lines defined by Eq. (22), taking equality

\[
(\alpha_t, \beta_t) = \left( \frac{\gamma(t)}{2t}, \frac{\gamma(t)}{2t} \right). \tag{23}
\]

As expected \((\alpha_S, \beta_S)\) and \((\alpha_N, \beta_N)\) lie in the interior of \( J \) and the nontrivial witness on the boundary of \( J \), namely \((\alpha_t, \beta_t)\), will detect a larger set of bound entangled states. The expectation value of \( W_E \) in the state \( \varrho_{xy} \) assumes the same form as Eq. (13) with \( M_N \) replaced by

\[
M_E = \left( x^2 + \frac{\alpha_S s}{d-1} \left( \frac{x(2y+1)}{d-1} + \frac{(y+1)^2}{d-1} \right) + xy + \beta s y^2 \right). \tag{24}
\]

Since the state is invariant under the exchanging of two qudits and \( x \) and \( y \) we can obtain a similar entanglement witness \( W'_E \) from \( W_E \) by exchanging two qudits. Its expectation value in \( \varrho_{xy} \) is determined by the matrix \( M'_E \) obtained form \( M_E \) by exchanging \( x \) and \( y \). In order to have an entangled PPT state \( \varrho_{xy} \) it suffice to have det \( M_E \) < 0 or det \( M'_E \) < 0 which turns out to be the condition \((x, y) \in D_E \) (see supplementary material).

| \( d \) | \((x, y)\) | \( s \) | \( a \) | Max violation |
|---|---|---|---|---|
| 3 | \((0.473, 0.182)\) | 0.5413 | 0.851 | \(3.2655 \times 10^{-3}\) |
| 4 | \((0.434, 0.154)\) | 0.5370 | 0.887 | \(2.0082 \times 10^{-3}\) |
| 5 | \((0.400, 0.136)\) | 0.5370 | 0.908 | \(1.3277 \times 10^{-3}\) |
| 6 | \((0.372, 0.123)\) | 0.5373 | 0.923 | \(9.3813 \times 10^{-4}\) |
| 7 | \((0.349, 0.114)\) | 0.5377 | 0.933 | \(6.9687 \times 10^{-4}\) |
| 8 | \((0.330, 0.106)\) | 0.5380 | 0.941 | \(5.3768 \times 10^{-4}\) |
| 9 | \((0.313, 0.099)\) | 0.5382 | 0.947 | \(4.2729 \times 10^{-4}\) |

**TABLE II:** The maximal violation of the steering inequality by the PPT state \( \varrho_{xy} \) with measurement settings determined by \( a \) and \( s \) in the case of \( 3 \leq d \leq 9 \).
Conclusions and discussions — We have constructed a family of bound entangled states and proposed a Bell inequality, a steering inequality, and a family of entanglement witnesses to detect their nonlocality, steerability, and entanglement. Our entanglement witnesses can also help detect other bound entangled states and entangled states for which other criteria might fail. Our proposed bound entangled states may find applications in the nonlocality-based or and semi-device dependent quantum information tasks. Their preparation in various physical systems might be facilitated by the symmetry of $\Theta_{xy}$ exhibited via $\Theta_{xy}$. We believe that all the proposed states are entangled, as suggested by numerical evidences, even though they cannot be comprehensively detected by our entanglement witness. The questions of its generalization to continuous variable systems and bi-partite systems with unequal local dimensions are left open.

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[1] J. S. Bell, *On the EPR paradox*, Physics 1, 195 (1964).
[2] N. Brunner, D. Cavalcanti, S. Pironio, V. Scarani, and S. Wehner, *Bell nonlocality*, Rev. Mod. Phys. 86, 419 (2014).
[3] R.F. Werner, *Quantum states with Einstein-Podolsky-Rosen correlations admitting a hidden-variable model*, Phys. Rev. A 40, 4277 (1989).
[4] R. Horodecki, P. Horodecki, M. Horodecki, and K. Horodecki, *Quantum entanglement*, Rev. Mod. Phys. 81, 865 (2009).
[5] N. Gisin, *Bell’s inequality holds for all non-product states*, Phys. Lett. A 154, 201 (1991).
[6] S. Popescu and D. Rohrlich, *Generic quantum nonlocality*, Phys. Lett. A 166, 293 (1992).
[7] D. Cavalcanti, M.L. Almeida, V. Scarani, A. Acín, *Quantum networks reveal quantum nonlocality*, Nat. Comm. 2, 184 (2011).
[8] S. Yu, Q. Chen, C.J. Zhang, C.H. Lai, and C.H. Oh, *All entangled pure states violate a single Bell’s inequality*, Phys. Rev. Lett. 109, 120402 (2012).
[9] C.H. Bennett, G. Brassard, S. Popescu, B. Schumacher, J.A. Smolin, W.K. Wootters, *Purification of Noisy Entanglement and Faithful Teleportation via Noisy Channels*, Phys. Rev. Lett. 76, 722 (1996).
[10] M. Horodecki, P. Horodecki, and R. Horodecki, *Mixed-State Entanglement and Distillation: Is there a Bound Entanglement in Nature?*, Phys. Rev. Lett. 80, 5239 (1998).
[11] A. Peres, *Separability Criterion for Density Matrices*, Phys. Rev. Lett. 77, 1413 (1996).
[12] M. Horodecki, P. Horodecki, and R. Horodecki, *Separability of mixed states: necessary and sufficient conditions*, Phys. Lett. A 223, 210 (1996).
[13] K. Horodecki, M. Horodecki, P. Horodecki, J. Oppenheim, *Secure key from bound entanglement*, Phys. Rev. Lett. 94, 160502 (2005).
[14] M. Epping and C. Brukner, *Bound entanglement helps to reduce communication complexity*, Phys. Rev. A 87, 032305 (2013).
[15] A. Peres, *All the Bell inequalities*, Found Phys. 29, 589 (1999).
[16] W. Dür, *Multipartite Bound Entangled States that Violate Bells Inequality*, Phys. Rev. Lett. 87, 230402 (2001).
[17] T. Vértesi and N. Brunner, *Quantum nonlocality does not imply entanglement distillability*, Phys. Rev. Lett. 108, 030403 (2012).
[18] T. Moroder, O. Gittsovich, M. Huber, and O. Gühne, *Steering bound entangled states: A counterexample to the stronger Peres conjecture*, Phys. Rev. Lett. 113, 050404 (2014).
[19] T. Vérisi and N. Brunner, *Disproving the Peres conjecture by showing Bell nonlocality from bound entanglement*, Nat. Comm. 5, 5297 (2014).
[20] M.F. Pusey, *Negativity and steering: A stronger Peres conjecture*, Phys. Rev. A 88, 032313 (2013).
[21] E. Schrödinger, *Discussion of probability relations between separated systems*, Proc. Camb. Phil. Soc. 31, 555 (1935).
[22] H.M. Wiseman, S.J. Jones, and A.C. Doherty, *Steering, Entanglement, Nonlocality, and the Einstein-Podolsky-Rosen Paradox*, Phys. Rev. Lett. 98, 140402 (2007).
[23] D. Chruściński and G. Sarbicki, *Entanglement witnesses: construction, analysis and classification*, J. Phys. A 47, 483001 (2014).
[24] S. Yu and N.-L. Liu, *Entanglement detection by local orthogonal observables*, Phys. Rev. Lett. 95, 150504 (2005).
SUPPLEMENTAL MATERIAL

Construction of $\Theta_d$ — For examples we have $\Theta_2 = \{\pm |1\rangle\}$ and $\Theta_3 = \{\pm \sqrt{3}|1\rangle - |2\rangle)/2, |2\rangle\}$. In general $\Theta_d$ with $d \geq 3$ is defined recursively by $\Theta_{d-1}$ via

$$|\theta_p\rangle_{d-1} = \frac{\sqrt{d(d-2)}|\theta_p\rangle_{d-2} - |d-1\rangle}{d-1}$$

(S1)

for $0 \leq p \leq d - 2$ and $|\theta_{d-1}\rangle_{d-1} = |d-1\rangle$. All the coefficients of $|\theta_p\rangle$ in the computational basis are real numbers, i.e., $|\theta_p\rangle = |k\rangle\langle k|$ for all $k$. Since the Gramm matrix of those $d$ states in $\Theta_d$ has rank $d - 1$ there are exactly $d - 1$ independent state in $\Theta_d$ and it holds

$$\sum_{p=0}^{d-1} |\theta_p\rangle = 0, \quad \sum_{p=0}^{d-1} |\theta_p\rangle \langle \theta_p| = \frac{d}{d-1} \bar{P}_0,$$

(S2)

where $\bar{P}_0 = I - P_0$ with $P_0 = |0\rangle\langle 0|$. is the projection to the $d - 1$ dimensional subspace.

Partial transpose of $\varrho_{xy}$ — We shall prove that the state $\varrho_{xy}$ defined in Eq. (3) has positive partial transpose for all $(x, y) \in D$, i.e., $x, y, \Delta > 0$ by showing that $\varrho_{xy} = \varrho_{xy}^{T_1}$ with $T_1$ denoting the partial transpose made on the first qudit. To proceed we introduce a $d - 1$ dimensional maximally entangled state

$$|\Phi\rangle := \sum_{k=1}^{d-1} |k, k\rangle = \frac{d-1}{d} \sum_{p=0}^{d-1} |\theta_p\rangle \otimes |\theta_p\rangle$$

(S3)

in which we have taken into account Eq. (S2). For simplicity we shall denote by a hatted letter, e.g., $\hat{\theta}_p$, the projection of the corresponding pure state, e.g., $|\theta_p\rangle\langle \theta_p|$, in what follows. First, since $|\Psi\rangle = |00\rangle + |\Phi\rangle$, we have

$$\hat{\psi}_{T_1} = |00\rangle\langle 00| + \bar{\Phi}^{T_1} + \sum_{k=1}^{d-1} (|0, k\rangle\langle k, 0| + |k, 0\rangle\langle 0, k|).$$

(S4)

Second, from the identity

$$\sum_{i, j=1}^{d-1} \hat{\psi}_{ij} = \sum_{i, j=1}^{d-1} (|i, j\rangle\langle i, j| - |i, j\rangle\langle j, i|) = \bar{P}_0 \otimes P_0 - \bar{\Phi}^{T_1},$$

it follows that

$$\sum_{i, j=1}^{d-1} (\hat{\psi}_{ij} - \hat{\psi}_{ij}^{T_1}) = \bar{\Phi} - \bar{\Phi}^{T_1}.$$  

(S5)

Third, by taking into account the fact that $\sum_{k=1}^{d-1} |k\rangle\langle k| = \bar{P}_0$, $\bar{P}_0|\theta_p\rangle = |\theta_p\rangle$, and $|\theta_p\rangle\langle \theta_p| = \delta_{p-1}^{d-1}$, we obtain

$$\sum_{k=1}^{d-1} |0, k\rangle\langle \phi_k| = \frac{(d-1)\bar{\varrho}}{d\sqrt{d-2}} \sum_{p=0}^{d-1} |0\rangle\langle \theta_p| \otimes |\theta_p\rangle\langle \theta_p|,$$

(S6)

and

$$d^2(d-2) \sum_{k=1}^{d-1} \bar{\varrho}_k = \sum_{p, q=0}^{d-1} |\theta_p\rangle\langle \theta_q| \otimes |\theta_p\rangle \langle \theta_q| \sum_{k=1}^{d-1} \langle \theta_p|k\rangle\langle k|\theta_q\rangle$$

$$= \sum_{p, q=0}^{d-1} |\theta_p\rangle\langle \theta_q| \otimes |\theta_p\rangle \langle \theta_q| \frac{d\delta_{pq} - 1}{d-1}$$

$$= \frac{d}{d-1} \sum_{p=0}^{d-1} \bar{\theta}_p \otimes \bar{\theta}_p - \frac{d^2}{(d-1)^3} \bar{\Phi},$$

(S7)

from which it follows that

$$\sum_{k=1}^{d-1} (\hat{\psi}_k - \hat{\psi}_k^{T_1}) = xy \sum_{k=1}^{d-1} (|0, k\rangle\langle k, 0| + |k, 0\rangle\langle 0, k|)$$

$$-xy(|\Phi\rangle\langle 00| + |00\rangle\langle \Phi|) + \frac{z^2(\hat{\Phi}^{T_1} - \bar{\Phi})}{d-2}.$$  

(S8)

Putting together Eq. (S4), Eq. (S3), and Eq. (S8) and recalling that $\Delta = \frac{d^2 - 2}{2} - xy$, we obtain $\varrho_{xy} - \varrho_{xy}^{T_1} = 0$.

Bounding triangles for $D_N^S$ and $D_S^N$ — If $(x, y) \in D_N^S$ then from condition Eq. (5) it follows that $x > d_+ y$ and

$$\frac{z}{y} > \frac{\tilde{\lambda}^2 - 1 - \sqrt{1 + \tilde{\lambda}^2}(\tilde{\lambda} - \tilde{d}_+)(\tilde{\lambda} + \tilde{d}_-)}{\sqrt{1 + \tilde{\lambda}^2} - \sqrt{1 + \tilde{\lambda}^2}(\tilde{\lambda} - \tilde{d}_-)}$$

$$\geq \tilde{\lambda}d\sqrt{d-2} + \frac{(d-1)(d-2)}{2} - 2 > (d-1)^{\frac{1}{2}}$$

$$\tilde{\lambda} = x/(y\sqrt{d-1})$$

$$d_+ = d_+/\sqrt{d-1} = d\sqrt{d-2} = (d-1)^{\frac{1}{2}}.$$  

As a result we obtain $x < x_N$ and, considering $x > y$, also $(x, y) \in D_S^N$ for $(x, y) \in D_N^S$ and even if Eq. (5) is an equality, i.e., $D_N^S \subset D_S^N$. If $(x, y) \in D_S^N$ then we have condition Eq. (6) which reads

$$2 + \frac{z}{y} > \left(1 + \frac{1}{\sqrt{\lambda}}\right) \frac{(d-1)\lambda + 1}{2} := K_{\lambda}.$$  

(S9)

with $\lambda = x/y$. Because $\lambda > 1$ we have $(d-1)\sqrt{\lambda+1}/\sqrt{\lambda} > d$ from which it follows $2z > (d-1)x$, i.e., $x < x_S$.

Derivation of Eq. (13) — Recalling that $A_p = |A_p\rangle\langle A_p|$ and $\bar{A}_p = I - A_p$ with $|A_p\rangle = a|0\rangle + b|\theta_p\rangle$ and identity

$$\sum_{p=0}^{d-1} A_p = da^2 P_0 + \frac{db^2}{d-1} \bar{P}_0$$

(S10)
we can rewrite
\[
W_N = A_0 \otimes P_0 - \sum_{p=0}^{d-1} A_p \otimes P_0 - \sum_{p=0}^{d-1} A_p \otimes B_p
\]
\[
= (1 - db^2)P_0 \otimes P_0 - \left( d - 1 - \frac{db^2}{d - 1} \right) P_0 \otimes P_0
\]
\[
- \sum_{p=0}^{d-1} A_p \otimes B_p. \tag{S11}
\]
Since \( B_p = |B_p\rangle\langle B_p| \) and \( |B_p\rangle = a_0|0\rangle + b_0|\theta_p\rangle \) with \( a_0 = 1/\sqrt{d} \) and \( b_0 = \sqrt{(d-1)/d} \) and by denoting \( |A_p, B_p\rangle = |A_p\rangle \otimes |B_p\rangle \), we have \( \langle \Psi | A_p, B_p \rangle = a_0 b_0 + b_0 |\theta_p\rangle \).
Since \( |A_p, B_p\rangle \) is symmetric and \( |\psi_ij\rangle \) is antisymmetric in the subspace spanned by \{\( |i\rangle \}_{i=1}^{d-1} \}, we have \( \langle \psi_ij | A_p, B_p \rangle = 0 \) for all \( i \neq j \). Furthermore, from the identity
\[
\langle \phi_k | A_p, B_p \rangle = \frac{(d-1)!}{d!} \sum_{q=0}^{d-1} \theta_q^p |A_p\rangle \langle \theta_q | B_p \rangle \langle \theta_p | k \rangle
\]
\[
= b b_0 \frac{(d-1)!}{d!} \sum_{q=0}^{d-1} \theta_q^p (\theta_q | \theta_p \rangle \langle \theta_q | \theta_p \rangle \langle \theta_p | k \rangle
\]
\[
= b b_0 (\theta_p | k \rangle \langle \theta_p | d \rangle \frac{d-2}{d-1} \langle \theta_p | k \rangle \tag{S12}
\]
for each \( k = 1, 2, \ldots, d-1 \), where we have used the facts \( \langle \theta_q | \theta_p \rangle = \frac{d b_0^p}{d-1} \) and \( \sum_p |\theta_p\rangle = 0 \), it follows
\[
\langle \psi_i | A_p, B_p \rangle = \left( x a b_0 + y b a_0 + z b b_0 \sqrt{\frac{d-2}{d-1}} \langle \theta_p | k \rangle
\]
and thus
\[
\sum_{k=1}^{d-1} (|\psi_i | A_p, B_p \rangle |^2 = \frac{(x a \sqrt{d-1} + y b + z b)^2}{d}.
\]
As a result we have
\[
\sum_{p=0}^{d-1} (|A_p \otimes B_p \rangle |_{e_{xy}}^2 = \frac{xy}{R} \left( a + \sqrt{d-1}b \right)^2 + \frac{1}{R} \frac{x a \sqrt{d-1} + (y + z) b}{(x^2 + \frac{xy}{d-1}) \sqrt{\frac{x(y+z)}{d-1} + xy}} \left( a \right) \left( b \right) \tag{S13}
\]
Taking into account \( a^2 + b^2 = 1 \) and
\[
\langle P_0 \otimes P_0 \rangle |_{e_{xy}} = \frac{xy}{R}, \quad \langle \bar{P}_0 \otimes P_0 \rangle |_{e_{xy}} = \frac{(d-1)y^2}{R} \tag{S14}
\]
we finally obtain Eq.\( [13] \) with two by two matrix \( M_N \) given by Eq.\([14]\). In the case of steerability \( W_S \) and entanglement witness \( W_E \), which assume a similar form as \( W_N \), we can obtain similar expression of the expectation value \( \text{Tr}(e_{xy} W_N) \) as Eq.\([13]\) with \( M_N \) replaced by \( M_S \) and \( M_E \) respectively.

**Analytical violation to the Bell inequality** — To have a nonzero violation we need \( M_N < 0 \), which turns out to be exactly \((x, y) \in \mathcal{D}_N^2 \) defined by Eq.\([5] \), or equivalently,
\[
\left| \frac{\bar{d}}{y} + 1 - \lambda^2 \right| \leq \sqrt{(1 + \lambda^2)(\bar{d} + \lambda + \bar{d})} := \Gamma \lambda \tag{S15}
\]
where \( \bar{d} = x'(y \sqrt{d - 1}) \) satisfying \( \lambda > \bar{d} = \bar{d}/(y \sqrt{d - 1}) \). We can parametrize each \((x, y) \in \mathcal{D}_N^2 \) giving rise to a nonlocal bound entangled state with a real number \( \lambda > \bar{d} \) and an angle \( 0 < \theta < \pi \) as following
\[
y = \left( \frac{(\bar{d}^2 - 1 - \Gamma \lambda \cos \theta)^2}{d - 2} + (d - 1) \lambda^2 + 1 \right)^{-1/2} \tag{S16}
\]
and recalling that \( \bar{d} = \sqrt{(d - 2)(1 - x^2 - y^2)} \). The blue curve shown in the inset of Fig.1 corresponds to \( \theta = \frac{\pi}{2} \).
Each given \( \lambda > \bar{d} \) and \( \theta \in (0, \pi) \) define a state \( e_{xy} \) via \((x, y) \) given above. For this state we have
\[
\text{det } M_N = -y^4 \Gamma^2 \lambda^2 \sin^2 \theta \tag{S18}
\]
and we take \((a, b)\) to be the eigenstate, which can be analytically determined by \( M_N \), corresponding to the negative eigenvalue
\[
\frac{2 \text{det } M_N}{\text{Tr} M_N + \sqrt{(\text{Tr} M_N)^2 - 4 \text{det } M_N}} \tag{S19}
\]
of \( M_N \) and we obtain analytically the nonzero violation
\[
\text{Tr}(e_{xy} W_N) = \frac{2(d - 1)R^{-1}y^4 \Gamma^2 \lambda^2 \sin^2 \theta}{\text{Tr} M_N + \sqrt{(\text{Tr} M_N)^2 - 4 \text{det } M_N}}. \tag{S20}
\]

Though the maximal violations over all possible states in \( \mathcal{D}_N^2 \) in the case of finite dimensions can be carried out only numerically, in the large \( d \) limit, we obtain the asymptotic maximal violation as follows. Since \( \bar{d} \approx 2d^{3/2} \) we choose \( \lambda = (2 + \epsilon) d^{3/2} \) for some \( \epsilon > 0 \) then we have \( \Gamma^2 \lambda \approx \epsilon (2 + \epsilon) d^{3/2} \) so that \( 1/y \approx (2 + \epsilon)^2 + \mu \sqrt{\epsilon (2 + \epsilon)^3} d^{3/2} \). Because \( \text{Tr} M_N \approx 1 \), and \( R \approx 2d \) we obtain the asymptotic violation \( \approx \frac{2}{\sqrt{5}} \lambda^2 \sin^2 \theta \) which attains its maximum at \( \sin^2 \theta = 2/\sqrt{5} \) and \( \epsilon = 5/2 \) giving rise to the asymptotic maximal violation \( \approx \frac{1}{20}d^{-4} \). The optimal measurement setting reads \( a \approx 1 - x^2/2 \), which is determined by the corresponding eigenstate.

**Proof of Eq.\([18]\)** — The inequality holds outside the 2-dimensional subspace spanned by \{\( |0\rangle, |\theta_0\rangle \)\} and within this subspace the left hand side of Eq.\([18]\) becomes
\[
\begin{pmatrix} a^2 & ab \\ ab & b^2/s \end{pmatrix} \geq 0. \tag{S21}
\]
Derivation of Eq. (6) — From \( \det M_S < 0 \) for some \( 0 < s < 1 \) it follows that

\[
\frac{x^2(2y + z)^2}{d - 1} > x^2 + \frac{xy^3}{d - 1} + s \frac{xyL}{d - 1} + \frac{1}{s} x^2 y^2 \\
geq (x\sqrt{L} + y\sqrt{xy/((d-1)})^2
\]

(S22)

where we have denoted \( L = \frac{(x^2 + y^2}{d - 1} + xy - y^2 \) and taken

\( s = \sqrt{((d-1)xy/L} \) to equalize the second inequality. By denoting \( \lambda = x/y \) and \( v = \bar{z}/y \) we obtain

\[
2 + v > \sqrt{(1+v)^2 + (d-1)(\lambda - 1) + \frac{1}{\sqrt{\lambda}}\ }
\]

(S23)

from which it follows

\[
1 - \frac{1}{\sqrt{\lambda}} > \frac{(d-1)(\lambda - 1) + 1 + v}{(1 + v)^2 + (d-1)(\lambda - 1) + 1 + v}
\]

(S24)

If \( \lambda \leq 1 \) then from Eq. S24 it follows \( 1 + v \leq (d-1)(\lambda + \sqrt{\lambda}) \) and \( 2 + v < K_\lambda \). Taking into account \( v \geq (d - 2)\sqrt{\lambda} \) we obtain a contradiction

\[
\frac{1}{d - 1} \leq \lambda + \frac{\sqrt{\lambda}}{d - 1} \leq \lambda + \frac{2\sqrt{\lambda}}{d - 1} < \frac{1}{d - 1}
\]

(S25)

so that we have \( \lambda > 1 \). If \( 1 + v \leq (d-1)(\lambda + \sqrt{\lambda}) \) then Eq.(S10) follows from Eq.(S24). If \( 1 + v > (d-1)(\lambda + \sqrt{\lambda}) \) then Eq.(S10) follows from \( K_\lambda \leq (d-1)\lambda + 1 < 1 + v \) since \( \lambda > 1 \). Thus from det \( M_S < 0 \) for some \( 0 < s < 1 \) it follows condition Eq.(6) and \( x > y \) and vice versa.

Asymptotic violation to the steering inequality — Let us denote \( \lambda = x/y \) and from the condition Eq.(6) for steerability it follows that there is \( \nu > 1 \) such that

\[
y = \frac{\sqrt{d-2}}{\sqrt{\nu K_\lambda - 2) + (d-2)(1 + \lambda^2)} \}
\]

(S25)

with \( K_\lambda \) defined in Eq.(S9). That is to say every pair \( (x,y) \in D_\lambda \) is characterized by two real numbers \( \lambda, \nu > 1 \). In the large \( d \) limit we have \( 1/y \approx \frac{1}{2} \nu (\lambda + \sqrt{\lambda})/d \) and therefore the largest eigenvalue of \(-\tilde{M}_S \) approaches

\[
-\det M_S \approx xy \left( \frac{2x}{\sqrt{d}} - x^2 + xy - s \frac{xy}{d} - \frac{x y}{s} \right)
\]

(S25)

\[
\leq 16(\nu - 1)(\sqrt{\lambda} - 1) \frac{\nu ^4 (\lambda + 1)^3 d^2}{d - 1}
\]

(S27)

attains its maximum at \( \nu = 4/3 \) and \( \lambda = 4 \), yielding the asymptotic violation as listed in Table II. We have the optimal \( s = \sqrt{xy} \) to attain the above inequality.

Entanglement witness — For \( W_E \) to be candidate of entanglement witness it should hold for every pure state \( \left| \psi \right> \) of the first qubit that \( Tr_A(\left| \psi \otimes I \right> W_E) \leq 0 \), i.e.,

\[
\sum_{p=0}^{d-1} s_p B_p \geq h_{\alpha \beta} P_0
\]

(S28)

with \( h_{\alpha \beta} = (1 - \alpha) a^2 - \beta b^2 s^2 \), where \( s_p = \left| \left< \psi \left| A_p \right> \right|^2 \) and \( s = \left| \left< \psi \left| 0 \right> \right|^2 \) with \( s = 1 - s \). If \( s = 1 \), i.e., \( \left< \psi \right| = 0 \), then \( s_p = a^2 \) so that we obtain the condition \( \alpha \geq 0 \). In the case of \( s \neq 1 \) we introduce

\[
t : = \frac{|a|\sqrt{s}}{|b|\sqrt{s}}
\]

(S29)

If \( t \leq 1 \) then for any given \( p \) we can always choose \( \left| \psi \right> \) such that \( s_p = 0 \). Thus we have only to require \( (1 - \alpha) t^2 \leq \beta \) for all \( t \leq 1 \), from which it follows \( \beta \geq 0 \), to ensure Eq.(S28) in this case. As a result we obtain the condition \( \alpha < 1 \) otherwise \( W_E \) would be negative semi-definite. Now we consider \( t > 1 \) and in this case

\[
\left| \left< \psi \left| A_p \right> \right| = |a\left< \psi \left| 0 \right> + b\left< \psi \left| \theta \right> \right| \geq |a|\sqrt{s} - |b|\sqrt{s} > 0,
\]

since \( \left| \left< \psi \left| \theta \right> \right| \leq \sqrt{s} \), so that we always have \( s_p > 0 \) for all \( p \), i.e., \( B_p = \sum_p s_p B_p \) is full rank. The condition Eq.(S28) now becomes equivalent to

\[
1 \geq h_{\alpha \beta} \left< 0 \left| B_p \right> \right|^2 \geq \frac{(1 - \alpha) t^2 - \beta}{d} \sum_{p=0}^{d-1} \frac{1}{s_p}
\]

(S30)

where we have denoted \( \tilde{s}_p = s_p/(b^2 s) \) for which it holds

\[
\tilde{s}_p \geq (t - 1)^2, \sum_{p=0}^{d-1} \frac{\tilde{s}_p}{d} = dt^2 + \frac{d}{d - 1}
\]

(S31)

We denote by \( S_t \) the simplex \( \left( \tilde{s}_0, \tilde{s}_1, \ldots, \tilde{s}_{d-1} \right) \) defined by two conditions above for a given \( t \). The extremal points of \( S_t \) are of form

\[
\left[ \tilde{s}_p \right] = (t - 1)^2, \left[ \tilde{s}_q \right] = \left( t + \frac{1}{d - 1} \right)^2 := t_+ (q \neq p)
\]

for each \( p = 0,1, \ldots, d - 1 \). This is because firstly for the extremal point there is at least one \( p \) such that \( \tilde{s}_p = (t - 1)^2 \), due to condition Eq.(S31), and in this case it holds \( a\left< \psi \left| 0 \right> = \frac{t}{b}\left< \psi \left| \theta \right> \right| \) and \( \left| \left< \psi \left| \theta \right> \right| \leq \sqrt{s} \). Secondly, for a general \( \tilde{s} = \left( \tilde{s}_0, \tilde{s}_1, \ldots, \tilde{s}_{d-1} \right) \), with a component, say \( \tilde{s}_p \), being equal to \( (t - 1)^2 \), it holds the inequality

\[
t_+ = \sum_{q \neq p} \tilde{s}_q \geq \frac{\sum_{q \neq p} \frac{\sqrt{\tilde{s}_q}}{d - 1}}{d - 1} \frac{\sqrt{\tilde{s}_q}}{d - 1}\sum_{q \neq p} \left| \left< \psi \left| A_p \right> \right|^2
\]

(S32)

where the first equality stems from Eq.(S31), from which it follows \( \tilde{s}_q = t_+ \), with \( q \neq p \). As a result we obtain

\[
\max_{s \in S_t} \sum_{p=0}^{d-1} \frac{1}{s_p} \geq \frac{1}{(t - 1)^2} + \frac{d - 1}{t + \frac{1}{d - 1}} := \hat{\gamma}(t)
\]

(S32)

because the left hand side is a convex function of \( \tilde{s} \) so that its maximum in the simplex \( S_t \) is attained at the extremal points of \( S_t \). Since \( \hat{\gamma}(t) = t^2 - d/\hat{\gamma}(t) \) we obtain condition Eq.(S22) from Eq.(S30) together with Eq.(S32).
That is to say $W_E$ is a possible entanglement witness, i.e., nonpositive on all separable states, if and only if the condition Eq. (22) holds for all $1 \leq t \leq 1 + (d - 1)/(d - 2) := t_1$ with $t_1$ being the unique solution to $\alpha_t = 0$ with $t \geq 1$ where, with $u = (d - 1) (t - 1)$,

$$\alpha_t = \frac{(d - 1)(d + 2u)(d - (d - 2)u)}{(d + u - 1)(d + 2u + u^2)^2}, \quad (S33)$$

$$\beta_t = \frac{u(d + u)(d^2 + 3du + 3u^2)}{(d - 1)(d + 2u + u^2)^2}, \quad (S34)$$

is the envelop, given by Eq. (23), of the straight lines in the $(\alpha, \beta)$ plane defined by Eq. (22) taking equality. It is straightforward to check that $W_E$ with $(\alpha, \beta) \in J$ can detect the entanglement of $\Psi$.

By applying the entanglement witness $W_E$ on the boundary of $J$, i.e., $(\alpha_t, \beta_t)$ with $1 \leq t \leq t_1$, to the state $\varrho_{xy}$ we obtain a similar expression of the expectation value $\text{Tr}(g_{xy} W_E)$ as Eq. (13) with $M_N$ replaced by $M_E$. Thus the state is entangled if $\det M_E < 0$ for some $1 \leq t \leq t_1$ so that the region enclosed by the envelop of the family of curves in the $x, y$ plane defined by $\det M_E = 0$ parametrized by $t$, which is illustrated in Fig. 3 in the case of $d = 3$, gives rise to bound entangled states. From the equation $\det M_E = 0$, i.e.,

$$\frac{x^2(2y + \bar{z})^2}{d - 1} = \left(\frac{x^2 + \alpha_t x y}{d - 1}\right) \left(\frac{(y + \bar{z})^2}{d - 1} + xy + \beta_t y^2\right),$$

and its derivative with respect to $t$ the envelop is determined by the following two equations

$$d - 1) \lambda + \alpha_t = \frac{(2 + v)}{t} \sqrt{\lambda}, \quad (S35)$$

$$\frac{(1 + v)^2}{d - 1} + \lambda + \beta_t = \frac{(2 + v)}{t} \sqrt{\lambda}, \quad (S36)$$

with $\lambda = x/y$ and $v = \bar{z}/y$. From Eq. (S35) it follows that $v = (d - 1) t \sqrt{\lambda} + \alpha_t/t \sqrt{\lambda} = -2$ so that Eq. (S36) becomes a quartic equation $(r - r_0)f(r) = 0$ of $r = \sqrt{\lambda}$ where

$$r_0 = \frac{d + 2u}{d + 2u + u^2}, \quad u = (d - 1)(t - 1) \quad (S37)$$

and

$$f(r) = r^3 - r^2 - \frac{d + 2u - du}{(d + 2u + u^2)^2} g(r/r_1) \quad (S38)$$

in which

$$g(r) = 1 - (1 + u)r + \left((1 + u)^2 - \frac{1}{r_0}\right) r^2$$

$$= \left((1 + u)^2 - \frac{1}{r_0}\right) (r - r_c)^2 + g(r_c) \quad (S39)$$

is a quadratic function of $r$ whose minimum

$$g(r_c) = \frac{3}{4}(1 + u)^2 - \frac{1}{r_0} \quad (S40)$$

is attained at $r = r_c$ where

$$r_1 = \frac{d + 2u - du}{d + 2u + u^2}, \quad r_c = \frac{1 + u}{2(1 + u)^2 - \frac{1}{r_0}} \quad (S41)$$

As will be shown below $f(r) < 0$ for $r < 1$ so that we obtain the unique solution to Eq. (S35) and Eq. (S36) for $r < 1$ as $r = r_0$, i.e.,

$$\sqrt{\frac{x}{y}} = r_0, \quad v = \frac{z \sqrt{d - 2} - y}{y} = (d - 2) \sqrt{\frac{x}{y}} \quad (S42)$$

with $0 \leq u \leq d/(d - 2)$, which is exactly the curve $\Delta = 0$ with $(d - 2)/(d - 1) \leq \sqrt{x/y} \leq 1$. Together with the curve defined by $\det M_E = 0$ with $t = 1 + d/(d - 1)(d - 2)$ the envelop Eq. (S42) gives rise to Eq. (7) in the case of $x < y$. If we consider $W_E$ with two qudits exchanged we obtain in the same manner Eq. (7) in the case of $x > y$.

Now we shall prove $f(r) < 0$ when $r < 1$. It suffices to show that $g(r/r_1) \geq 0$ for $r < 1$ which is true if $g(r_c) \geq 0$. If $g(r_c) < 0$ then, since $1/r_0 < 1 + u$, it holds $\frac{3}{4}(1 + u)^2 < 1/r_0 < 1 + u$ from which it follows $u < 1/3$ and

$$2(d + 2u - du) - (1 + u)(d + 2u + u^2)$$

$$= (1 - 3u)d + 2u - 3u^2 - u^3 > 0 \quad (S43)$$

i.e., $r_1 > (1 + u)/2$. As a result we obtain $r_c > 2/(1 + u) > 1/r_1$, considering $\frac{3}{4}(1 + u)^2 < 1/r_0$, so that the function $g(r/r_1)$ of $r$ is decreasing for $r \leq 1$. Thus

$$g(r/r_1) \geq g(1/r_1) = 1 - \frac{1 + u}{r_1} + \frac{(1 + u)^2 - 1/r_0}{r_1^2}$$

$$\geq \frac{1}{r_1} \left(r_1 + u - \frac{1}{r_0}\right) \geq 0.$$

FIG. 3: (Color online) Illustration of the entanglement region $D^E$ in the case of $d = 3$ that is defined by the envelop of $\det M_E < 0$ with $1 \leq t \leq t_1$. 

\[ \begin{align*}
\text{FIG. 3: (Color online) Illustration of the entanglement region } D^E \text{ in the case of } d = 3 \text{ that is defined by the envelop of } \det M_E < 0 \text{ with } 1 \leq t \leq t_1. \\
\text{That is to say } W_E \text{ is a possible entanglement witness, i.e., nonpositive on all separable states, if and only if the condition Eq. (22) holds for all } 1 \leq t \leq 1 + \frac{d}{(d - 1)(d - 2)} := t_1 \text{ with } t_1 \text{ being the unique solution to } \alpha_t = 0 \text{ with } t \geq 1 \text{ where, with } u = (d - 1)(t - 1),
\end{align*} \]