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Letter

Entanglement criterion and strengthened Bell inequalities based on the Pearson correlation

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A R T I C L E I N F O

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A B S T R A C T

Entanglement is a property associated with quantum correlations and represents a key resource in several applications of quantum technology. Therefore, the ability to characterize entanglement is important at both foundational and practical levels. This work demonstrates how the Pearson correlation coefficient can be used to establish an entanglement criterion for quantum systems of two qubits. This criterion is then used to prove that a proposed conjecture is correct for the case of two qubits, which allows to efficiently identify entanglement without the need of complete prior knowledge of the quantum state. For higher dimensional quantum states the conjecture is demonstrated to be false through counter-examples, therefore a modified version of it is proposed. Finally, two new strengthened Bell inequalities are derived, which are also efficient in entanglement identification.

1. Introduction

Entanglement [1,2] is a type of correlation found in composite quantum systems [3,4]. This correlation is connected with phenomena such as the violation of Bell inequalities [5,6], which is a characteristic example of how the predictions of quantum mechanics fundamentally deviate from what it would be classically expected. Entanglement plays a key role in quantum information applications such as quantum computing [7], quantum communication [8], and quantum sensing [9].

The identification of entanglement is in general a nondeterministic polynomial-time (NP) hard problem [10,11], but for certain systems with low dimensions or a particular symmetry efficient criteria have been derived [12–14]. The first criterion that was formulated to identify entanglement is the violation of Bell inequalities [15,16]. Another important criterion, called the Peres-Horodecki criterion, is based on checking whether the application of the partial transpose map on a quantum state is a completely positive operation [17–19]. Various criteria have been derived through Heisenberg-like uncertainty relations [20–27] and through entropic uncertainty relations [28–31]. Other criteria include the estimation of concurrence [32], the covariance matrix of locally measurable observables [33,34], the cross-norm criterion along with its extensions [35–37], optimization methods on entanglement witnesses [38–40], and the sum of joint probabilities for complementary observables [41].

The above criteria are able to identify correlations in quantum systems, but differ significantly from the ones used in classical systems [42,43], where correlations are typically assessed through the Pearson correlation coefficient (PCC) [44] or the mutual information (MI) [45]. An entanglement criterion through the MI was already successfully established [46], but a criterion through the PCC remains an open problem.

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The main contribution of this work is the derivation of a PCC-based entanglement criterion, which can be used to develop experimentally efficient methods to identify entanglement. In particular, the PCC-based entanglement criterion is used to prove that the Maccone–Bruß–Macchiavello (MBM) conjecture [46] is correct for the case of qubits. For higher dimensional states, counterexamples of this conjecture are constructed which lead to the establishment of a modified version of this conjecture. Another contribution of this work is the establishment of two strengthened Clauser–Horne–Shimony–Holt (CHSH) inequalities, one based on the covariance and another based on the PCC of the observables. Those expressions generalize the original strengthened CHSH inequality [47–49], which is an expectation value-based expression. The violation of any of the above inequalities is itself an entanglement criterion.

The paper is structured as in the following. In Section 2, preliminary definitions are provided on the PCC, bipartite entanglement, complementarity, orthogonality, and the Fano form of quantum states. The entanglement criterion for qubits through the PCC is presented in Section 3. In Section 4, the MBM conjecture is proven for the case of qubits and counterexamples for higher-dimensional states are provided that lead to a new conjecture. The derivation of the covariance-based and the PCC-based strengthened CHSH inequalities is given in Section 5. Finally, our conclusion is given in Section 6.

2. Preliminary definitions

This section introduces the necessary definitions required for the rest of the paper.

2.1. Pearson correlation coefficient

2.1.1. PCC in classical systems

In classical probability theory [42,43], the linear correlation between two real random variables $\mathsf{x} \in \mathcal{R}$ and $\mathsf{y} \in \mathcal{R}$ is measured through the PCC [44]

$$\mathbb{C}\mathrm{or}\{\mathsf{x},\mathsf{y}\} := \frac{\mathbb{E}\{\mathsf{xy}\} - \mathbb{E}\{\mathsf{x}\}\,\mathbb{E}\{\mathsf{y}\}}{\sqrt{\mathbb{V}\{\mathsf{x}\}\,\mathbb{V}\{\mathsf{y}\}}} = \frac{\mathbb{C}\mathrm{ov}\{\mathsf{x},\mathsf{y}\}}{\sqrt{\mathbb{V}\{\mathsf{x}\}\,\mathbb{V}\{\mathsf{y}\}}}, \tag{1}$$

where $\mathbb{E}\{\mathsf{x}\} := \sum_i x_i \mathbb{P}\{x_i\}$ is the expectation value of a random variable x, with x_i being a possible outcome occurred with probability $\mathbb{P}\{x_i\}$, $\mathbb{C}\mathrm{ov}\{\mathsf{x},\mathsf{y}\} := \mathbb{E}\{\mathsf{xy}\} - \mathbb{E}\{\mathsf{x}\}\mathbb{E}\{\mathsf{y}\}$ the covariance between x and y, and $\mathbb{V}\{\mathsf{x}\} := \mathbb{E}\{\mathsf{x}^2\} - \mathbb{E}\{\mathsf{x}\}^2$ the variance of x. The PCC is symmetric, i.e., $\mathbb{C}\mathrm{or}\{\mathsf{x},\mathsf{y}\} = \mathbb{C}\mathrm{or}\{\mathsf{y},\mathsf{x}\}$, and its range is $[-1,1]$. For vanishing variances, $\mathbb{C}\mathrm{or}\{\mathsf{x},\mathsf{y}\}$ is undefined. The random variables x and y are linearly dependent when $\mathbb{C}\mathrm{or}\{\mathsf{x},\mathsf{y}\} = \pm 1$ (perfectly correlated for +1 and anti-correlated for -1). On the other hand, when x and y are not correlated, then $\mathbb{C}\mathrm{or}\{\mathsf{x},\mathsf{y}\} = 0$, while the converse is not in general true. Finally recall that under an affine transformation $\check{\mathsf{x}} = \alpha_x \mathsf{x} + \beta_x$ and $\check{\mathsf{y}} = \alpha_y \mathsf{y} + \beta_y$, where $\alpha_x, \alpha_y \in \mathcal{R}/\{0\}$, $\beta_x, \beta_y \in \mathcal{R}$, the absolute value of the PCC is constant, i.e., $\left|\mathbb{C}\mathrm{or}\{\mathsf{x},\mathsf{y}\}\right| = \left|\mathbb{C}\mathrm{or}\{\check{\mathsf{x}},\check{\mathsf{y}}\}\right|$.

2.1.2. PCC in quantum systems

In quantum systems [2] we are interested in assessing the correlations within a bipartite quantum state, $\boldsymbol{S}^{\mathrm{AB}} \in \mathcal{H}_d^{\mathrm{A}} \otimes \mathcal{H}_d^{\mathrm{B}}$, where d is the dimension of the Hilbert space for each party, $\mathcal{H}_d$. Given two arbitrary observables, i.e., Hermitian matrices, $\boldsymbol{X} \in \mathcal{H}_d^{\mathrm{A}}$ and $\boldsymbol{Y} \in \mathcal{H}_d^{\mathrm{B}}$, the PCC is defined as

$$\mathbb{C}\mathrm{or}\{\boldsymbol{X},\boldsymbol{Y}\} := \frac{\mathbb{E}\{\boldsymbol{X}\otimes\boldsymbol{Y}\} - \mathbb{E}\{\boldsymbol{X}\}\,\mathbb{E}\{\boldsymbol{Y}\}}{\sqrt{\mathbb{V}\{\boldsymbol{X}\}\,\mathbb{V}\{\boldsymbol{Y}\}}} = \frac{\mathbb{C}\mathrm{ov}\{\boldsymbol{X},\boldsymbol{Y}\}}{\sqrt{\mathbb{V}\{\boldsymbol{X}\}\,\mathbb{V}\{\boldsymbol{Y}\}}}, \tag{2}$$

where $\mathbb{E}\{\boldsymbol{X}\} := \mathrm{tr}\{\boldsymbol{S}^{\mathrm{AB}}(\boldsymbol{X}\otimes\boldsymbol{I})\}$, $\mathbb{E}\{\boldsymbol{Y}\} := \mathrm{tr}\{\boldsymbol{S}^{\mathrm{AB}}(\boldsymbol{I}\otimes\boldsymbol{Y})\}$, and $\mathbb{E}\{\boldsymbol{X}\otimes\boldsymbol{Y}\} := \mathrm{tr}\{\boldsymbol{S}^{\mathrm{AB}}(\boldsymbol{X}\otimes\boldsymbol{Y})\}$ are the expectation values of $\boldsymbol{X}$ and $\boldsymbol{Y}$, $\mathbb{C}\mathrm{ov}\{\boldsymbol{X},\boldsymbol{Y}\} := \mathbb{E}\{\boldsymbol{X}\otimes\boldsymbol{Y}\} - \mathbb{E}\{\boldsymbol{X}\}\mathbb{E}\{\boldsymbol{Y}\}$ is the covariance between $\boldsymbol{X}$ and $\boldsymbol{Y}$, and $\mathbb{V}\{\boldsymbol{X}\} := \mathrm{tr}\{\boldsymbol{S}^{\mathrm{AB}}(\boldsymbol{X}\otimes\boldsymbol{I})^2\} - \mathrm{tr}\{\boldsymbol{S}^{\mathrm{AB}}(\boldsymbol{X}\otimes\boldsymbol{I})\}^2$ and $\mathbb{V}\{\boldsymbol{Y}\} := \mathrm{tr}\{\boldsymbol{S}^{\mathrm{AB}}(\boldsymbol{I}\otimes\boldsymbol{Y})^2\} - \mathrm{tr}\{\boldsymbol{S}^{\mathrm{AB}}(\boldsymbol{I}\otimes\boldsymbol{Y})\}^2$ are the variances of $\boldsymbol{X}$ and $\boldsymbol{Y}$, respectively. Similar to the classical case, the PCC is symmetric, i.e., $\mathbb{C}\mathrm{or}\{\boldsymbol{X},\boldsymbol{Y}\} = \mathbb{C}\mathrm{or}\{\boldsymbol{Y},\boldsymbol{X}\}$. In the Lemma below, it is shown that the absolute value of the PCC is invariant under affine transformations.

Lemma 1. *Consider two observables, $\boldsymbol{X} \in \mathcal{H}_d^{\mathrm{A}}$ and $\boldsymbol{Y} \in \mathcal{H}_d^{\mathrm{B}}$. Under affine transformations*

$$\check{\boldsymbol{X}} = \alpha_x \boldsymbol{X} + \beta_x \boldsymbol{I} \quad \text{and} \quad \check{\boldsymbol{Y}} = \alpha_y \boldsymbol{Y} + \beta_y \boldsymbol{I}, \tag{3}$$

with $\alpha_x, \alpha_y \in \mathcal{R}/\{0\}$, $\beta_x, \beta_y \in \mathcal{R}$, and $\boldsymbol{I} \in \mathcal{H}_d$ denoting the identity matrix, the absolute value of the PCC is constant, i.e., $\left|\mathbb{C}\mathrm{or}\{\boldsymbol{X},\boldsymbol{Y}\}\right| = \left|\mathbb{C}\mathrm{or}\{\check{\boldsymbol{X}},\check{\boldsymbol{Y}}\}\right|$.

Proof. See Appendix A. ⊠

2.2. Bipartite entanglement

A bipartite quantum state $\boldsymbol{S}^{\mathrm{AB}} \in \mathcal{H}_d^{\mathrm{A}} \otimes \mathcal{H}_d^{\mathrm{B}}$ is called *entangled* when it cannot be written as a convex combination of product states [1,2],

$$\boldsymbol{S}^{\mathrm{AB}} \neq \sum_k p_k\, \boldsymbol{S}_k^{\mathrm{A}} \otimes \boldsymbol{S}_k^{\mathrm{B}}, \tag{4}$$

where $\sum_k p_k = 1$ and $\boldsymbol{S}^{\mathrm{A}} \in \mathcal{H}_d^{\mathrm{A}}$ and $\boldsymbol{S}^{\mathrm{B}} \in \mathcal{H}_d^{\mathrm{B}}$ are marginal quantum states. A state that is not entangled is called separable.

2.3. Complementarity and orthogonality

Two finite-dimensional observables, $\boldsymbol{X}_1 \in \mathcal{H}_d$ and $\boldsymbol{X}_2 \in \mathcal{H}_d$, are called *complementary* [2,50] if and only if the orthonormal bases $\{|e_k\rangle\}_{k=0}^{d-1}$ and $\{|h_k\rangle\}_{k=0}^{d-1}$ of their corresponding spectral decompositions,

$$\boldsymbol{X}_1 = \sum_{k=0}^{d-1} \lambda_{1_k} |e_k\rangle\langle e_k| \quad \text{and} \quad \boldsymbol{X}_2 = \sum_{k=0}^{d-1} \lambda_{2_k} |h_k\rangle\langle h_k|, \tag{5}$$

are mutually unbiased in $\mathcal{H}_d$, i.e.,

$$\left|\langle e_k|h_\ell\rangle\right|^2 = \frac{1}{d} \quad \forall k,\ell \in \{0,1,\cdots,d-1\}, \tag{6}$$

and the eigenvalues $\lambda_{1_k}, \lambda_{2_k} \in \mathcal{R}\ \forall k \in \{0,1,\cdots,d-1\}$ are non-degenerate. The property of complementarity implies that when a measurement outcome of an observable $\boldsymbol{X}_1$ can be predicted with certainty, then the potential measurement outcomes of its complementary observable $\boldsymbol{X}_2$ are equally probable, i.e., the outcome is uncertain.

Remark 1. There exist at most $d+1$ mutually unbiased bases in a Hilbert space $\mathcal{H}_d$ [51].

Lemma 2. *When two complementary observables $\boldsymbol{X}_1, \boldsymbol{X}_2 \in \mathcal{H}_2$ have dichotomic outcomes ± 1, then they are: (i) orthogonal to each other and (ii) unitary.*

Proof. See Appendix B. ⊠

2.4. Fano representation

Consider a unitary operator basis $\{\boldsymbol{I}, \boldsymbol{\Lambda}_1, \boldsymbol{\Lambda}_2, \boldsymbol{\Lambda}_3\}$, where $\boldsymbol{I} \in \mathcal{H}_2$ is the identity matrix and $\boldsymbol{\Lambda}_k \in \mathcal{H}_2\ \forall k \in \{1,2,3\}$ are the Pauli matrices:

$$\boldsymbol{\Lambda}_1 := \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \ \boldsymbol{\Lambda}_2 := \begin{bmatrix} 0 & -\imath \\ \imath & 0 \end{bmatrix}, \text{ and } \boldsymbol{\Lambda}_3 := \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \tag{7}$$

where $\imath := \sqrt{-1}$.

The state of a bipartite two-qubit quantum system, $\boldsymbol{S}^{\mathrm{AB}} \in \mathcal{H}_2^{\mathrm{A}} \otimes \mathcal{H}_2^{\mathrm{B}}$, can be written in the Fano representation [52,53] as follows

$$\boldsymbol{S}^{\mathrm{AB}}=\frac{1}{4}\Big(\boldsymbol{I}\otimes\boldsymbol{I}+\sum_{k=1}^{3}n_k\,\boldsymbol{\Lambda}_k\otimes\boldsymbol{I}+\sum_{\ell=1}^{3}s_\ell\,\boldsymbol{I}\otimes\boldsymbol{\Lambda}_\ell+\sum_{k,\ell=1}^{3}t_{k\ell}\,\boldsymbol{\Lambda}_k\otimes\boldsymbol{\Lambda}_\ell\Big),\quad(8)$$

where $n_k=\mathbb{E}\{\boldsymbol{\Lambda}_k\otimes\boldsymbol{I}\}$, $s_\ell=\mathbb{E}\{\boldsymbol{I}\otimes\boldsymbol{\Lambda}_\ell\}$ and $t_{k\ell}=\mathbb{E}\{\boldsymbol{\Lambda}_k\otimes\boldsymbol{\Lambda}_\ell\}$ take real values. The marginal quantum states on $\mathcal{H}_2^{\mathrm{A}}$ and $\mathcal{H}_2^{\mathrm{B}}$ are given by

$$\boldsymbol{S}^{\mathrm{A}}=\frac{1}{2}\Big(\boldsymbol{I}+\sum_{k=1}^{3}n_k\,\boldsymbol{\Lambda}_k\Big)\quad\text{and}\quad\boldsymbol{S}^{\mathrm{B}}=\frac{1}{2}\Big(\boldsymbol{I}+\sum_{\ell=1}^{3}s_\ell\,\boldsymbol{\Lambda}_\ell\Big).\quad(9)$$

The marginal states are associated with the Bloch vectors $|n\rangle=[n_1,n_2,n_3]^{\mathrm{T}}$ and $|s\rangle=[s_1,s_2,s_3]^{\mathrm{T}}$, satisfying $\big\||n\rangle\big\|_2\leqslant 1$ and $\big\||s\rangle\big\|_2\leqslant 1$, where $\big\||v\rangle\big\|_2:=\sqrt{\langle v|v\rangle}$ denotes the Euclidean norm. $\boldsymbol{C}$ is the correlation matrix with elements $[\boldsymbol{C}]_{k\ell}=t_{k\ell}-n_k s_\ell$.

An arbitrary 2-dimensional observable $\boldsymbol{X}\in\mathcal{H}_2$ can be written as [2]

$$\boldsymbol{X}=x_0\,\boldsymbol{I}+\sum_{k=1}^{3}x_k\,\boldsymbol{\Lambda}_k\,,\quad(10)$$

where $x_0=\mathrm{tr}\{\boldsymbol{X}\}/2$ and $x_k=\mathrm{tr}\{\boldsymbol{X}\boldsymbol{\Lambda}_k\}/2$, for $k\in\{1,2,3\}$, take real values.

In the following Lemma, we derive an expression of the PCC for 2-dimensional observables.

Lemma 3. *The PCC for two observables, $\boldsymbol{X}=x_0\,\boldsymbol{I}+\sum_{k=1}^{3}x_k\,\boldsymbol{\Lambda}_k\in\mathcal{H}_2^A$ and $\boldsymbol{Y}=y_0\,\boldsymbol{I}+\sum_{\ell=1}^{3}y_\ell\,\boldsymbol{\Lambda}_\ell\in\mathcal{H}_2^B$ on $\boldsymbol{S}^{AB}\in\mathcal{H}_2^A\otimes\mathcal{H}_2^B$, is given by*

$$\mathbb{C}\mathrm{or}\{\boldsymbol{X},\boldsymbol{Y}\}=\frac{\langle\check{x}|\boldsymbol{C}|\check{y}\rangle}{\sqrt{1-\langle\check{x}|n\rangle^2}\sqrt{1-\langle\check{y}|s\rangle^2}}\,,\quad(11)$$

where $|\check{x}\rangle=[\check{x}_1,\check{x}_2,\check{x}_3]^{\mathrm{T}}$ and $|\check{y}\rangle=[\check{y}_1,\check{y}_2,\check{y}_3]^{\mathrm{T}}$, in which $\check{x}_k=x_k/\sqrt{x_1^2+x_2^2+x_3^2}$ and $\check{y}_k=y_k/\sqrt{y_1^2+y_2^2+y_3^2}$.

Proof. See Appendix C. ⊠

In the following Lemma, we derive a condition of complementarity for 2-dimensional observables.

Lemma 4. *Two observables $\boldsymbol{X}_1=x_{1_0}\,\boldsymbol{I}+\sum_{k=1}^{3}x_{1_k}\,\boldsymbol{\Lambda}_k\in\mathcal{H}_2$ and $\boldsymbol{X}_2=x_{2_0}\,\boldsymbol{I}+\sum_{k=1}^{3}x_{2_k}\,\boldsymbol{\Lambda}_k\in\mathcal{H}_2$ are complementary if and only if*

$$\sum_{k=1}^{3}x_{1_k}x_{2_k}=0\,.\quad(12)$$

Proof. See Appendix D. ⊠

Remark 2. When two observables $\boldsymbol{X}_1,\boldsymbol{X}_2\in\mathcal{H}_2$ are unitary and complementary, then they anti-commute [50], i.e.,

$$\big[\boldsymbol{X}_1,\boldsymbol{X}_2\big]_+:=\boldsymbol{X}_1\boldsymbol{X}_2+\boldsymbol{X}_2\boldsymbol{X}_1=0\,.\quad(13)$$

In the following Lemma, we derive a condition for orthogonality for 2-dimensional observables.

Remark 3. Two observables $\boldsymbol{X}_1=x_{1_0}\,\boldsymbol{I}+\sum_{k=1}^{3}x_{1_k}\,\boldsymbol{\Lambda}_k\in\mathcal{H}_2$ and $\boldsymbol{X}_2=x_{2_0}\,\boldsymbol{I}+\sum_{k=1}^{3}x_{2_k}\,\boldsymbol{\Lambda}_k\in\mathcal{H}_2$ are orthogonal if and only if

$$\sum_{k=0}^{3}x_{1_k}x_{2_k}=0\,.\quad(14)$$

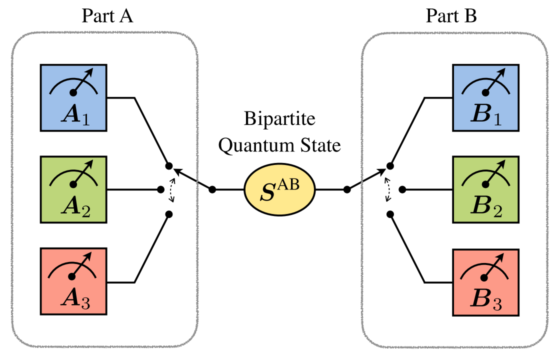


Fig. 1. Schematic representation of the three complementary observables measured on each part of a bipartite quantum state $\boldsymbol{S}^{\mathrm{AB}}\in\mathcal{H}_2^{\mathrm{A}}\otimes\mathcal{H}_2^{\mathrm{B}}$.

3. Entanglement criterion

This section presents an entanglement criterion for quantum systems of two qubits based on the PCC between the measurement outcomes of complementary observables.

3.1. PCC-based entanglement criterion

Consider a bipartite quantum state $\boldsymbol{S}^{\mathrm{AB}}\in\mathcal{H}_2^{\mathrm{A}}\otimes\mathcal{H}_2^{\mathrm{B}}$. Having as a goal to identify entanglement, measurements are performed in a set of three complementary observables: $\boldsymbol{A}_1,\boldsymbol{A}_2,\boldsymbol{A}_3\in\mathcal{H}_2^{\mathrm{A}}$ for part A, and $\boldsymbol{B}_1,\boldsymbol{B}_2,\boldsymbol{B}_3\in\mathcal{H}_2^{\mathrm{B}}$ for part B. For a schematic representation see Fig. 1. The number of measurements corresponds to the maximum number of complementary observables existing in $\mathcal{H}_2$, which is equal to three according to Remark 1.

Theorem 1 *(PCC-based entanglement criterion). A bipartite quantum state $\boldsymbol{S}^{AB}\in\mathcal{H}_2^A\otimes\mathcal{H}_2^B$ is entangled if there exist pairwise complementary observables $\boldsymbol{A}_1,\boldsymbol{A}_2,\boldsymbol{A}_3\in\mathcal{H}_2^A$ and $\boldsymbol{B}_1,\boldsymbol{B}_2,\boldsymbol{B}_3\in\mathcal{H}_2^B$, such that*

$$\sum_{i=1}^{3}\Big|\mathbb{C}\mathrm{or}\{\boldsymbol{A}_i,\boldsymbol{B}_i\}\Big|>1\,.\quad(15)$$

Proof. Based on Lemma 3, we have

$$\begin{aligned}\sum_{i=1}^{3}\Big|\mathbb{C}\mathrm{or}\{\boldsymbol{A}_i,\boldsymbol{B}_i\}\Big|&=\sum_{i=1}^{3}\frac{\big|\langle\check{a}_i|\boldsymbol{C}|\check{b}_i\rangle\big|}{\sqrt{1-\langle\check{a}_i|n\rangle^2}\sqrt{1-\langle\check{b}_i|s\rangle^2}}&(16a)\\&\leqslant\frac{\sum_{i=1}^{3}\big|\langle\check{a}_i|\boldsymbol{C}|\check{b}_i\rangle\big|}{\sqrt{1-\langle n|n\rangle}\sqrt{1-\langle s|s\rangle}}\,,&(16b)\end{aligned}$$

where (16b) follows from the Cauchy-Schwarz inequality, i.e., $\langle\check{a}_i|n\rangle^2\leqslant\big\||\check{a}_i\rangle\big\|_2^2\big\||n\rangle\big\|_2^2=\big\||n\rangle\big\|_2^2=\langle n|n\rangle$, and analogously $\langle\check{b}_i|s\rangle^2\leqslant\langle s|s\rangle\ \forall i\in\{1,2,3\}$. Lemma 4 implies that $\{|\check{a}_1\rangle,|\check{a}_2\rangle,|\check{a}_3\rangle\}$ and $\{|\check{b}_1\rangle,|\check{b}_2\rangle,|\check{b}_3\rangle\}$ are sets of orthonormal vectors. Thus, by introducing the 3×3 orthonormal matrices:

$$\boldsymbol{O}_A=\begin{bmatrix}\langle\check{a}_1|\\\langle\check{a}_2|\\\langle\check{a}_3|\end{bmatrix}\quad\text{and}\quad\boldsymbol{O}_B=\big[\,|\check{b}_1\rangle\quad|\check{b}_2\rangle\quad|\check{b}_3\rangle\,\big]\,,\quad(17)$$

the numerator of the right-hand side of (16b) can be written as

$$\begin{aligned}\sum_{i=1}^{3}\big|\langle\check{a}_i|\boldsymbol{C}|\check{b}_i\rangle\big|&=\sum_{i=1}^{3}\Big|\big[\boldsymbol{O}_A\boldsymbol{C}\boldsymbol{O}_B\big]_{ii}\Big|&(18a)\\&=\mathrm{tr}\,\{\boldsymbol{D}\,\boldsymbol{O}_A\boldsymbol{C}\,\boldsymbol{O}_B\}&(18b)\\&=\mathrm{tr}\{\boldsymbol{U}\boldsymbol{C}\}&(18c)\\&\leqslant\big\|\boldsymbol{C}\big\|_{\mathrm{tr}}\,,&(18d)\end{aligned}$$

where $\boldsymbol{D}$ in (18b) is a diagonal matrix with elements $\left[\boldsymbol{D}\right]_{ii} = 1$ for $\left[\boldsymbol{O}_A \boldsymbol{C} \boldsymbol{O}_B\right]_{ii} \geqslant 0$ and $\left[\boldsymbol{D}\right]_{ii} = -1$ otherwise. $\boldsymbol{U} = \boldsymbol{O}_B \boldsymbol{D} \boldsymbol{O}_A$ in (18c) is a unitary matrix since it is a product of unitary matrices. Inequality (18d) follows from the fact that for unitary operators $\boldsymbol{U}$ we have $\left\|\boldsymbol{C}\right\|_{\text{tr}} = \max_{\boldsymbol{U}}\left\{\text{tr}\left\{\boldsymbol{U}\boldsymbol{C}\right\}\right\}$ (see Corollary 7.4.1.3 in [54]), where $\left\|\boldsymbol{X}\right\|_{\text{tr}} := \sum_i \sigma_i\left\{\boldsymbol{X}\right\}$ denotes the trace norm of a matrix $\boldsymbol{X}$, and $\sigma_i\left\{\boldsymbol{X}\right\}$ are its singular values. Combining (18d) and (16b), we obtain

$$\sum_{i=1}^{3}\left|\,\mathbb{C}\text{or}\left\{\boldsymbol{A}_i, \boldsymbol{B}_i\right\}\right| \leqslant \frac{\left\|\boldsymbol{C}\right\|_{\text{tr}}}{\sqrt{1-\langle n|n\rangle}\sqrt{1-\langle s|s\rangle}} \,. \tag{19}$$

In Theorem 1 of [37] and equivalently in Proposition IV.2 of [34] it was shown that for all separable states we have $\left\|\boldsymbol{C}\right\|_{\text{tr}} \leqslant \sqrt{1-\langle n|n\rangle}\sqrt{1-\langle s|s\rangle}$. So, for every separable state the following inequality holds

$$\sum_{i=1}^{3}\left|\,\mathbb{C}\text{or}\left\{\boldsymbol{A}_i, \boldsymbol{B}_i\right\}\right| \leqslant 1\,, \tag{20}$$

which completes the proof. ⊠

Theorem 1 proves that if for a given quantum state there exist two sets of three pairwise complementary observables violating the inequality (20), then the state must be entangled. The above entanglement criterion is closely connected to the extended cross norm criterion [37] and the covariance matrix criterion [33]. The critical aspect that differentiates the PCC-based (and the MI-based [46]) entanglement criterion from other existing methods is that it provides a unified perspective of statistical correlations in both classical and quantum systems. This result reveals the key role that complementarity plays in quantum systems by allowing a type of correlations with no classical counterpart.

3.2. Application examples

The effectiveness of the PCC-based entanglement criterion in Theorem 1 is illustrated below by considering some examples of separable and entangled $(2 \otimes 2)$-dimensional quantum states.

3.2.1. Product states

Product mixed states, defined as

$$\boldsymbol{S}^{\text{AB}}_{\text{prod}} := \boldsymbol{S}^{\text{A}} \otimes \boldsymbol{S}^{\text{B}} \tag{21}$$

vanish PCC for any set of measured observables,

$$\boldsymbol{S}^{\text{AB}} = \boldsymbol{S}^{\text{AB}}_{\text{prod}} \Rightarrow \sum_{i=1}^{3}\left|\,\mathbb{C}\text{or}\left\{\boldsymbol{A}_i, \boldsymbol{B}_i\right\}\right| = 0\,, \tag{22}$$

since $\mathbb{E}\left\{\boldsymbol{A}_i \otimes \boldsymbol{B}_i\right\} = \mathbb{E}\left\{\boldsymbol{A}_i\right\}\mathbb{E}\left\{\boldsymbol{B}_i\right\}\ \forall i \in \left\{1,2,3\right\}$.

3.2.2. Bell states

Bell states are defined as

$$\boldsymbol{S}^{\text{AB}}_{\text{Bell, k}} := |\phi_k\rangle\langle\phi_k|\ \forall k \in \{1,2,3,4\}\,, \tag{23}$$

with

$$|\phi_1\rangle := \frac{|0\rangle\otimes|0\rangle + |1\rangle\otimes|1\rangle}{\sqrt{2}}\,,\ |\phi_2\rangle := \frac{|0\rangle\otimes|0\rangle - |1\rangle\otimes|1\rangle}{\sqrt{2}}\,,$$
$$|\phi_3\rangle := \frac{|0\rangle\otimes|1\rangle + |1\rangle\otimes|0\rangle}{\sqrt{2}}\,,\ |\phi_4\rangle := \frac{|0\rangle\otimes|1\rangle - |1\rangle\otimes|0\rangle}{\sqrt{2}}\,. \tag{24}$$

For $\boldsymbol{S}^{\text{AB}} = \boldsymbol{S}^{\text{AB}}_{\text{Bell, k}}$ the PCC is maximized when $\boldsymbol{A}_i = \boldsymbol{B}_i = \boldsymbol{\Lambda}_i\ \forall i \in \left\{1,2,3\right\}$,

$$\sum_{i=1}^{3}\left|\,\mathbb{C}\text{or}\left\{\boldsymbol{A}_i, \boldsymbol{B}_i\right\}\right| = 3 \tag{25}$$

for $k \in \{1,2,3,4\}$, since $\mathbb{E}\left\{\boldsymbol{A}_i \otimes \boldsymbol{B}_i\right\} = 1$, $\mathbb{E}\left\{\boldsymbol{A}_i\right\} = \mathbb{E}\left\{\boldsymbol{B}_i\right\} = 0$, and $\mathbb{V}\left\{\boldsymbol{A}_i\right\} = \mathbb{V}\left\{\boldsymbol{B}_i\right\} = 1\ \forall i \in \left\{1,2,3\right\}$.

3.2.3. Bell states through single-qubit quantum channels

Three typical decohering single-qubit quantum channels, $\mathcal{C}_\ell(\boldsymbol{S})$ for $\ell \in \left\{1,2,3\right\}$, are: (i) the bit flip channel $\mathcal{C}_1$; (ii) the bit-phase flip channel $\mathcal{C}_2$; (iii) and the phase flip channel $\mathcal{C}_3$, defined as follows:

$$\mathcal{C}_\ell(\boldsymbol{S}) = \left(1-p\right)\boldsymbol{S} + p\,\boldsymbol{\Lambda}_\ell \boldsymbol{S} \boldsymbol{\Lambda}_\ell\ \forall \ell \in \left\{1,2,3\right\} \tag{26}$$

where $p \in \left[0,1\right]$ is the error probability. Another common quantum channel is the depolarizing channel $\mathcal{C}_{\text{dep}}$, defined as

$$\mathcal{C}_{\text{dep}}(\boldsymbol{S}) = \left(1-p\right)\boldsymbol{S} + \frac{p}{2}\,\boldsymbol{I}\,, \tag{27}$$

where $p \in [0,1]$ is the error probability.

Consider the case where one party of the Bell state $\boldsymbol{S}^{\text{AB}}_{\text{Bell, k}}$ passes through the channels above. The output states are given by

$$\mathcal{C}_\ell\left(\boldsymbol{S}^{\text{AB}}_{\text{Bell, k}}\right) = \left(1-p\right)\boldsymbol{S}^{\text{AB}}_{\text{Bell, k}} + p\left(\boldsymbol{\Lambda}_\ell \otimes \boldsymbol{I}\right)\boldsymbol{S}^{\text{AB}}_{\text{Bell, k}}\left(\boldsymbol{\Lambda}_\ell \otimes \boldsymbol{I}\right) \tag{28}$$

and

$$\mathcal{C}_{\text{dep}}\left(\boldsymbol{S}^{\text{AB}}_{\text{Bell, k}}\right) = \left(1-p\right)\boldsymbol{S}^{\text{AB}}_{\text{Bell, k}} + \frac{p}{2}\left(\boldsymbol{S}^{\text{A}}_{\text{Bell, k}} \otimes \boldsymbol{I}\right), \tag{29}$$

where $\boldsymbol{S}^{\text{A}}_{\text{Bell, k}} = \text{tr}_{\text{B}}\left\{\boldsymbol{S}^{\text{AB}}_{\text{Bell, k}}\right\} = \boldsymbol{I}/2$ corresponds to the marginal Bell state that passes through the channel. The PCC for $\boldsymbol{S}^{\text{AB}} = \mathcal{C}_\ell(\boldsymbol{S}^{\text{AB}}_{\text{Bell, k}})$ when $\boldsymbol{A}_i = \boldsymbol{B}_i = \boldsymbol{\Lambda}_i\ \forall i \in \left\{1,2,3\right\}$ is

$$\sum_{i=1}^{3}\left|\,\mathbb{C}\text{or}\left\{\boldsymbol{A}_i, \boldsymbol{B}_i\right\}\right| = 1 + 2\left|1-2p\right|, \tag{30}$$

and thus the output state in (28) is always entangled apart from the case when $p = 1/2$. The PCC for $\boldsymbol{S}^{\text{AB}} = \mathcal{C}_{\text{dep}}(\boldsymbol{S}^{\text{AB}}_{\text{Bell, k}})$ is

$$\sum_{i=1}^{3}\left|\,\mathbb{C}\text{or}\left\{\boldsymbol{A}_i, \boldsymbol{B}_i\right\}\right| = 3\left(1-p\right). \tag{31}$$

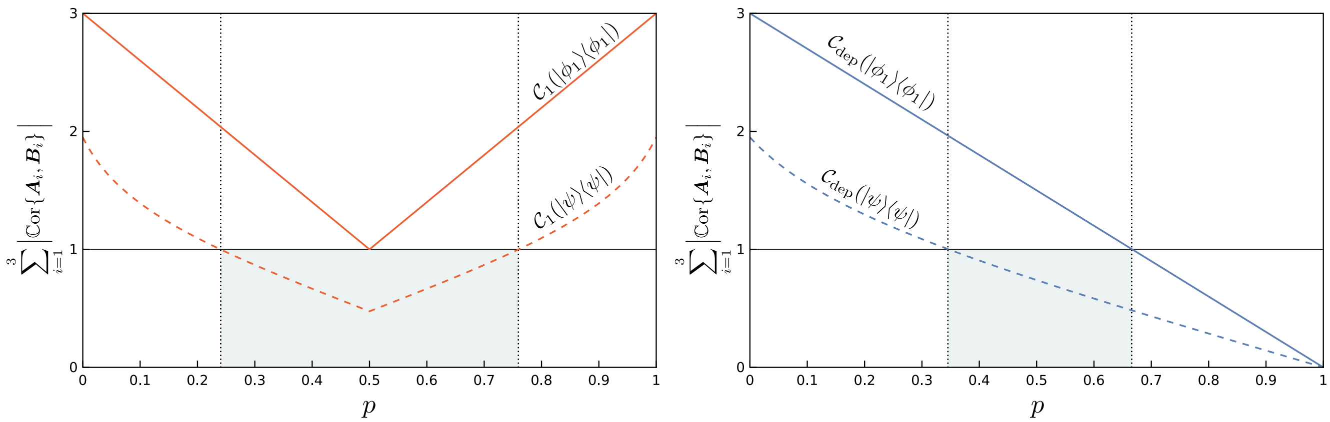
Note that the output state in (29) is known as the Werner state [1], which is separable for $p \geqslant 2/3$ and entangled for $p < 2/3$. Thus, if there is any entanglement left after a Bell state has passed through any of the above four channels, the PCC-based entanglement criterion is always able to identify it. However, it should be noted that not all entangled states can be identified through this method. A specific example is presented in Fig. 2, where we compare the above states with the case of a non-maximally entangled state that passes through the same quantum channels. It can be observed that for certain values of p the entanglement is not identified despite this state is known to be entangled.

3.2.4. Bell-diagonal states

Bell-diagonal states are defined as $\boldsymbol{S}^{\text{AB}}_{\text{BDS}} := \sum_{k=1}^{4} p_k\, \boldsymbol{S}^{\text{AB}}_{\text{Bell, k}}$ where $\sum_{k=1}^{4} p_k = 1$, and their PCC for $\boldsymbol{A}_i = \boldsymbol{B}_i = \boldsymbol{\Lambda}_i\ \forall i \in \{1,2,3\}$ is equal to

$$\sum_{i=1}^{3}\left|\,\mathbb{C}\text{or}\left\{\boldsymbol{A}_i, \boldsymbol{B}_i\right\}\right| = \sum_{k=2}^{4}\left|1-2(p_1+p_k)\right|. \tag{32}$$

Bell-diagonal states are separable when $p_k \leqslant 1/2\ \forall k \in \left\{1,2,3,4\right\}$ [55]. Thus, it can be seen from the above expression that several Bell-diagonal states can saturate the bound (20) in Theorem 1, e.g., $\boldsymbol{S}^{\text{AB}}_{\text{BDS}_{12}} = \left(\boldsymbol{S}^{\text{AB}}_{\text{Bell}_1} + \boldsymbol{S}^{\text{AB}}_{\text{Bell}_2}\right)/2$. In [56], analogous expressions for the value $\sum_{i=1}^{3}\left|\,\mathbb{C}\text{or}\left\{\boldsymbol{A}_i, \boldsymbol{B}_i\right\}\right|$ were derived based on the Fano form of Bell-diagonal states that pass through bit flip, phase flip, and bit-phase flip quantum channels.



(a) Bit flip channel (b) Depolarizing channel

Fig. 2. The PCC is plotted for quantum states passing through a bit flip channel (red lines) in subfigure (a) and a depolarizing channel (blue lines) in subfigure (b). Solid lines correspond to a Bell input state $|\phi_1\rangle\langle\phi_1|$ and the dashed lines to the pure non-maximally entangled input state $|\psi\rangle\langle\psi|$, where $|\psi\rangle = \sqrt{\mu}\,|0\rangle \otimes |0\rangle + \sqrt{1-\mu}\,|1\rangle \otimes |1\rangle$ with $\mu = 0.06$. When the input is the Bell state entanglement can always be identified on the output state, since both blue and red solid lines are above the unity threshold (horizontal black line) for: (a) $p \neq 1/2$ in the case of the bit flip channel; and (b) $p < 2/3$ in the case of the depolarizing channel. On the other hand, when the input state is $|\psi\rangle\langle\psi|$ there is a range of the values of p, represented by the gray area in the subfigures, for which entanglement cannot be identified even though it is present.

4. On the MBM conjecture

The number of measurements needed in the PCC-based entanglement criterion is equal to the one required for reconstructing the density matrix of a $(2\otimes 2)$-dimensional quantum state, a process called quantum tomography [57]. The number of measurements needed for quantum tomography grows exponentially with the number of quantum states [12], which makes it an experimentally very demanding task especially in applications that require to identify entanglement in large-scale quantum networks.

A more practical method to identify entanglement that does not presume knowledge of the density matrix $\boldsymbol{S}^{\mathrm{AB}}$ was proposed by Maccone, Bruß, and Macchiavello in [46]. A bipartite entangled state $\boldsymbol{S}^{\mathrm{AB}} \in \mathcal{H}_d^{\mathrm{A}} \otimes \mathcal{H}_d^{\mathrm{B}}$ is shared between two parts and measurements are performed selected between a pair of complementary observables: $\boldsymbol{A}_1, \boldsymbol{A}_2 \in \mathcal{H}_d^{\mathrm{A}}$ for part A, and $\boldsymbol{B}_1, \boldsymbol{B}_2 \in \mathcal{H}_d^{\mathrm{B}}$ for part B. In [46] it was conjectured that when the inequality $\sum_{i=1}^{2}\left|\mathbb{C}\mathrm{or}\{\boldsymbol{A}_i, \boldsymbol{B}_i\}\right| > 1$ is satisfied the state $\boldsymbol{S}^{\mathrm{AB}}$ is entangled, that we refer below as the MBM conjecture. The MBM conjecture for systems of two qubits is explored in [46], showing that, if true, is able to identify entangled states missed by other entanglement criteria. This method to identify entanglement can be seen as a special case of the PCC-based entanglement criterion, where each party possesses three complementary observables. Recently, the MBM conjecture was proven to be true for pure states and particular $(2\otimes 2)$-dimensional mixed states [58]. The proof of the MBM conjecture for any $(2\otimes 2)$-dimensional quantum state is given as a corollary of Theorem 1.

Corollary 1. *A bipartite quantum state $\boldsymbol{S}^{AB} \in \mathcal{H}_2^A \otimes \mathcal{H}_2^B$ is entangled if there exist complementary observables $\boldsymbol{A}_1, \boldsymbol{A}_2 \in \mathcal{H}_2^A$ and $\boldsymbol{B}_1, \boldsymbol{B}_2 \in \mathcal{H}_2^B$, such that*

$$\sum_{i=1}^{2}\left|\mathbb{C}\mathrm{or}\{\boldsymbol{A}_i, \boldsymbol{B}_i\}\right| > 1\,. \tag{33}$$

Proof. Based on Theorem 1, for any separable state we have

$$\sum_{i=1}^{2}\left|\mathbb{C}\mathrm{or}\{\boldsymbol{A}_i, \boldsymbol{B}_i\}\right| \leqslant \sum_{i=1}^{3}\left|\mathbb{C}\mathrm{or}\{\boldsymbol{A}_i, \boldsymbol{B}_i\}\right| \leqslant 1\,, \tag{34}$$

which completes the proof. ⊠

The MBM conjecture has already been employed for entanglement identification in several works [56,58–63], so its validation, i.e., Corollary 1, provides a solid basis on the results of those works.

In higher, but finite, dimensional states, we show that the MBM conjecture is violated, and thus propose an appropriate generalization. In particular, consider a $(d\otimes d)$-dimensional separable quantum state

$$\tilde{\boldsymbol{S}}_{\mathrm{sep}}^{\mathrm{AB}} := \sum_{k=0,1}\frac{\boldsymbol{\Pi}_{e_k}\otimes\boldsymbol{\Pi}_{e_k} + \boldsymbol{\Pi}_{h_k}\otimes\boldsymbol{\Pi}_{h_k}}{4}\,, \tag{35}$$

where $\boldsymbol{\Pi}_{e_k} = |e_k\rangle\langle e_k|$ and $\boldsymbol{\Pi}_{h_k} = |h_k\rangle\langle h_k|$. The mutually unbiased orthonormal bases $\{|e_k\rangle\}_{k=0}^{d-1}$ and $\{|h_k\rangle\}_{k=0}^{d-1}$ are connected through the discrete Fourier transform, $|h_\ell\rangle = \frac{1}{\sqrt{d}}\sum_{k=0}^{d-1} w^{k\ell}|e_k\rangle$ with $w = e^{2\pi\imath/d}$. Consider also the d-dimensional complementary observables, given by:

$$\boldsymbol{A}_1 = \boldsymbol{B}_1 = \boldsymbol{\Pi}_{e_0} - \boldsymbol{\Pi}_{e_1} + \epsilon\sum_{k=2}^{d-1} k\,\boldsymbol{\Pi}_{e_k}\,, \tag{36a}$$

$$\boldsymbol{A}_2 = \boldsymbol{B}_2 = \boldsymbol{\Pi}_{h_0} - \boldsymbol{\Pi}_{h_1} + \epsilon\sum_{k=2}^{d-1} k\,\boldsymbol{\Pi}_{h_k}\,, \tag{36b}$$

with $\epsilon \in \mathcal{R}/\{0\}$. Note that the expressions $\epsilon\sum_{k=2}^{d-1} k\,\boldsymbol{\Pi}_{e_k}$ and $\epsilon\sum_{k=2}^{d-1} k\,\boldsymbol{\Pi}_{h_k}$ are employed in order the eigenvalues of the observables to be non-degenerate. In the limit of $\epsilon \to 0$ we retrieve (see Appendix E): $\mathbb{E}\{\boldsymbol{A}_i\} = \mathbb{E}\{\boldsymbol{B}_i\} = 0$, $\mathbb{E}\{\boldsymbol{A}_i\otimes\boldsymbol{B}_i\} = 1/2$, and $\mathbb{E}\{(\boldsymbol{A}_i)^2\} = \mathbb{E}\{(\boldsymbol{B}_i)^2\} = 1/2 + 1/d$ for $i \in \{1,2\}$. Using the results above it follows that

$$\boldsymbol{S}^{\mathrm{AB}} = \tilde{\boldsymbol{S}}_{\mathrm{sep}}^{\mathrm{AB}} \Rightarrow \sum_{i=1}^{2}\left|\mathbb{C}\mathrm{or}\{\boldsymbol{A}_i, \boldsymbol{B}_i\}\right| = 2 - \frac{4}{2+d}\,, \tag{37}$$

which violates the MBM Conjecture for $d \geqslant 3$. Under thorough numerical investigation we have not found separable states in $\mathcal{H}_d^{\mathrm{A}} \otimes \mathcal{H}_d^{\mathrm{B}}$ for which $\left|\mathbb{C}\mathrm{or}\{\boldsymbol{A}_1, \boldsymbol{B}_1\}\right| + \left|\mathbb{C}\mathrm{or}\{\boldsymbol{A}_2, \boldsymbol{B}_2\}\right|$ surpasses the right-hand side of (37),[5] therefore we introduce the following conjecture.

[5] The random separable states were generated following the method described in [64]. The random complementary observables were created by randomly assigning eigenvalues to the spectral decompositions of two observables that have mutually unbiased orthonormal bases as in (5).

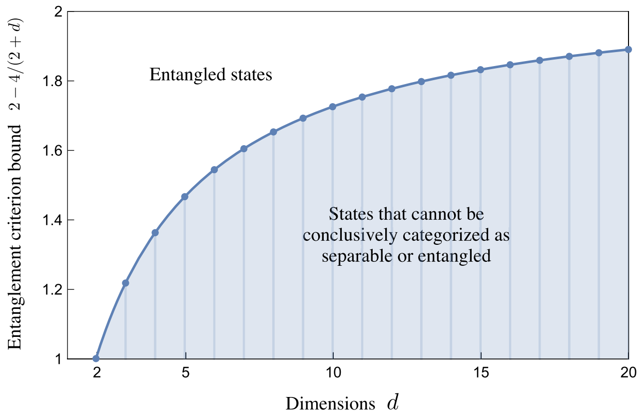


Fig. 3. The conjectured entanglement identification method in (38) is presented for $(d \otimes d)$-dimensional states as a function of d. The dark blue line indicates the bound above which a quantum state is conjectured to be entangled. The light blue region, below the bound, corresponds to states where this criterion is inconclusive regarding their separability. It is apparent that the ability to identify entanglement through this method diminishes as the dimensions of the Hilbert space increase.

Conjecture. *A bipartite quantum state $\boldsymbol{S}^{AB} \in \mathcal{H}_d^A \otimes \mathcal{H}_d^B$ is entangled if there exist complementary observables $\boldsymbol{A}_1, \boldsymbol{A}_2 \in \mathcal{H}_d^A$ and $\boldsymbol{B}_1, \boldsymbol{B}_2 \in \mathcal{H}_d^B$, such that*

$$\sum_{i=1}^{2} \left| \mathbb{C}\mathrm{or}\left\{ \boldsymbol{A}_i, \boldsymbol{B}_i \right\} \right| > 2 - \frac{4}{2+d}\,. \tag{38}$$

Inequality (38) implies that the ability to identify entanglement through the PCC diminishes with the dimension of the underlying Hilbert space, as also shown in Fig. 3. It is worth mentioning that the dependence on d in (38) is not surprising since an analogous dependence is also present in the MI-based entanglement criterion [46], which is also based on correlations between the outcomes of complementary observables. Conditioned on the validity of the conjecture, identifying high-dimensional entanglement through (38) has the same merits as the method discussed in Corollary 1, as the density matrix of the quantum state is not required to be known.

For the sake of completeness, the case of infinite-dimensional quantum states can be analyzed as well, even though it goes beyond the scope of the MBM conjecture. In Appendix F, a family of separable Gaussian states is considered for which it is shown that the expression $\left| \mathbb{C}\mathrm{or}\left\{ \boldsymbol{A}_1, \boldsymbol{B}_1 \right\} \right| + \left| \mathbb{C}\mathrm{or}\left\{ \boldsymbol{A}_2, \boldsymbol{B}_2 \right\} \right|$ becomes greater than one. This result implies that this type of entanglement identification method is not appropriate for infinite-dimensional quantum states.

5. Strengthened Bell inequalities

In this section generalized strengthened Bell inequalities are derived, based on the covariance and the PCC.

5.1. Bell inequalities

Consider a quantum state $\boldsymbol{S}^{\mathrm{AB}} \in \mathcal{H}_2^{\mathrm{A}} \otimes \mathcal{H}_2^{\mathrm{B}}$ and two pairs of observables $\boldsymbol{A}_1, \boldsymbol{A}_2 \in \mathcal{H}_2^{\mathrm{A}}$ and $\boldsymbol{B}_1, \boldsymbol{B}_2 \in \mathcal{H}_2^{\mathrm{B}}$ with dichotomic outcomes ± 1. The CHSH inequality [6]:

$$\mathbb{E}\left\{ \boldsymbol{A}_1 \otimes \boldsymbol{B}_1 \right\} + \mathbb{E}\left\{ \boldsymbol{A}_1 \otimes \boldsymbol{B}_2 \right\} + \mathbb{E}\left\{ \boldsymbol{A}_2 \otimes \boldsymbol{B}_1 \right\} - \mathbb{E}\left\{ \boldsymbol{A}_2 \otimes \boldsymbol{B}_2 \right\} \leqslant 2 \tag{39}$$

is satisfied for any so-called local-realistic theory. It has been shown that the violation of (39) is a sufficient (but not necessary) condition to identify entanglement in a quantum state [15,16]. Note that the CHSH inequality belongs to the family of Bell inequalities [5] (see [65–68] for an analysis of the assumptions and the implications of the Bell inequalities).

Recently, a generalization of (39) was derived in [69] considering the covariance as

$$\mathbb{C}\mathrm{ov}\left\{ \boldsymbol{A}_1, \boldsymbol{B}_1 \right\} + \mathbb{C}\mathrm{ov}\left\{ \boldsymbol{A}_1, \boldsymbol{B}_2 \right\} + \mathbb{C}\mathrm{ov}\left\{ \boldsymbol{A}_2, \boldsymbol{B}_1 \right\} - \mathbb{C}\mathrm{ov}\left\{ \boldsymbol{A}_2, \boldsymbol{B}_2 \right\} \leqslant \frac{16}{7}\,. \tag{40}$$

Considering the PCC, a generalization of (39) was derived in [70] as

$$\mathbb{C}\mathrm{or}\left\{ \boldsymbol{A}_1, \boldsymbol{B}_1 \right\} + \mathbb{C}\mathrm{or}\left\{ \boldsymbol{A}_1, \boldsymbol{B}_2 \right\} + \mathbb{C}\mathrm{or}\left\{ \boldsymbol{A}_2, \boldsymbol{B}_1 \right\} - \mathbb{C}\mathrm{or}\left\{ \boldsymbol{A}_2, \boldsymbol{B}_2 \right\} \leqslant \frac{5}{2}\,. \tag{41}$$

As it was shown in [69], (40) serves as a device-independent witness for the shared randomness in a Bell experiment. Contrary to (39), (40) and (41) are nonlinear, a property that can offer efficiency in the identification of quantum correlations in quantum networks, as discussed in [71–73].

5.2. Strengthened Bell inequalities

A tighter version of (39), known as the strengthened CHSH inequality, asserts that for all separable $(2 \otimes 2)$-dimensional quantum states and complementary observables $\boldsymbol{A}_1, \boldsymbol{A}_2 \in \mathcal{H}_2^{\mathrm{A}}$ and $\boldsymbol{B}_1, \boldsymbol{B}_2 \in \mathcal{H}_2^{\mathrm{B}}$, with dichotomic outcomes ± 1, the following inequality is satisfied [47–49]:

$$\mathbb{E}\left\{ \boldsymbol{A}_1 \otimes \boldsymbol{B}_1 \right\} + \mathbb{E}\left\{ \boldsymbol{A}_1 \otimes \boldsymbol{B}_2 \right\} + \mathbb{E}\left\{ \boldsymbol{A}_2 \otimes \boldsymbol{B}_1 \right\} - \mathbb{E}\left\{ \boldsymbol{A}_2 \otimes \boldsymbol{B}_2 \right\} \leqslant \sqrt{2}\,. \tag{42}$$

The violation of (42) constitutes a sufficient condition for entanglement. Thus, on the one hand (42) is more restrictive than (39) for the considered observables, but on the other hand it has a smaller violation threshold.

Below, we derive a strengthened CHSH inequality based on the covariance of the observables.

Theorem 2. *For all bipartite separable quantum states $\boldsymbol{S}_{\mathrm{sep}}^{AB} \in \mathcal{H}_2^A \otimes \mathcal{H}_2^B$ measured by complementary observables $\boldsymbol{A}_1, \boldsymbol{A}_2 \in \mathcal{H}_2^A$ and $\boldsymbol{B}_1, \boldsymbol{B}_2 \in \mathcal{H}_2^B$, with dichotomic outcomes ± 1, the following inequality is satisfied*

$$\mathbb{C}\mathrm{ov}\left\{ \boldsymbol{A}_1, \boldsymbol{B}_1 \right\} + \mathbb{C}\mathrm{ov}\left\{ \boldsymbol{A}_1, \boldsymbol{B}_2 \right\} + \mathbb{C}\mathrm{ov}\left\{ \boldsymbol{A}_2, \boldsymbol{B}_1 \right\} - \mathbb{C}\mathrm{ov}\left\{ \boldsymbol{A}_2, \boldsymbol{B}_2 \right\} \leqslant \sqrt{2}\,. \tag{43}$$

Proof. Based on Lemma 2 the observables $\boldsymbol{A}_1, \boldsymbol{A}_2, \boldsymbol{B}_1$ and $\boldsymbol{B}_2$ are unitary and pairwisely orthogonal. Due to Lemma 4 and Remark 3, we know that for the observables $\boldsymbol{B}_1 = b_{1_0}\boldsymbol{I} + \sum_{k=1}^{3} b_{1_k}\boldsymbol{A}_k$ and $\boldsymbol{B}_2 = b_{2_0}\boldsymbol{I} + \sum_{k=1}^{3} b_{2_k}\boldsymbol{A}_k$, we have $b_{1_0} = b_{2_0} = 0$, and thus $\boldsymbol{B}_i^2 = \sum_{k=1}^{3} b_{i_k}^2 \boldsymbol{I} + 2b_{i_0}\sum_{k=1}^{3} b_{i_k}\boldsymbol{A}_k$ with $\sum_{k=1}^{3} b_{i_k}^2 = 1\ \forall i \in \left\{1,2\right\}$. Let us define the orthogonal observables $\boldsymbol{B}_+ := \boldsymbol{B}_1 + \boldsymbol{B}_2$ and $\boldsymbol{B}_- := \boldsymbol{B}_1 - \boldsymbol{B}_2$, which, based on Lemma 4, are complementary as $\sum_{k=1}^{3}\left(b_{1_k} + b_{2_k}\right)\left(b_{1_k} - b_{2_k}\right) = \sum_{k=1}^{3}\left(b_{1_k}^2 - b_{2_k}^2\right) = 0$. Then, using Corollary 1, we obtain

$$1 \geqslant \left| \mathbb{C}\mathrm{or}\left\{ \boldsymbol{A}_1, \boldsymbol{B}_+ \right\} \right| + \left| \mathbb{C}\mathrm{or}\left\{ \boldsymbol{A}_2, \boldsymbol{B}_- \right\} \right| \tag{44a}$$

$$= \left| \frac{\mathbb{E}\left\{\boldsymbol{A}_1 \otimes \boldsymbol{B}_1\right\} - \mathbb{E}\left\{\boldsymbol{A}_1\right\}\mathbb{E}\left\{\boldsymbol{B}_1\right\} + \mathbb{E}\left\{\boldsymbol{A}_1 \otimes \boldsymbol{B}_2\right\} - \mathbb{E}\left\{\boldsymbol{A}_1\right\}\mathbb{E}\left\{\boldsymbol{B}_2\right\}}{\sqrt{\mathbb{V}\left\{\boldsymbol{A}_1\right\}\mathbb{V}\left\{\boldsymbol{B}_+\right\}}} \right| + \left| \frac{\mathbb{E}\left\{\boldsymbol{A}_2 \otimes \boldsymbol{B}_1\right\} - \mathbb{E}\left\{\boldsymbol{A}_2\right\}\mathbb{E}\left\{\boldsymbol{B}_1\right\} - \mathbb{E}\left\{\boldsymbol{A}_2 \otimes \boldsymbol{B}_2\right\} + \mathbb{E}\left\{\boldsymbol{A}_2\right\}\mathbb{E}\left\{\boldsymbol{B}_2\right\}}{\sqrt{\mathbb{V}\left\{\boldsymbol{A}_2\right\}\mathbb{V}\left\{\boldsymbol{B}_-\right\}}} \right|. \tag{44b}$$

Taking into account Remark 2, the observables $\boldsymbol{B}_1$ and $\boldsymbol{B}_2$ anti-commute, i.e., $\left[\boldsymbol{B}_1, \boldsymbol{B}_2\right]_+ = 0$, thus leading to $\boldsymbol{B}_\pm^2 = \left(\boldsymbol{B}_1 \pm \boldsymbol{B}_2\right)^2 = \boldsymbol{B}_1^2 + \boldsymbol{B}_2^2 \pm \left[\boldsymbol{B}_1, \boldsymbol{B}_2\right]_+ = 2\boldsymbol{I}$. Then, by noting that $\mathbb{V}\left\{\boldsymbol{A}_i\right\} = \mathbb{E}\left\{\boldsymbol{A}_i^2\right\} - \mathbb{E}\left\{\boldsymbol{A}_i\right\}^2 \leqslant 1\ \forall i \in \{1,2\}$ and $\mathbb{V}\left\{\boldsymbol{B}_\pm\right\} = \mathbb{E}\left\{\boldsymbol{B}_\pm^2\right\} - \mathbb{E}\left\{\boldsymbol{B}_\pm\right\}^2 \leqslant 2$, we obtain

$$1 \geqslant \left| \frac{\mathbb{E}\{\boldsymbol{A}_1 \otimes \boldsymbol{B}_1\} - \mathbb{E}\{\boldsymbol{A}_1\}\mathbb{E}\{\boldsymbol{B}_1\} + \mathbb{E}\{\boldsymbol{A}_1 \otimes \boldsymbol{B}_2\} - \mathbb{E}\{\boldsymbol{A}_1\}\mathbb{E}\{\boldsymbol{B}_2\}}{\sqrt{2}} \right| + \left| \frac{\mathbb{E}\{\boldsymbol{A}_2 \otimes \boldsymbol{B}_1\} - \mathbb{E}\{\boldsymbol{A}_2\}\mathbb{E}\{\boldsymbol{B}_1\} - \mathbb{E}\{\boldsymbol{A}_2 \otimes \boldsymbol{B}_2\} + \mathbb{E}\{\boldsymbol{A}_2\}\mathbb{E}\{\boldsymbol{B}_2\}}{\sqrt{2}} \right| \tag{45a}$$

$$\geqslant \frac{1}{\sqrt{2}} \Big(\mathbb{C}\mathrm{ov}\{\boldsymbol{A}_1, \boldsymbol{B}_1\} + \mathbb{C}\mathrm{ov}\{\boldsymbol{A}_1, \boldsymbol{B}_2\} + \mathbb{C}\mathrm{ov}\{\boldsymbol{A}_2, \boldsymbol{B}_1\} - \mathbb{C}\mathrm{ov}\{\boldsymbol{A}_2, \boldsymbol{B}_2\} \Big), \tag{45b}$$

which completes the proof. ⊠

Below, we also derive a strengthened CHSH inequality based on the PCC of the observables.

Theorem 3. *For all bipartite separable quantum states $\boldsymbol{S}_{\mathrm{sep}}^{AB} \in \mathcal{H}_2^A \otimes \mathcal{H}_2^B$ measured by complementary observables $\boldsymbol{A}_1, \boldsymbol{A}_2 \in \mathcal{H}_2^A$ and $\boldsymbol{B}_1, \boldsymbol{B}_2 \in \mathcal{H}_2^B$, the following inequality is satisfied*

$$\mathbb{C}\mathrm{or}\{\boldsymbol{A}_1, \boldsymbol{B}_1\} + \mathbb{C}\mathrm{or}\{\boldsymbol{A}_1, \boldsymbol{B}_2\} + \mathbb{C}\mathrm{or}\{\boldsymbol{A}_2, \boldsymbol{B}_1\} - \mathbb{C}\mathrm{or}\{\boldsymbol{A}_2, \boldsymbol{B}_2\} \leqslant \sqrt{2}. \tag{46}$$

Proof. Based on Lemma 3 the left-hand side of (46), denoted as γ, can be written as

$$\gamma = \sum_{i=1}^{2} \frac{\langle \check{a}_1 | \boldsymbol{C} | \check{b}_i \rangle}{\sqrt{1 - \langle \check{a}_1 | n \rangle^2} \sqrt{1 - \langle \check{b}_i | s \rangle^2}} + \sum_{i=1}^{2} \frac{(-1)^{i-1} \langle \check{a}_2 | \boldsymbol{C} | \check{b}_i \rangle}{\sqrt{1 - \langle \check{a}_2 | n \rangle^2} \sqrt{1 - \langle \check{b}_i | s \rangle^2}}, \tag{47}$$

where, according to Lemma 4, we have $\langle \check{a}_i | \check{a}_j \rangle = \delta_{ij}$ and $\langle \check{b}_i | \check{b}_j \rangle = \delta_{ij}$ $\forall i, j \in \{1, 2\}$. In order to simplify (47) we set $\langle a_+ | = \langle \check{a}_1 | / \sqrt{1 - \langle \check{a}_1 | n \rangle^2}$, $\langle a_- | = \langle \check{a}_2 | / \sqrt{1 - \langle \check{a}_2 | n \rangle^2}$, $|b_+\rangle = \sum_{i=1}^{2} |\check{b}_i\rangle / \sqrt{1 - \langle \check{b}_i | s \rangle^2}$, and $|b_-\rangle = \sum_{i=1}^{2} (-1)^{i-1} |\check{b}_i\rangle / \sqrt{1 - \langle \check{b}_i | s \rangle^2}$, thus obtaining

$$\gamma = \langle a_+ | \boldsymbol{C} | b_+ \rangle + \langle a_- | \boldsymbol{C} | b_- \rangle. \tag{48}$$

Let us define the 2×3 and 3×2 matrices:

$$\boldsymbol{G} = \begin{bmatrix} \langle a_+ | \\ \langle a_- | \end{bmatrix} \quad \text{and} \quad \boldsymbol{J} = \begin{bmatrix} |b_+\rangle & |b_-\rangle \end{bmatrix}, \tag{49}$$

from which it follows that

$$\gamma = \mathrm{tr}\{\boldsymbol{G}\boldsymbol{C}\boldsymbol{J}\} = \mathrm{tr}\{\boldsymbol{C}\boldsymbol{L}\}, \tag{50}$$

where $\boldsymbol{L} = \boldsymbol{J}\boldsymbol{G} = |b_+\rangle\langle a_+| + |b_-\rangle\langle a_-|$.

Using von Neumann's trace theorem (see Theorem 8.7.6 in [54]), we obtain

$$\gamma = \mathrm{tr}\{\boldsymbol{C}\boldsymbol{L}\} \leqslant \sum_{i=1}^{3} \sigma_i\{\boldsymbol{C}\} \sigma_i\{\boldsymbol{L}\} \leqslant \sigma_1\{\boldsymbol{L}\} \left\| \boldsymbol{C} \right\|_{\mathrm{tr}}, \tag{51}$$

where $\sigma_i\{\cdot\}$ denotes the i-th singular value arranged in a decreasing order, i.e., $\sigma_1\{\cdot\} \geqslant \sigma_2\{\cdot\} \geqslant \sigma_3\{\cdot\}$. By definition $\sigma_1\{\boldsymbol{L}\} = \sqrt{\lambda_1\{\boldsymbol{L}^\dagger \boldsymbol{L}\}}$, where $\lambda_1\{\boldsymbol{L}^\dagger \boldsymbol{L}\}$ denotes the largest eigenvalue of the positive semidefinite matrix $\boldsymbol{L}^\dagger \boldsymbol{L}$. In the orthonormal basis $\{|\check{a}_1\rangle, |\check{a}_2\rangle, |\check{a}_3\rangle\}$ the matrix $\boldsymbol{L}^\dagger \boldsymbol{L}$ can be written as

$$\boldsymbol{L}^\dagger \boldsymbol{L} = \boldsymbol{M}\boldsymbol{K}\boldsymbol{M}, \tag{52}$$

with

$$\boldsymbol{M} = \begin{bmatrix} \frac{1}{\sqrt{1 - \langle \check{a}_1 | n \rangle^2}} & 0 & 0 \\ 0 & \frac{1}{\sqrt{1 - \langle \check{a}_2 | n \rangle^2}} & 0 \\ 0 & 0 & 0 \end{bmatrix} \tag{53}$$

and

$$\boldsymbol{K} = \begin{bmatrix} \langle b_+ | b_+ \rangle & \langle b_+ | b_- \rangle & 0 \\ \langle b_- | b_+ \rangle & \langle b_- | b_- \rangle & 0 \\ 0 & 0 & 0 \end{bmatrix}. \tag{54}$$

Based on Theorem 5.6.9 in [54], we have

$$\lambda_1\{\boldsymbol{M}\boldsymbol{K}\boldsymbol{M}\} \leqslant \left\| \boldsymbol{M}\boldsymbol{K}\boldsymbol{M} \right\|_2, \tag{55}$$

where $\left\| \boldsymbol{X} \right\|_2 := \max_{\| |v\rangle \|_2 = 1} \left\| \boldsymbol{X} |v\rangle \right\|_2 = \sigma_1\{\boldsymbol{X}\}$ is the spectral norm. Matrix norms are submultiplicative, which implies that

$$\left\| \boldsymbol{M}\boldsymbol{K}\boldsymbol{M} \right\|_2 \leqslant \left\| \boldsymbol{M} \right\|_2 \left\| \boldsymbol{K} \right\|_2 \left\| \boldsymbol{M} \right\|_2. \tag{56}$$

$\boldsymbol{M}$ and $\boldsymbol{K}$ are positive semidefinite matrices, therefore

$$\left\| \boldsymbol{M} \right\|_2 = \lambda_1\{\boldsymbol{M}\}, \tag{57a}$$

$$\left\| \boldsymbol{K} \right\|_2 = \lambda_1\{\boldsymbol{K}\}. \tag{57b}$$

By using $\langle \check{a}_i | n \rangle^2 \leqslant \langle n | n \rangle$ and $\langle \check{b}_i | s \rangle^2 \leqslant \langle s | s \rangle$ for $i \in \{1, 2\}$, we have

$$\lambda_1\{\boldsymbol{M}\} = \max\left\{ \frac{1}{\sqrt{1 - \langle \check{a}_1 | n \rangle^2}}, \frac{1}{\sqrt{1 - \langle \check{a}_2 | n \rangle^2}} \right\} \leqslant \frac{1}{\sqrt{1 - \langle n | n \rangle}}, \tag{58a}$$

$$\lambda_1\{\boldsymbol{K}\} = \max\left\{ \frac{2}{1 - \langle \check{b}_1 | n \rangle^2}, \frac{2}{1 - \langle \check{b}_2 | n \rangle^2} \right\} \leqslant \frac{2}{1 - \langle s | s \rangle}. \tag{58b}$$

Combining (55) – (58), $\sigma_1\{\boldsymbol{L}\}$ is upper-bounded as follows:

$$\sigma_1\{\boldsymbol{L}\} \leqslant \frac{\sqrt{2}}{\sqrt{1 - \langle n | n \rangle} \sqrt{1 - \langle s | s \rangle}}, \tag{59}$$

and thus

$$\gamma \leqslant \frac{\sqrt{2} \left\| \boldsymbol{C} \right\|_{\mathrm{tr}}}{\sqrt{1 - \langle n | n \rangle} \sqrt{1 - \langle s | s \rangle}}. \tag{60}$$

Utilizing the fact that for all separable states the condition $\left\| \boldsymbol{C} \right\|_{\mathrm{tr}} \leqslant \sqrt{1 - \langle n | n \rangle} \sqrt{1 - \langle s | s \rangle}$ is satisfied [34,37], we conclude that

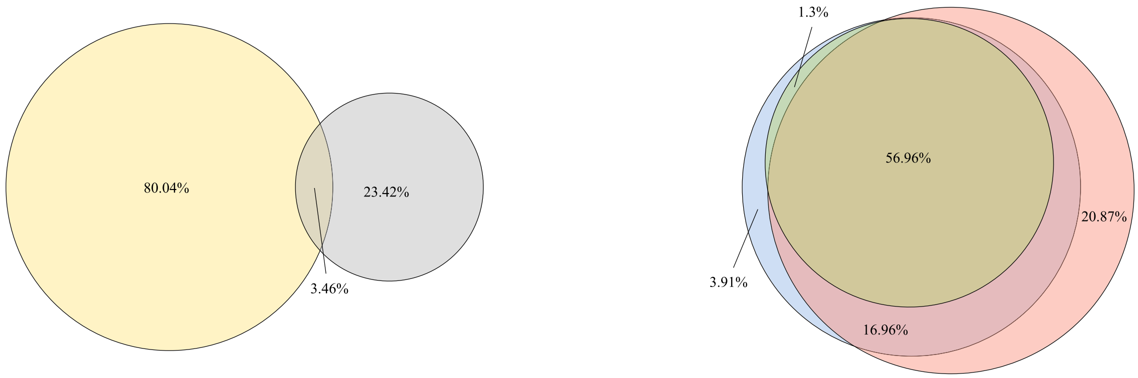
$$\mathbb{C}\mathrm{or}\{\boldsymbol{A}_1, \boldsymbol{B}_1\} + \mathbb{C}\mathrm{or}\{\boldsymbol{A}_1, \boldsymbol{B}_2\} + \mathbb{C}\mathrm{or}\{\boldsymbol{A}_2, \boldsymbol{B}_1\} - \mathbb{C}\mathrm{or}\{\boldsymbol{A}_2, \boldsymbol{B}_2\} \leqslant \sqrt{2}, \tag{61}$$

which completes the proof. ⊠

Inequality (46) is a more general formulation of (43) since it only requires the observables to be complementary. All three strengthened CHSH inequalities can identify entanglement through their violation.

In Fig. 4 we consider 10^6 randomly created entangled quantum states (see footnote 5 regarding the generation of those random states) and a fixed set of observables: $\boldsymbol{A}_1 = \boldsymbol{B}_1 = \boldsymbol{\Lambda}_1$ and $\boldsymbol{A}_2 = \boldsymbol{B}_2 = \boldsymbol{\Lambda}_2$. Using Venn diagrams we compare the effectiveness of the four entanglement criteria discussed in this paper, i.e., the criterion in (33) and the violation of the three strengthened CHSH inequalities in (42), (43), and (46). With that specific set of observables 0.79% of the entangled states were able to be identified from at least one of the four methods.[6] Considering the set of all identified states, in Fig. 4 (a) we represent in yellow the percentage of states that were identified using (33) and with gray the ones that were identified by the violation of at least one of the three strengthened CHSH inequalities. In Fig. 4 (b) we provide a more detailed representation of the gray-colored set of states. It can be seen that the states identified by the violation of (43), represented in green, is a subset of the states identified by the violation of (46), represented in blue. With red are represented the states that are identified

[6] The percentage of identified entangled states can be significantly increased if we perform an optimization over the set of observables, as shown in [46].



(a) Entangled states identified by any method

(b) Entangled states identified by the violation of at least one of the strengthened CHSH inequalities

Fig. 4. Comparison among the four entanglement identification methods discussed in this paper is presented through Venn diagrams, i.e., the criterion in (33) and the violation of the three strengthened CHSH inequalities in (42), (43), and (46). We consider 10^6 randomly created entangled quantum states and a fixed set of observables: $\boldsymbol{A}_1 = \boldsymbol{B}_1 = \boldsymbol{\Lambda}_1$ and $\boldsymbol{A}_2 = \boldsymbol{B}_2 = \boldsymbol{\Lambda}_2$. For this particular set of observables 0.79% of the entangled states are identified by at least one of the four methods. From the total number of entangled states that are identified by any method we represent in subfigure (a) with yellow the ones that (33) is identifying and with gray the ones that are identified by the violation of at least one of the strengthened CHSH inequalities. In subfigure (b) we break down the gray-colored set of subfigure (a) into the contribution of each strengthened CHSH inequality. In particular, with red we represent the states that are identified due to the violation of (42), with green the corresponding states due to the violation of (43), and with blue the corresponding states due to the violation of (46).

from the violation of (42), which is a set that partially overlaps with both of the previous sets. The fact that (42) is a linear CHSH inequality while (43) and (46) are nonlinear, explains the partial overlap of their corresponding sets. On the other hand, it is numerically evident that the violation of (46) implies the violation of (43). This is not surprising as the left-hand side of both inequalities, has to exceed the same threshold to identify entanglement. Taking into account that the PCC of two observables for a given state is by definition the normalized covariance of the same system [see (2)], one can consider the special case where the variances of all four observables are equal in value. For that case, the value of the variance, which is always in the range $[0, 1]$, is multiplied with $\sqrt{2}$, and thus decreasing the threshold. So, inequality (46) is easier to be violated than (43).

6. Conclusion

In this paper we showed how the classical method of assessing correlations through the PCC can be extended to quantum systems, providing a new perspective on the characterization of non-classical correlations. Specifically, we focused on how the property of entanglement can be identified.

We derived an entanglement criterion that is able to identify entanglement through the PCC of the measurement outcomes of complementary observables for quantum systems of two qubits. This criterion was then used to assess a previously proposed conjecture [46], which was indeed found to be true for the case of qubits, but violated for higher-dimensional quantum states (for which an appropriate modification is proposed). We also derived new strengthened CHSH inequalities, in terms of the covariance and the PCC of the corresponding observables, which can also be used as entanglement criteria.

The results of this work make evident that the critical aspect that differentiates quantum correlations from classical ones is ascribed to the complementarity of the properties measured by each party.

CRediT authorship contribution statement

Spyros Tserkis: Writing – review & editing, Writing – original draft, Methodology. **Syed M. Assad:** Writing – review & editing, Writing – original draft, Methodology. **Andrea Conti:** Writing – review & editing, Writing – original draft, Methodology. **Moe Z. Win:** Writing – review & editing, Writing – original draft, Supervision, Methodology.

Declaration of competing interest

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Data availability

No data was used for the research described in the article.

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Appendix A. Proof of Lemma 1

Given a quantum state $\boldsymbol{S}^{\mathrm{AB}} \in \mathcal{H}_d^{\mathrm{A}} \otimes \mathcal{H}_d^{\mathrm{B}}$, we obtain: $\mathbb{E}\{\check{\boldsymbol{X}}\} = \alpha_x \mathbb{E}\{\boldsymbol{X}\} + \beta_x$, $\mathbb{E}\{\check{\boldsymbol{Y}}\} = \alpha_y \mathbb{E}\{\boldsymbol{Y}\} + \beta_y$, $\mathbb{E}\{\check{\boldsymbol{X}} \otimes \check{\boldsymbol{Y}}\} = \alpha_x\alpha_y \mathbb{E}\{\boldsymbol{X} \otimes \boldsymbol{Y}\} + \alpha_x\beta_y \mathbb{E}\{\boldsymbol{X}\} + \alpha_y\beta_x \mathbb{E}\{\boldsymbol{Y}\} + \beta_x\beta_y$, $\mathbb{V}\{\check{\boldsymbol{X}}\} = \alpha_x^2 \mathbb{V}\{\boldsymbol{X}\}$, and $\mathbb{V}\{\check{\boldsymbol{Y}}\} = \alpha_y^2 \mathbb{V}\{\boldsymbol{Y}\}$. So, the PCC is $\mathbb{C}\mathrm{or}\{\check{\boldsymbol{X}}, \check{\boldsymbol{Y}}\} = \frac{\alpha_x\alpha_y}{|\alpha_x||\alpha_y|} \mathbb{C}\mathrm{or}\{\boldsymbol{X}, \boldsymbol{Y}\}$, which implies that $\left|\mathbb{C}\mathrm{or}\{\boldsymbol{X}, \boldsymbol{Y}\}\right| = \left|\mathbb{C}\mathrm{or}\{\check{\boldsymbol{X}}, \check{\boldsymbol{Y}}\}\right|$, and completes the proof.

Appendix B. Proof of Lemma 2

Two complementary observables $\boldsymbol{X}_1, \boldsymbol{X}_2 \in \mathcal{H}_2$ with dichotomic outcomes ± 1 have the following spectral decompositions

$$\boldsymbol{X}_1 = |e_0\rangle\langle e_0| - |e_1\rangle\langle e_1|, \tag{B.1a}$$

$$\boldsymbol{X}_2 = |h_0\rangle\langle h_0| - |h_1\rangle\langle h_1|, \tag{B.1b}$$

where the orthonormal bases $\{|e_0\rangle, |e_1\rangle\}$ and $\{|h_0\rangle, |h_1\rangle\}$ are mutually unbiased, i.e., $\left|\langle e_k|h_\ell\rangle\right|^2 = 1/2\ \forall k,\ell \in \{0,1\}$. Then, it is easy to see that $\mathrm{tr}\{\boldsymbol{X}_1^\dagger \boldsymbol{X}_2\} = 0$, which implies orthogonality, i.e., $\boldsymbol{X}_1 \perp \boldsymbol{X}_2$. Simple calculations also reveal that $\boldsymbol{X}_1\boldsymbol{X}_1^\dagger = \boldsymbol{X}_1^\dagger\boldsymbol{X}_1 = \boldsymbol{I}$ and $\boldsymbol{X}_2\boldsymbol{X}_2^\dagger = \boldsymbol{X}_2^\dagger\boldsymbol{X}_2 = \boldsymbol{I}$, i.e., $\boldsymbol{X}_1$ and $\boldsymbol{X}_2$ are unitary, which completes the proof.

Appendix C. Proof of Lemma 3

Based on Lemma 1, the PCC $\mathbb{C}\mathrm{or}\{\boldsymbol{X},\boldsymbol{Y}\}$ for any two 2-dimensional observables $\boldsymbol{X} = x_0\,\boldsymbol{I} + \sum_{k=1}^3 x_k\,\boldsymbol{\Lambda}_k$ and $\boldsymbol{Y} = y_0\,\boldsymbol{I} + \sum_{k=1}^3 y_k\boldsymbol{\Lambda}_k$ is equal to $\mathbb{C}\mathrm{or}\{\check{\boldsymbol{X}},\check{\boldsymbol{Y}}\}$ where $\check{\boldsymbol{X}} = \sum_{k=1}^3 \check{x}_k\,\boldsymbol{\Lambda}_k$ and $\check{\boldsymbol{Y}} = \sum_{k=1}^3 \check{y}_k\,\boldsymbol{\Lambda}_k$, with $\check{x}_k = x_k/\sqrt{x_1^2+x_2^2+x_3^2}$ and $\check{y}_k = y_k/\sqrt{y_1^2+y_2^2+y_3^2}$, i.e.,

$$\mathbb{C}\mathrm{or}\{\boldsymbol{X},\boldsymbol{Y}\} = \mathbb{C}\mathrm{or}\{\check{\boldsymbol{X}},\check{\boldsymbol{Y}}\}\,. \tag{C.1}$$

For the observable $\check{\boldsymbol{X}}$ and the marginal state $\boldsymbol{S}^{\mathrm{A}}$ given in (9), we obtain $\mathbb{E}\{\check{\boldsymbol{X}}\} = \sum_{k=1}^3 n_k\check{x}_k = \langle\check{x}|n\rangle$ and $\mathbb{V}\{\check{\boldsymbol{X}}\} = \sum_{k=1}^3 \check{x}_k^2 - \langle\check{x}|n\rangle^2 = 1-\langle\check{x}|n\rangle^2$. Analogously, for the observable $\check{\boldsymbol{Y}}$ and the marginal state $\boldsymbol{S}^{\mathrm{B}}$ given in (9) we have $\mathbb{E}\{\check{\boldsymbol{Y}}\} = \langle s|\check{y}\rangle$ and $\mathbb{V}\{\check{\boldsymbol{Y}}\} = 1-\langle s|\check{y}\rangle^2$. For the tensor product $\check{\boldsymbol{X}}\otimes\check{\boldsymbol{Y}}$ and the global state $\boldsymbol{S}^{\mathrm{AB}}$, we obtain $\mathbb{E}\{\check{\boldsymbol{X}}\otimes\check{\boldsymbol{Y}}\} = \sum_{k,\ell=1}^3 t_{k\ell}\check{x}_k\check{y}_\ell = \langle\check{x}|\boldsymbol{T}|\check{y}\rangle$. Then, by setting $\boldsymbol{C} = \boldsymbol{T} - |n\rangle\langle s|$ with elements $[\boldsymbol{C}]_{k\ell} = t_{k\ell} - n_k s_\ell$ it follows

$$\mathbb{C}\mathrm{or}\{\boldsymbol{X},\boldsymbol{Y}\} = \frac{\langle\check{x}|\boldsymbol{C}|\check{y}\rangle}{\sqrt{1-\langle\check{x}|n\rangle^2}\sqrt{1-\langle\check{y}|s\rangle^2}}\,, \tag{C.2}$$

which completes the proof.

Appendix D. Proof of Lemma 4

Consider two complementary 2-dimensional observables with spectral decomposition $\boldsymbol{X}_1 = \lambda_{1_0}|e_0\rangle\langle e_0| + \lambda_{1_1}|e_1\rangle\langle e_1|$ and $\boldsymbol{X}_2 = \lambda_{2_0}|h_0\rangle\langle h_0| + \lambda_{2_1}|h_1\rangle\langle h_1|$, where the orthonormal bases $\{|e_0\rangle,|e_1\rangle\}$ and $\{|h_0\rangle,|h_1\rangle\}$ are mutually unbiased, i.e., $\left|\langle e_k|h_\ell\rangle\right|^2 = 1/2$ and also $\lambda_{1_0}\neq\lambda_{1_1}$ and $\lambda_{2_0}\neq\lambda_{2_1}$. The above observables can be equivalently written as $\boldsymbol{X}_1 = x_{1_0}\,\boldsymbol{I} + \sum_{k=1}^3 x_{1_k}\boldsymbol{\Lambda}_k$ and $\boldsymbol{X}_2 = x_{2_0}\,\boldsymbol{I} + \sum_{k=1}^3 x_{2_k}\boldsymbol{\Lambda}_k$. Taking into account the resolution identity, i.e., $\boldsymbol{I} = |e_0\rangle\langle e_0| + |e_1\rangle\langle e_1| = |h_0\rangle\langle h_0| + |h_1\rangle\langle h_1|$, we obtain another pair of complementary observables through the transformations $\boldsymbol{X}_1 \to \check{\boldsymbol{X}}_1 = \boldsymbol{X}_1 - x_{1_0}\boldsymbol{I}$ and $\boldsymbol{X}_2 \to \check{\boldsymbol{X}}_2 = \boldsymbol{X}_2 - x_{2_0}\boldsymbol{I}$, which have the following spectral decomposition

$$\check{\boldsymbol{X}}_1 = \check{\lambda}_{1_0}|e_0\rangle\langle e_0| + \check{\lambda}_{1_1}|e_1\rangle\langle e_1|\,, \tag{D.1a}$$

$$\check{\boldsymbol{X}}_2 = \check{\lambda}_{2_0}|h_0\rangle\langle h_0| + \check{\lambda}_{2_1}|h_1\rangle\langle h_1|\,, \tag{D.1b}$$

with

$$\check{\lambda}_{1_0} = -\check{\lambda}_{1_1} \quad\text{and}\quad \check{\lambda}_{2_0} = -\check{\lambda}_{2_1}\,, \tag{D.2}$$

since the Pauli matrices $\boldsymbol{\Lambda}_k$ have eigenvalues ±1 and they are traceless. By noticing that $\mathrm{tr}\{\check{\boldsymbol{X}}_1^\dagger\check{\boldsymbol{X}}_2\} = 2\sum_{k=1}^3 x_{1_k}x_{2_k}$ and using (D.1) and (D.2) it follows that $\mathrm{tr}\{\check{\boldsymbol{X}}_1^\dagger\check{\boldsymbol{X}}_2\} = 0$, implying that $\sum_{k=1}^3 x_{1_k}x_{2_k} = 0$.

To prove the opposite direction, consider the observables $\check{\boldsymbol{X}}_1 = \sum_{k=1}^3 x_{1_k}\boldsymbol{\Lambda}_k = \check{\lambda}_{1_0}|e_0\rangle\langle e_0| + \check{\lambda}_{1_1}|e_1\rangle\langle e_1|$ and $\check{\boldsymbol{X}}_2 = \sum_{k=1}^3 x_{2_k}\boldsymbol{\Lambda}_k = \check{\lambda}_{2_0}|h_0\rangle\langle h_0| + \check{\lambda}_{2_1}|h_1\rangle\langle h_1|$ with $\check{\lambda}_{1_0}\neq\check{\lambda}_{1_0}$ and $\check{\lambda}_{2_0}\neq\check{\lambda}_{2_0}$. When the condition $\sum_{k=1}^3 x_{1_k}x_{2_k} = 0$ is satisfied, we have $\sum_{k=1}^3 x_{1_k}x_{2_k} = 0 \Leftrightarrow \mathrm{tr}\{\check{\boldsymbol{X}}_1^\dagger\check{\boldsymbol{X}}_2\} = 0$, which implies

$$\left|\langle h_0|e_0\rangle\right|^2 - \left|\langle h_1|e_0\rangle\right|^2 - \left|\langle h_0|e_1\rangle\right|^2 + \left|\langle h_1|e_1\rangle\right|^2 = 0\,. \tag{D.3}$$

For the orthonormal bases $\{|e_0\rangle,|e_1\rangle\}$ and $\{|h_0\rangle,|h_1\rangle\}$ the Euclidean norm $\left\|\,|e_\ell\rangle\right\|_2 = \sqrt{\sum_{k=0}^1|\langle h_k|e_\ell\rangle|^2} = 1\ \forall\ell\in\{0,1\}$ takes the form

$$\left|\langle h_0|e_0\rangle\right|^2 + \left|\langle h_1|e_0\rangle\right|^2 = 1\,, \tag{D.4a}$$

$$\left|\langle h_0|e_1\rangle\right|^2 + \left|\langle h_1|e_1\rangle\right|^2 = 1\,, \tag{D.4b}$$

and the norm $\left\|\,|h_\ell\rangle\right\|_2 = \sqrt{\sum_{k=0}^1|\langle h_\ell|e_k\rangle|^2} = 1\ \forall\ell\in\{0,1\}$ takes the form

$$\left|\langle h_0|e_0\rangle\right|^2 + \left|\langle h_0|e_1\rangle\right|^2 = 1\,, \tag{D.5a}$$

$$\left|\langle h_1|e_0\rangle\right|^2 + \left|\langle h_1|e_1\rangle\right|^2 = 1\,. \tag{D.5b}$$

From the above relations it follows

$$(\text{D.4a}) - (\text{D.5b}) \Rightarrow \left|\langle h_0|e_0\rangle\right|^2 - \left|\langle h_1|e_1\rangle\right|^2 = 0\,, \tag{D.6a}$$

$$(\text{D.4b}) - (\text{D.5b}) \Rightarrow \left|\langle h_0|e_1\rangle\right|^2 - \left|\langle h_1|e_0\rangle\right|^2 = 0\,. \tag{D.6b}$$

Applying the above six conditions, (D.4a) – (D.6b), onto (D.3) we end up with the following four conditions:

$$\left|\langle h_0|e_0\rangle\right|^2 = 1/2\,, \tag{D.7a}$$

$$\left|\langle h_1|e_0\rangle\right|^2 = 1/2\,, \tag{D.7b}$$

$$\left|\langle h_0|e_1\rangle\right|^2 = 1/2\,, \tag{D.7c}$$

$$\left|\langle h_1|e_1\rangle\right|^2 = 1/2\,, \tag{D.7d}$$

which imply that $\boldsymbol{X}_1$ and $\boldsymbol{X}_2$ are complementary, which completes the proof.

Appendix E. Counterexample for $(d\otimes d)$-dimensional states

Considering the state in (35) and taking the limit $\epsilon\to0$, the expectation value of the observables $\boldsymbol{A}_1$ in (36a) is given by $\lim_{\epsilon\to0}\mathbb{E}\{\boldsymbol{A}_1\} = \mathbb{E}\{\boldsymbol{\Pi}_{e_0}\} - \mathbb{E}\{\boldsymbol{\Pi}_{e_1}\} = 0$, since $\mathbb{E}\{\boldsymbol{\Pi}_{e_0}\} = \mathbb{E}\{\boldsymbol{\Pi}_{e_1}\} = \frac{d+2}{4d}$. Analogously, we have $\lim_{\epsilon\to0}\mathbb{E}\{\boldsymbol{A}_2\} = \lim_{\epsilon\to0}\mathbb{E}\{\boldsymbol{B}_1\} = \lim_{\epsilon\to0}\mathbb{E}\{\boldsymbol{B}_2\} = 0$.

For $\lim_{\epsilon\to0}\mathbb{E}\{\boldsymbol{A}_1\otimes\boldsymbol{B}_1\}$, we obtain $\lim_{\epsilon\to0}\mathbb{E}\{\boldsymbol{A}_1\otimes\boldsymbol{B}_1\} = \mathbb{E}\{\boldsymbol{\Pi}_{e_0}\otimes\boldsymbol{\Pi}_{e_0}\} - \mathbb{E}\{\boldsymbol{\Pi}_{e_0}\otimes\boldsymbol{\Pi}_{e_1}\} - \mathbb{E}\{\boldsymbol{\Pi}_{e_1}\otimes\boldsymbol{\Pi}_{e_0}\} + \mathbb{E}\{\boldsymbol{\Pi}_{e_1}\otimes\boldsymbol{\Pi}_{e_1}\} = \frac{1}{2}$, since $\mathbb{E}\{\boldsymbol{\Pi}_{e_0}\otimes\boldsymbol{\Pi}_{e_0}\} = \mathbb{E}\{\boldsymbol{\Pi}_{e_1}\otimes\boldsymbol{\Pi}_{e_1}\} = \frac{d^2+2}{4d^2}$ and $\mathbb{E}\{\boldsymbol{\Pi}_{e_0}\otimes\boldsymbol{\Pi}_{e_1}\} = \mathbb{E}\{\boldsymbol{\Pi}_{e_1}\otimes\boldsymbol{\Pi}_{e_0}\} = \frac{2}{4d^2}$. Analogously, we obtain $\lim_{\epsilon\to0}\mathbb{E}\{\boldsymbol{A}_2\otimes\boldsymbol{B}_2\} = \frac{1}{2}$.

Finally, we have $\lim_{\epsilon\to0}\mathbb{E}\{\boldsymbol{A}_1^2\} = \mathbb{E}\{\boldsymbol{\Pi}_{e_0}\} + \mathbb{E}\{\boldsymbol{\Pi}_{e_1}\} = \frac{1}{2}+\frac{1}{d}$, and analogously $\lim_{\epsilon\to0}\mathbb{E}\{\boldsymbol{A}_2^2\} = \lim_{\epsilon\to0}\mathbb{E}\{\boldsymbol{B}_1^2\} = \lim_{\epsilon\to0}\mathbb{E}\{\boldsymbol{B}_2^2\} = \frac{1}{2}+\frac{1}{d}$. So, the variances become equal to $\mathbb{V}\{\boldsymbol{A}_1\} = \mathbb{E}\{\boldsymbol{A}_1^2\} - \mathbb{E}\{\boldsymbol{A}_1\}^2 = \mathbb{E}\{\boldsymbol{A}_1^2\}$ and similarly, $\mathbb{V}\{\boldsymbol{A}_2\} = \mathbb{E}\{\boldsymbol{A}_2^2\}$, $\mathbb{V}\{\boldsymbol{B}_1\} = \mathbb{E}\{\boldsymbol{B}_1^2\}$, and $\mathbb{V}\{\boldsymbol{B}_2\} = \mathbb{E}\{\boldsymbol{B}_2^2\}$. Therefore, using these results, we have

$$\left|\,\mathbb{C}\mathrm{or}\{\boldsymbol{A}_1,\boldsymbol{B}_1\}\right| + \left|\,\mathbb{C}\mathrm{or}\{\boldsymbol{A}_2,\boldsymbol{B}_2\}\right| = 2 - \frac{4}{2+d}\,. \tag{E.1}$$

Appendix F. Infinite-dimensional quantum states

For infinite-dimensional quantum states $\boldsymbol{S}_\infty^{\mathrm{AB}} \in \mathcal{H}_\infty^{\mathrm{A}}\otimes\mathcal{H}_\infty^{\mathrm{B}}$, the notion of complementarity cannot be defined through (6), so a slightly different analysis is required. In infinite-dimensional Hilbert spaces two observables $\boldsymbol{Q}$ and $\boldsymbol{P}$ with eigensets $\{|q\rangle\}_{q\in\mathcal{R}}$ and $\{|p\rangle\}_{p\in\mathcal{R}}$ are complementary if they satisfy [74]

$$\left|\langle q|p\rangle\right|^2 = \frac{1}{2\pi\hbar}\,, \tag{F.1}$$

where $\hbar$ denotes the reduced Planck constant. Typical complementary observables in those systems are the position, $\boldsymbol{Q}$, and momentum, $\boldsymbol{P}$

quadratures, where in what follows we set $\hbar = 2$, so the vacuum state has a quadrature variance equal to one.

Consider a bipartite (two-mode) Gaussian state $\boldsymbol{S}_{\mathrm{G}}^{\mathrm{AB}}$. Given a vectorial operator defined as $\boldsymbol{R} := \left[\boldsymbol{Q}_1, \boldsymbol{P}_1, \boldsymbol{Q}_2, \boldsymbol{P}_2\right]^{\mathrm{T}}$, Gaussian states are fully described by a covariance matrix $\boldsymbol{V}$ with elements $\left[\boldsymbol{V}\right]_{ij} = \mathbb{E}\left\{\left[\Delta \boldsymbol{R}_i, \Delta \boldsymbol{R}_j\right]_+\right\}/2$, where $\Delta \boldsymbol{X} := \boldsymbol{X} - \mathbb{E}\{\boldsymbol{X}\}$ [75]. Under local operations and assuming vanishing first moments, the covariance matrix of a Gaussian state can be brought to its standard form [19,20]

$$\boldsymbol{V}_{\boldsymbol{S}_{\mathrm{G}}^{\mathrm{AB}}} = \begin{bmatrix} \mathbb{E}\{\boldsymbol{Q}_1^2\} & 0 & \mathbb{E}\{\boldsymbol{Q}_1 \otimes \boldsymbol{Q}_2\} & 0 \\ 0 & \mathbb{E}\{\boldsymbol{P}_1^2\} & 0 & \mathbb{E}\{\boldsymbol{P}_1 \otimes \boldsymbol{P}_2\} \\ \mathbb{E}\{\boldsymbol{Q}_1 \otimes \boldsymbol{Q}_2\} & 0 & \mathbb{E}\{\boldsymbol{Q}_2^2\} & 0 \\ 0 & \mathbb{E}\{\boldsymbol{P}_1 \otimes \boldsymbol{P}_2\} & 0 & \mathbb{E}\{\boldsymbol{P}_2^2\} \end{bmatrix}. \tag{F.2}$$

In the context of our analysis, let us set $\boldsymbol{A}_1 = \boldsymbol{Q}_1$, $\boldsymbol{A}_2 = \boldsymbol{P}_1$, $\boldsymbol{B}_1 = \boldsymbol{Q}_2$, and $\boldsymbol{B}_2 = \boldsymbol{P}_2$. Let us have a Gaussian state with the following covariance matrix

$$\boldsymbol{V}_{\boldsymbol{S}_{\mathrm{G,sep}}} = \begin{bmatrix} \upsilon & 0 & \upsilon-1 & 0 \\ 0 & \upsilon & 0 & \upsilon-1 \\ \upsilon-1 & 0 & \upsilon & 0 \\ 0 & \upsilon-1 & 0 & \upsilon \end{bmatrix} = \begin{bmatrix} \boldsymbol{V}_A & \boldsymbol{V}_C \\ \boldsymbol{V}_C^{\mathrm{T}} & \boldsymbol{V}_B \end{bmatrix}, \tag{F.3}$$

with $\upsilon \geqslant 1$, where $\upsilon = \mathbb{V}\{\boldsymbol{A}_i\} = \mathbb{V}\{\boldsymbol{B}_i\}$ for $i \in \{1,2\}$. Based on the necessary and sufficient PPT separability criterion [19,20], a bipartite Gaussian state is separable when the lowest symplectic eigenvalue of the partially transposed covariance matrix, i.e., $\lambda_-\{\boldsymbol{V}_{\boldsymbol{S}_{\mathrm{G,sep}}}^{\Gamma}\}$, is greater or equal to one. This eigenvalue is calculated through

$$\lambda_-\{\boldsymbol{V}_{\boldsymbol{S}_{\mathrm{G,sep}}}^{\Gamma}\} = \sqrt{\frac{\boldsymbol{V}_E - \sqrt{\boldsymbol{V}_E^2 - 4\det\left(\boldsymbol{V}_{\boldsymbol{S}_{\mathrm{G,sep}}}\right)}}{2}}, \tag{F.4}$$

with $\upsilon_E = \det\left(\boldsymbol{V}_A\right) + \det\left(\boldsymbol{V}_B\right) - 2\det\left(\boldsymbol{V}_C\right)$. So, we obtain

$$\lambda_-\{\boldsymbol{V}_{\boldsymbol{S}_{\mathrm{G,sep}}}^{\Gamma}\} = \sqrt{2\upsilon - 1}, \tag{F.5}$$

meaning that it is greater or equal to one for any $\upsilon \geqslant 1$, and thus the state $\boldsymbol{V}_{\boldsymbol{S}_{\mathrm{G,sep}}}$ is separable. For those states, we obtain

$$\boldsymbol{S}^{\mathrm{AB}} = \boldsymbol{S}_{\mathrm{G,sep}}^{\mathrm{AB}} \Rightarrow \sum_{i=1}^{2} \left|\mathbb{C}\mathrm{or}\{\boldsymbol{A}_i, \boldsymbol{B}_i\}\right| = 2 - \frac{2}{\upsilon}, \tag{F.6}$$

since $\left|\mathbb{C}\mathrm{or}\{\boldsymbol{A}_1, \boldsymbol{B}_1\}\right| = \left|\mathbb{C}\mathrm{or}\{\boldsymbol{A}_2, \boldsymbol{B}_2\}\right| = (\upsilon-1)/\upsilon$. Thus, for $\upsilon > 2$, even though the state $\boldsymbol{S}_{\mathrm{G,sep}}^{\mathrm{AB}}$ is by construction separable, the expression $\left|\mathbb{C}\mathrm{or}\{\boldsymbol{A}_1, \boldsymbol{B}_1\}\right| + \left|\mathbb{C}\mathrm{or}\{\boldsymbol{A}_2, \boldsymbol{B}_2\}\right|$ becomes larger than one. The above counterexamples provide further support on the validity of the proposed Conjecture in (38), since they are consistent with the trend that the larger the dimensions of the Hilbert space the harder it is to identify entanglement through this method (see Fig. 3).

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