We present a framework for deciding whether a quantum state is separable or entangled using covariance matrices of locally measurable observables. This leads to the covariance matrix criterion as a general separability criterion. We demonstrate that this criterion allows to detect many states where the familiar criterion of the positivity of the partial transpose fails. It turns out that a large number of criteria which have been proposed to complement the positive partial transpose criterion – the computable cross norm or realignment criterion, the criterion based on local uncertainty relations, criteria derived from extensions of the realignment map, and others – are in fact a corollary of the covariance matrix criterion.

I. INTRODUCTION

Entanglement is the feature of quantum theory that renders it crucially different from a classical statistical theory. It also plays the central role in quantum information science, as a resource for information processing tasks. Consequently, a lot of effort has been made in the last decade to understand the meaning and the structure of entangled states [1, 2]. One of the most elementary yet notorious questions is how to find good criteria to decide whether a state is entangled or classically correlated in the first place. Formally, one asks whether a given state \( \rho \) in a bipartite system is contained in the convex hull of product states and can hence be written as

\[
\rho = \sum_k p_k |a_k\rangle \langle a_k| \otimes |b_k\rangle \langle b_k| ,
\]

where the coefficients \( p_k \) form a probability distribution. If so, all correlations can come from classical shared randomness, and a state is called classically correlated or separable. Otherwise, \( \rho \) is an entangled state. The decision problem of deciding whether a state is entangled or separable is known to be a computationally hard problem in the physical dimension, for a certain scaling of the error in the weak membership problem [3]. Yet, the problem one typically faces is the one where one has just a physical state given – having some fixed dimension – and one aims at finding criteria to make a judgment based on these criteria. Not surprisingly, given the central status of entanglement in quantum information theory, a lot of effort has been devoted to identifying such good and practical and computable criteria for separability in composite quantum states.

Historically, the first criterion of this sort was derived from the observation that every separable state will have a positive partial transpose, and that the positivity of the latter can hence be used as an entanglement criterion (PPT criterion) [4, 5]. This criterion later turned out to be necessary and sufficient for separability for low dimensional systems (\( 2 \times 2 \) and \( 2 \times 3 \)), whereas in higher dimensions this is no longer the case [6]. The PPT criterion is an example of a criterion based on positive maps: In fact, it has been proven that a state \( \rho \) is separable if and only if for any positive map \( \Lambda \) the operator \( (1 \otimes \Lambda)(\rho) \) is also positive [6]. Consequently, the systematic investigation of positive maps has led to a number of new separability criteria [6]. A quite remarkable criterion of this type is the reduction criterion, which is equivalent to the PPT criterion for \( 2 \times 2 \) and \( 2 \times 3 \) cases and weaker for higher dimensions [8]. There are also other criteria that turned out to be directly related to the PPT criterion: The majorization criterion [9] and also entropic criteria [10] have been shown to be weaker than the PPT criterion [11, 12]. Moreover, one can extend the PPT condition to a test based on a complete hierarchy of symmetric extensions, where each step constitutes a semidefinite program [13] (another complete family of semidefinite tests has been described in [14]). In such a hierarchy, every entangled state is necessarily detected as such in some step of the hierarchy. However, the steps in the hierarchy require more and more computational effort, which makes this approach difficult already for modest system sizes.

Apart from these criteria that are directly related to the PPT criterion, a number of other separability criteria have been suggested where such a connection seemingly does not exist. The most prominent criterion of this type is the computable cross-norm or realignment criterion (CCNR) [15]. Other criteria in this category use the Bloch representation of density matrices [14, 15], local uncertainty relations (LURs) [16], local orthogonal observables [17], or extensions of the realignment map [18, 19, 20]. These criteria are complementing the PPT criterion in an interesting way: In fact they detect some states as being entangled where the PPT criterion fails.
They also do not rely on positive maps.

At first sight, one might think that these criteria form a collection of quite beautiful, but strangely disconnected results. They have been derived using a variety of unrelated methods, and their connection often seems quite unclear. It is the main purpose of this work to develop a framework for the systematic understanding of all these latter approaches.

In Ref. [22] we have proposed to investigate the separability problem using covariance matrices (CMs) of certain observables. In this context we have developed a separability criterion in terms of covariance matrices (covariance matrix criterion or CMC). We have shown that the CMC is, when augmented with appropriate local filtering, despite its simplicity a surprisingly strong entanglement criterion, which can detect states where the PPT criterion fails and which is at the same time necessary and sufficient for two qubits. Here we complete this approach and present new results in various directions. Specifically, we show that a number of criteria which have been proposed to improve the PPT criterion – namely the CCNR criterion [13], the LURS [18], and recent criteria from Refs. [16, 17], – follow directly from the CMC. In this way the CMC can be seen as complementary to the PPT criterion. We also tighten previous formulations of the CMC. We discuss several examples, and compare the performance of the criteria to instances of random states from a families of bound entangled states.

This manuscript is organized as follows: In the second section, we introduce CMs and discuss their mathematical properties. Those readers who are mainly interested in separability criteria may only consume Definitions II.1 and II.2 and Propositions II.3 and II.12 and may then directly jump to Section III. In that Section, we introduce the CMC and evaluate it in several different ways. By doing this we establish the mentioned connection to the other separability criteria which will turn out to be corollaries of the former. In Section IV of the paper we will consider the connection between the CMC and the LURs. In the fifth section we will scrutinize the CMC for the two qubit case. In Section VI we will assess the strength of the mentioned criteria by considering a family of bound entangled states. We will then conclude and elaborate on possible extensions of the work presented here. Some more technical proofs of our theorems will finally be presented in the Appendix.

II. COVARIANCE MATRICES

In this section we will investigate covariance matrices as our main tool. In the first subsection we will introduce the different definitions of CMs and fix our notation. In the second subsection we will address the question to which extent CMs can be used as a unique description of quantum states besides density matrices. Finally, in the third and fourth subsections we will mention and prove some useful properties of CMs, which will be used later in our study of entanglement.

A. Definition of covariance matrices

In what follows let $\rho$ be a pure or mixed quantum state, described by a (positive) density operator in a $d$-dimensional Hilbert space $\mathcal{H}$ and let $\{M_k : k = 1, \ldots, N\}$ a suitable set of observables. Unless stated otherwise, we will always assume that these observables are orthonormal observables with respect to the Hilbert-Schmidt scalar product between observables, i.e., they fulfill

$$\text{tr}(M_i M_j) = \delta_{i,j}. \quad (2)$$

Furthermore, we will typically assume that the $M_i$ form a complete basis and span the whole observable algebra. This implies that there are $N = d^2$ different $M_i$, and that any other observable can be expressed as a linear combination of the $M_i$.

As an example for such a set of observables for the case of a single qubit, one can consider the (appropriately normalized) Pauli matrices,

$$M_1 = \frac{1}{\sqrt{2}}, \quad M_2 = \frac{\sigma_x}{\sqrt{2}}, \quad M_3 = \frac{\sigma_y}{\sqrt{2}}, \quad M_4 = \frac{\sigma_z}{\sqrt{2}}. \quad (3)$$

We can now formulate the main definitions for this work.

Definition II.1 (Covariance matrix). The $d^2 \times d^2$ covariance matrix $\gamma = \gamma(\rho, \{M_k\})$ and the $d^2 \times d^2$ symmetrized covariance matrix $\gamma^S = \gamma^S(\rho, \{M_k\})$ are defined by their matrix entries as

$$\gamma i,j = \langle M_i M_j \rangle - \langle M_i \rangle \langle M_j \rangle, \quad (4)$$

$$\gamma^S i,j = \frac{\langle M_i M_j \rangle + \langle M_j M_i \rangle}{2} - \langle M_i \rangle \langle M_j \rangle. \quad (5)$$

Sometimes, the difference between the linear part of a CM and the nonlinear part becomes relevant. Therefore, we define the linear part of $\gamma$ as $g_{i,j} = \langle M_i M_j \rangle$ and the linear part of the symmetric CM as $g_{i,j}^S = \langle M_i M_j + M_j M_i \rangle/2$.

We will often for simplicity of notation also write $\gamma(\rho)$ or $\gamma(\{M_k\})$ instead of $\gamma(\rho, \{M_k\})$, or simply $\gamma$. We will also sometimes indicate with respect to what state an expectation value is taken, so $(M_i) = \langle M_i \rangle_\rho$. It is straightforward to see that $\gamma$ is a complex Hermitian matrix. The matrix $\gamma^S$ in turn is real and symmetric. Both $\gamma$ and $\gamma^S$ are positive semidefinite, $\gamma, \gamma^S \geq 0$ [24].

Note finally that for odd $d$, there is another basis of orthonormal observables that can equally be used and that is commonly employed in the mathematical physics literature in the context of discrete Weyl systems [23]. Let $A(0,0)$ be the parity operator that maps $P(0,0) : |x\rangle \mapsto |-x\rangle$, where $|x\rangle \in \{0, \ldots, d-1\}$, meant modulo $d$. Then, for $(q,p) \in \mathbb{Z}_d^2$ let

$$P(q,p) = W(q,p) P(0,0) W(q,p)^\dagger \quad (6)$$
Similarly, we can define a symmetric block covariance matrix which is another set of observables, connected to the \{M_k\} by a basis transformation \(K_i = \sum_{k=1}^{N} O_{i,j} M_j\) with some matrix \(O\) then \(\gamma(\{K_i\})\) is given by

\[
\gamma(\{K_i\}) = O\gamma(\{M_k\})O^T.
\]

Note that \(O\) is an orthogonal matrix if \(K_i\) and \(M_i\) are orthonormal bases.

**Proof:** A direct calculation gives

\[
\gamma(\{K_i\})_{i,j} = \sum_{l,m} (O_{i,l} M_l O_{j,m} M_m) - (O_{i,l} M_l) (O_{j,m} M_m) = \sum_{l,m} O_{i,l} \gamma(\{M_k\})_{l,m} O^T_{m,j},
\]

which proves the claim.

The main point is that the previous proposition allows us to choose the basis which we want to express our CM in arbitrarily, since we know how the CM will be transformed under a basis transformation in the space of observables.

We can now come back to the initial question: Suppose we are given some CM with a fixed basis of observables. Are we able to reconstruct the physical state from this CM uniquely? We will start answering this question by considering a single system.

**Proposition II.4** (Characterization of states via non-symmetric covariance matrices). Given a non-symmetric CM with tomographically complete set of observables, we can reconstruct the corresponding physical state unambiguously.

**Proof:** We choose the following basis of the observables:

\[
D_i = |i\rangle\langle i|, \quad i = 1, \ldots, d,
\]

\[
X_{i,j} = \frac{1}{\sqrt{2}}(|i\rangle\langle j| + |j\rangle\langle i|), \quad 1 \leq i < j \leq d,
\]

\[
Y_{k,l} = \frac{i}{\sqrt{2}}(|k\rangle\langle l| - |l\rangle\langle k|), \quad 1 \leq k < l \leq d.
\]

These observables form an orthonormal basis, and we will refer to this basis as to the standard basis later on. As in any basis \(M_k\), we can write the state as \(\rho = \sum_k \langle M_k | M_k \rangle\). From Eq. (1) one can see that \(\gamma_{i,j} = \langle i | J | k \rangle \langle k | J | j \rangle = \langle M_i | M_j \rangle\). In the following we will show that in the chosen basis, all first moments can be obtained from expectation values of commutators.

For the chosen standard basis we can explicitly calculate all commutators

\[
[D_{k}, X_{k,l}] = \frac{i}{\sqrt{2}} Y_{k,l}, \quad [D_{k}, Y_{k,l}] = -\frac{i}{\sqrt{2}} X_{k,l}, \quad [X_{k,l}, Y_{k,l}] = i(|k\rangle\langle k| - |l\rangle\langle l|).
\]

Hence, all expectation values of the \(X_{i,j}\) and \(Y_{k,l}\) can be calculated. The same is true for the diagonal elements: Using the fact that the trace of the density matrix is
equal to one, we can calculate all the diagonal elements from the mean values of \( [X_{k,1}, Y_{k,1}] \).

Clearly, the same approach can be used for bipartite systems, if we use the CM in the full (and not in a block) form. In this case we can use a product basis \( \{|i_1, i_2\}\). Identifying \((i_1, i_2) = i:\) we can define the standard basis as above and find all first moments from the covariance matrix.

As we have seen, the non-symmetric CM defined in Eq. (14) describes the physical state completely. The knowledge of the symmetric CM in Eq. (15) is, however, not enough:

**Proposition II.5** (Inequivalence of states and symmetric covariance matrices). The knowledge of the symmetric CM \( \gamma^S \) does, in general, not determine the state \( \rho \) completely.

**Proof:** We prove the claim by providing a counterexample. Let us take a single qubit. As observables we take the appropriate normalized Pauli matrices. The symmetric CM has the following entries

\[
\gamma_{0,j}^S = \frac{1}{4} \langle \sigma_j \rangle - \frac{1}{2} \langle \sigma_j \rangle = 0 = \gamma_{0,0}^S, \tag{17}
\]

\[
\gamma_{i,j}^S = \frac{1}{4} \langle \sigma_i \sigma_j \rangle - \frac{1}{2} \langle \sigma_i \sigma_j \rangle = \delta_{i,j} - \frac{\delta_{i,j}}{2}. \tag{18}
\]

From this we can determine the norm of the mean value of the spin component in a certain direction, but not its sign. Hence we know the length of the Bloch vector of the system, up to some reflection to the origin, which corresponds to simultaneous change of signs of all \( \langle \sigma_i \rangle \)'s.

One might think that the case of one qubit constitutes a special case. However, the same ambiguity will arise if one embedded a qubit in a higher dimensional, say, three level system. As it can be checked, the additional observables in the basis of observables \( \{ M_k \} \) will not provide any further information.

To summarize: The knowledge of the symmetric CM of a qubit alone is not sufficient to decide between two alternatives of states which have opposite (symmetric to the origin) Bloch vectors. Also, merely the additional knowledge of a single bit (the sign) is needed to make this correspondence unambiguous. This, however, is specific to the qubit case. We will now turn to investigating the same question for the block CM defined in Eq. (8):

**Proposition II.6** (Relationship between bipartite states and block covariance matrices). For block CMs \( \gamma \) and \( \gamma^S \) on a bipartite system, the following statements hold:

(i) The (non-symmetric) block CM \( \gamma \) determines the bipartite state \( \rho_{AB} \) completely.

(ii) The symmetric block \( \gamma^S \) does not determine \( \rho_{AB} \) completely.

**Proof:** Obviously, given a non-symmetric block CM for the set of variables \( A_k \otimes 1 \) and \( 1 \otimes B_l \) we can determine first all \( \langle A_k \rangle \) and \( \langle B_l \rangle \) for the reduced state \( \rho_A \) in the same way as in Proposition II.4 from the blocks \( A \) and \( B \) of \( \gamma \). Then, knowing the block \( C \) we can fix the rest \( \langle A_k \otimes B_l \rangle \) as

\[
\langle A_k \otimes B_l \rangle = C_{k,l} + \langle A_k \rangle \langle B_l \rangle \tag{19}
\]

and hence \((i)\) is proved.

The validity of \((ii)\) is straightforward to see for two qubit states, as there will be the same lack of information on the mean values of observables as in Proposition II.5 and hence \( \gamma^S_{AB} \) does not provide the whole information about the state.

The fact that the symmetric block CM \( \gamma^S \) does not determine the state completely will later be important for the discussion of our entanglement criteria. Therefore, let us investigate this correspondence for the case of two qubits in more detail. For that, let \( A_i \) and \( B_j \) be Pauli matrices. We may write the state in the form

\[
\rho_{AB} = \frac{1}{4} \sum_{i,j} \lambda_{i,j} \sigma_i^A \otimes \sigma_j^B, \tag{20}
\]

where \( \lambda_{i,j} = \text{tr}(\rho \sigma_i^A \otimes \sigma_j^B) \).

As one can see from Eq. (19) we have two possibilities of changing the \( \lambda_{i,j} \) while keeping the \( C_{i,j} \) invariant: We can (i) flip the signs of both of the Bloch vectors of the reduced density matrices, \( \lambda_{0,j} \) and \( \lambda_{i,0} \) for \( i,j = 1,2,3 \), while keeping the left hand side of Eq. (19) invariant. Alternatively, we can (ii) flip the sign of only one of them, which implies that we also have to change the left hand side of Eq. (19).

Concerning (i), one can directly calculate the transformed state \( \rho^{\text{inv}} \). It turns out that the eigenvalues of \( \rho \) and \( \rho^{\text{inv}} \) are the same, suggesting that they are connected by a unitary transformation maybe in addition with a global transposition which transforms one state to the other. Actually the unitary transformation is a local unitary one, and one has the following transformation:

\[
(\rho^{\text{inv}})^T = U^\dagger \rho_{AB} U, \quad U = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \otimes \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \tag{21}
\]

Since there is no physical process which corresponds to a transposition of a state, there are two physically different states \( \rho \) and \( \rho^{\text{inv}} \) which give rise to the same covariance matrix and which are connected by the simultaneous flip of the Bloch vectors of their subsystems. Nevertheless we can see from Eq. (21) that these states have the same entanglement properties, because there is a local unitary operation in addition to a global transposition connecting them. These transformations do not change the outcome of the PPT criterion, and in fact do not change the entanglement properties of any two-qubit quantum state.

Concerning (ii), it also possible to flip the Bloch vector of only one of the subsystems in a such a way that the
The rank is given by \( \text{Rank} (\rho_{\text{inv}}) = \text{Rank} (\rho_{c}) \).

Let \( \rho_{c} \) be a symmetric CM. The inverted form \( \rho_{\text{inv}} \) fulfills:

(i) The rank is given by \( \text{Rank} (\gamma) = d - 1 \).

(ii) The nonzero eigenvalues of \( \gamma \) are equal to 1, hence \( \text{tr} (\gamma) = d - 1 \).

(iii) Consequently, we have \( \gamma^2 = \gamma \).

Proof: Without any loss of generality we assume \( \rho = |1\rangle \langle 1 | \) and take as observables the ones of the standard basis \(|i\rangle\rangle_{\text{standard}}\). Calculating directly and reordering of the matrix elements afterwards gives a block structure \(28\):

\[
\gamma = \bigoplus_{k=1}^{d-1} [B_k] \bigoplus \Theta_{d^2 - 2d + 2} \quad \text{with} \quad B_k = \begin{pmatrix} 1/2 & i/2 \\ -i/2 & 1/2 \end{pmatrix},
\]

where \( \Theta_k \) denotes a \( k \times k \) matrix of zeros. This matrix has the desired properties.

From this we can directly read off the properties of the symmetric form of the covariance matrix:

**Corollary II.8 (Properties of symmetric CMs for pure states).** Let \( \{ G_i \} \) be a tomographically complete set of observables of a \( d \)-dimensional system. If \( \rho \) is a pure state, then \( \gamma^S \) (as \( d^2 \times d^2 \) symmetric matrix) fulfills:

(i) The rank is given by \( \text{Rank} (\gamma^S) = 2(d - 1) \).

(ii) The nonzero eigenvalues of \( \gamma^S \) are equal to 1/2, hence \( \text{tr} (\gamma^S) = d - 1 \).

We now turn to a proposition concerning the trace of a CM for mixed states.
Proposition II.9 (Trace of CMs). Let $\rho$ be a mixed state. Then
\[
\text{tr}[\gamma(\rho)] = d - \text{tr}(\rho^2)
\]
which implies that $d - 1/d \geq \text{tr}(\gamma(\rho)) \geq d - 1$. This holds also for $\gamma^{S}$.

Proof: By definition \(\text{tr}(\gamma) = \sum_i \gamma_{i,i} = \sum_i \delta^2(M_i) = \sum_i ((M_i^2) - (M_i^2))\). The first summation is trivial, since we have $\sum_k M_k = d I$. Furthermore we can write $\rho = \sum_k (M_k^2)M_k$ which implies that $\sum_k (M_k^2) = \text{tr}(\rho^2)$, and further $1/d \leq \text{tr}(\rho^2) \leq 1$. The statement for $\gamma^{S}$ follows directly from the fact that $\text{tr}(\gamma) = \text{tr}(\gamma^{S})$.

We can also estimate the operator norm (i.e., the maximal eigenvalue) of CMs.

Proposition II.10 (Operator norm of CMs). For the CM $\gamma(\rho)$ and its linear part $g(\rho)$ the operator norm is bounded by
\[
\|g(\rho)\| \leq \|\rho\| \quad \text{and} \quad \|\gamma(\rho)\| \leq \|\rho\|.
\]
The same bounds hold for symmetric CMs.

Proof: Let us first consider $g(\rho)$. We have $\|g(\rho)\| = \max_{|x\rangle}|\langle x|g(\rho)|x\rangle| = (\langle x_0|g(\rho)|x_0\rangle = \text{tr}(\rho AA^\dagger)$ with $\text{tr}(AA^\dagger) = 1$. This is clearly smaller than $\|\rho\|$. For $\gamma(\rho)$ this follows then from $\langle AA^\dagger \rangle - \langle A\rangle A^\dagger \leq \langle AA^\dagger \rangle$.

Finally, CMs also satisfy an interesting majorization relation. This has its root in the way how one can relate CMs to the rotated CMs of the pure states occurring in their convex decompositions in terms of pure states.

Proposition II.11 (Majorization relation for CMs). For any (mixed) state $\rho$, both the linear part $g(\rho)$ with entries $g_{i,j} = \langle M_i M_j \rangle$ as well as the CM $\gamma(\rho)$ satisfy
\[
\sum_{j=1}^k \lambda_j[g(\rho)], \sum_{j=1}^k \lambda_j[\gamma(\rho)] \leq \min(k,d - \delta, \frac{1}{d}),
\]
for the non-increasingly ordered eigenvalues, where $\delta_\gamma = 1$ for $\gamma(\rho)$ and $\delta_\gamma = 0$ if $g(\rho)$ is considered.

Proof: This is a consequence of $\|\gamma(\rho)\|, \|g(\rho)\| \leq 1$ as well as of $\text{tr}[\gamma(\rho)] \leq d - \frac{1}{d}$ and $\text{tr}(g(\rho)) \leq d$.

E. Mixing property of covariance matrices

Separable states are those states that can be written as convex combinations of product states. Therefore we have to understand the behavior of CMs under mixing of states for the derivation of separability criteria. An important property of covariance matrices which we refer to as concavity property is the following:

Proposition II.12 (Concavity property). Let $\rho = \sum_k p_k \rho_k$ be a convex combination of states $\rho_k$, then
\[
\gamma(\rho) \geq \sum_k p_k \gamma(\rho_k).
\]
Clearly, this implies the same relation for the symmetrized CM $\gamma^{S}$.

Proof: As shown in Ref. [29] this inequality holds for an arbitrary symmetric CM $\gamma$. Moreover, since $\langle M_i M_j \rangle_\rho = \sum_k p_k \langle M_i M_j \rangle_{\rho_k}$ for all $i,j$, we have for the non-linear part that
\[
- \langle M_i \rangle \langle M_j \rangle_\rho \geq - \sum_k p_k \langle M_i \rangle_{\rho_k} \langle M_j \rangle_{\rho_k},
\]
as a matrix inequality for the matrices $X_{i,j} = - \langle M_i \rangle \langle M_j \rangle_\rho$ and $Y_{i,j} = - \sum_k p_k \langle M_i \rangle_{\rho_k} \langle M_j \rangle_{\rho_k}$. From this, the above inequality follows for the non-symmetric CM $\gamma$.

This property will later be used to derive the separability criterion.

F. Transformations of observables and validity of covariance matrices

Transformations as generated by a general orthogonal matrix $O$ used in Proposition II.5 do in general not preserve the positivity of the state $\rho$ (see Ref. [19] for discussion). Only a subgroup will correspond to unitary transformations on the level of states. Here, we will clarify how unitary transformations of the state are reflected by orthogonal transformations on the level of CMs.

For this aim, let us consider the case that $\rho$ is transformed by some unitary transformation $\rho \mapsto U^\dagger U$. Equivalently, we can transform the operator basis, denoted as $\{G_i\}$, as
\[
G_i \mapsto H_i = U G_i U^\dagger = \sum_j O_{i,j} G_j.
\]
It is then easy to see that the transformation of the CM is
\[
\gamma(\rho) \mapsto O \gamma(\rho) O^T = \gamma(U^\dagger \rho U),
\]
We can now ask in what way $O$ depends on $U$, and which orthogonal $O \in O(d^2)$ correspond to a unitary $U \in U(d)$ acting in state space as described above. That is, we look for the group representation of $U(d)$ in the space of CMs (compare also the metaplectic representation of symplectic transformations in discrete Weyl systems, see Ref. [24]). The following theorem gives an answer to this question.

Proposition II.13 (Transformation laws for CMs). Let $U \in U(d)$. Then the $O \in O(d^2)$ representing $U$ as described above is given by
\[
O = \Gamma^T (U^T \otimes U^\dagger) \Gamma^*,
\]

where $\Gamma$ is a $d \times d$ matrix.
where $\Gamma$ is a $d^2 \times d^2$ square matrix constructed as $\Gamma_{\alpha,\beta}[i] = G^\alpha_{\beta}[i] = (|G_1\rangle, |G_2\rangle, \ldots)$, where we understand $\alpha, \beta$ as a row index, $G^\alpha_{\beta}$ as vectors and construct $\Gamma_{\alpha,\beta}[i]$ from them.

Proof: The proof is given in the Appendix. ■

It is an interesting open question to see how CMs are transformed under general completely positive maps, $\rho \to \sum_A A_i \rho A_i^\dagger$, where $\{A_i\}$ are Kraus operators, directly expressed in terms of the Kraus operators.

At the very beginning we have given two definitions of covariance matrices for the symmetric and non-symmetric case [33]. We will discuss this difference also later in the paper. However at this stage we mention a single connection between these two definitions for block CMs:

**Proposition II.14** (Block forms of CMs under local basis transformations). It is not possible to achieve for the block CMs $\gamma = \gamma^S$ via local basis transformations of the operator basis. The only states for which this relation holds have the reduced states $\rho_A = \text{tr}_B(\rho) = 1/d_A$ and $\rho_B = \text{tr}_A(\rho) = 1/d_B$, where $d_{A,B}$ are the dimensions of $\rho_{A,B}$. It follows that $\gamma = \gamma^S$ cannot be achieved by local unitary operations either.

Proof: The proof is given in the Appendix. ■

### III. THE COVARIANCE MATRIX CRITERION FOR SEPARABILITY

In this section, we introduce the covariance matrix criterion (CMC) for separability as our main topic of this paper. This is derived from the concavity property for CMs and the fact that the block CM for product states is block diagonal.

**Proposition III.1** (Covariance matrix criterion). Let $\rho$ be a separable state and $A_i (B_i)$ be orthogonal observables on $\mathcal{H}_A (\mathcal{H}_B)$, where the dimensions of the Hilbert spaces are $d_A (d_B)$, respectively. Define $M_i = A_i \otimes I$ for $i = 1, \ldots, d_A^2$ and $M_i = I \otimes B_i$ for $i = d_A^2 + 1, \ldots, d_A^2 + d_B^2$. Then there exist pure states $|\psi_k\rangle \langle \psi_k|$ for $A$ and $|\phi_k\rangle \langle \phi_k|$ for $B$ and convex weights $p_k$ such that if we define $\gamma = \sum_k p_k \gamma (|\psi_k\rangle \langle \psi_k|)$ and $\kappa = \sum_k p_k \gamma (|\phi_k\rangle \langle \phi_k|)$ the inequality

$$\gamma^S (\rho, \{M_i\}) \geq \kappa_A \oplus \kappa_B \Leftrightarrow \begin{pmatrix} A & C \\ \text{T} & B \end{pmatrix} \begin{pmatrix} \kappa_A & 0 \\ 0 & \kappa_B \end{pmatrix} \geq 0$$

holds. This means that the difference between left and right hand side must be positive-semidefinite. If there are no such $\kappa, \kappa_B$, then the state $\rho$ must be entangled.

Proof: First note that for this special choice of $M_i$, for any product state

$$\gamma (\rho_A \otimes \rho_B, \{M_i\}) = \gamma (\rho_A, \{A_i\}) \oplus \gamma (\rho_B, \{B_i\})$$

holds. Now, since any separable state can be written as $\rho = \sum_k p_k |\psi_k\rangle \langle \psi_k| \otimes |\phi_k\rangle \langle \phi_k|$, we can apply Prop. III.12 and arrive at the conclusion. ■

Note that the CMC is manifestly invariant under a change of the observables $\{A_k\}$ and $\{B_k\}$, as we know from Proposition II.13 (see also Eq. (37)); however, a suitable choice of them may simplify the evaluation a lot. Also, note that we have formulated the CMC for symmetric CMs, we will later discuss the case of non-symmetric CMs.

Obviously, as such, as formulated as in Prop. III.1 it is not clear that the CMC leads to an efficient and physically plausible test for separability: The main problem is to characterize the possible $\kappa_A$ and $\kappa_B$. As such, the formulation still contains an optimization over all pure product states. We will refer to an “evaluation of the CMC” hence whenever we can identify a property of $\kappa_A, \kappa_B$ that will render the above criterion an efficient test.

Some properties of we have derived above, notably

$$\text{tr}(\kappa_A) = d_A - 1$$

(see Proposition III.13), which we will use subsequently. We will now turn to feasible ways to evaluate the CMC. As a first step, we have to derive conditions on the blocks of a block matrix as in Eq. (34), which follow from the positivity condition in Eq. (33). Then, we ask how the observables $\{A_k\}$ and $\{B_k\}$ must be chosen in order to make a violation of Eq. (33) manifest.

Note the formal similarity of the condition $\gamma \geq \kappa_A \oplus \kappa_B$ to tests for separability for Gaussian states for systems with canonical coordinates. A CM in that context [30, 31] is any symmetric matrix satisfying $\gamma + i\sigma \geq 0$, where

$$\sigma = \bigoplus_{k=1}^n \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}.$$ (36)

A Gaussian state $\rho$ with CM $\gamma$ is now separable if and only if there exist covariance matrices $\gamma_A, \gamma_B$, each satisfying $\gamma_A, \gamma_B + i\sigma$ such that

$$\gamma \geq \gamma_A \oplus \gamma_B.$$ (37)

For non-Gaussian states, a violation of this condition is still sufficient to detect entanglement. Eq. (37), in turn, is simply a semi-definite program (SDP), so it can be efficiently decided [32]. The characterization of the right hand side is here an easy task, as these matrices are again constrained by a semi-definite constraint. We will see in section IV that for two qubits the CMC can be solved in a similar way as in the continuous variable case [34].

### IV. EVALUATION OF THE CMC

We would like to follow two strategies to evaluate the CMC as presented in the previous section. Both strategies are based on matrix invariants such as eigenvalues or singular values. Let us first characterize positive semi-definiteness of a block matrix of the type as in (33) in terms of singular values of its submatrices.
A. Evaluation of the CMC via singular values of submatrices

As a start, we state the following lemma:

**Lemma IV.1** (Block covariance matrices and unitarily invariant norms). If a positive matrix partitioned in block form is positive semi-definite,
\[
\begin{pmatrix}
A & C \\
C^T & B
\end{pmatrix} \geq 0,
\]
then
\[
\|A\| \|B\| \geq \|\|C\|\|^2,
\]
holds, where \(\|\cdot\|\) is any unitarily invariant norm. Specifically, this holds true for any Ky-Fan norm \(\|\cdot\|_{KF}\) defined as the sum of the largest \(k\) singular values. If we sum over all singular values, we arrive at the largest Ky-Fan norm, which is the trace norm.

**Proof:** The proof of this statement is actually a corollary of Theorem 3.5.15 of Ref. [23]. It is shown that
\[
\|A^p\| \|B^p\| \geq \|(C^1C)^{p/2}\|^2,
\]
for any \(p > 0\) and any unitarily invariant norm. For \(p = 1\) this is the result we are interested in. We will nevertheless present an alternative proof of this statement for Ky-Fan norms \(\|\cdot\|_{KF}\) defined as the sum of the largest \(k\) singular values, as the proof of Proposition IV.9 will make use of this proof.

Using the last Lemma we have:

**Proposition IV.2** (CMC evaluated using singular values). Let
\[
\gamma = \begin{pmatrix} A & C \\ C^T & B \end{pmatrix}
\]
be a CM. Then, if \(\rho\) is separable, we have
\[
\|C\|^2_{Tr} \leq \left[1 - \text{tr}(\rho_A^2)\right] \left[1 - \text{tr}(\rho_B^2)\right].
\]
If this inequality is violated, then \(\rho\) must be entangled.

**Proof:** We prove the claim applying the formula (39) directly, yielding
\[
\|C\|^2_{Tr} \leq \|A - \kappa_A\|_{Tr} \|B - \kappa_B\|_{Tr}
\]
Since \(A - \kappa_A\) as well as \(B - \kappa_B\) are Hermitian positive semi-definite matrices (due to concavity property of CMs) their trace norm will coincide with their trace. Hence \(\|A - \kappa_A\|_{Tr} = \text{tr}(A) - \text{tr}(\kappa_A) = 1 - \text{tr}(\rho_A^2)\), where we have used Corollary 1.19 and the fact that
\[
\sum_i A_{i,i} = \sum_i \langle A_i^2 \rangle - \langle A_i \rangle^2 = \langle d_{A} \rangle - \text{tr}(\rho_A^2),
\]
and \(\rho_A^2 = \sum_{i,j} (A_{i,j})^2 (A_{i,j})\).

Interestingly, this criterion has been proven already in a different context:

**Remark IV.3** (CMC and the criterion of Ref. [21]). The separability criterion in Proposition IV.2 is nothing but the separability criterion proposed in Theorem 1 of Ref. [21], hence the criterion of Ref. [21] is a corollary of the CMC.

Let us now connect the CMC to another type of entanglement criterion: There are several separability criteria in the literature which are based on the Bloch representation of density matrices. This representation in our case is just some particular choice of observables, namely one has to detach the identity from all others generators, which then have to be traceless. The fact that one of the observables is the identity, can simplify the CMC sometimes.

By definition the entries of the matrix \(C\) are given by
\[
C_{i,j} = \langle A_i \otimes B_j \rangle - \langle A_i \rangle \langle B_j \rangle,
\]
which consists of a linear (in the sense of mean values) and quadratic part. We define \(\mathcal{C}\) as the linear part of \(C\), i.e., \(\mathcal{C}_{i,j} = \langle A_i \otimes B_j \rangle\). Let us further consider \(\mathcal{C}\) as the submatrix of \(\mathcal{C}\), where the entries \(\langle 1_A \otimes B_j \rangle\) and \(\langle A_i \otimes 1_B \rangle\) are omitted, i.e., the first row and the first column are removed. Similarly, we can define matrices like \(\mathfrak{A}\) and \(\mathfrak{B}\) from \(A\) and \(B\). In the same spirit, we can define a submatrix of \(\kappa\) as \(\kappa^\text{red}\). Note that \(\text{tr}(\kappa^\text{red}) = \text{tr}(\kappa^\text{red})\), as the missing diagonal entry is the identity of \(\mathfrak{I}\), which is vanishing.

We are now able to establish a connection between the CMC and criteria based on the Bloch representation of density matrices:

**Proposition IV.4** (Relationship between CMC and criteria based on Bloch representations). Let
\[
\gamma = \begin{pmatrix} A & C \\ C^T & B \end{pmatrix}
\]
be a CM. Then if \(\rho\) is separable, we have
\[
\|\mathcal{C}\|^2_{Tr} \leq (1 - \frac{1}{d_A}) (1 - \frac{1}{d_B}).
\]
If this inequality is violated, then \(\rho\) must be entangled.

**Proof:** First, we can define two vectors \(|\psi^A\rangle|\psi^B\rangle\) with entries
\[
|\psi^A\rangle_i = \langle A_i |, \quad |\psi^B\rangle_i = \langle B_i |
\]
resulting in \(C = \mathcal{C} - |\psi^A\rangle\langle \psi^B|\). Similar relations hold for \(A\) and \(B\), so we can write the condition in CMC (33) in the form
\[
\frac{\langle \mathfrak{A} - \kappa_A | \mathcal{C} - \mathfrak{B} \rangle - \langle \psi^A \rangle - \langle \psi^B \rangle}{\langle \mathfrak{B} - \kappa_B \rangle} \text{tr} \geq 0.
\]
Positivity of the left hand side implies positivity of the first term \(X\) alone, since we subtract only one projector
which is itself positive. Concerning positivity of $X$ we can take $Q_{\text{red}}$, $B_{\text{red}}$, $C_{\text{red}}$, and $K_{\text{red}}$ instead, since positivity of a matrix implies positivity of all its main minors. Using Eq. (49), we get
\[ \| C_{\text{red}} \|_{\mathcal{T}_0} \leq \| Q_{\text{red}} - K_{\text{red}} \|_{\mathcal{T}_0} - \| B_{\text{red}} \|_{\mathcal{T}_0}. \]
Using that $\text{tr}(Q_{\text{red}}) = \sum_{i \geq 2} (A_i^2) = (dA/A) - (\langle A \rangle/dA)$ and $\text{tr}(K_{\text{red}}) = dA - 1$ proves the claim. ■

Interestingly, this separability criterion has also been proven before:

Remark IV.5 (CMC and the criterion of Ref. [16]). The separability criterion in Proposition IV.2 is nothing but the separability criterion for Bloch representations proposed in Ref. [16], hence the criterion of Ref. [16] is a corollary of the CMC.

Note that in Ref. [16] the observables have been normalized in a different way, leading to a slightly different formula.

Remark IV.6 (Connection between Propositions IV.1 and IV.2). Proposition IV.2 is strictly stronger than Proposition IV.1.
This fact was proven in version 5 of [21], which came out after submission of our paper to the arXiv.

Let us finish this subsection with a remark on the possible use of other Ky-Fan norms in the above argument. In fact, we do know more about the singular values (here eigenvalues) of $K_{\text{red}}$ and $K_{\text{red}}$ than their sum:

Lemma IV.7 (Ky-Fan norms of matrices in the CMC). The matrices $K_{\text{red}}$ (and similarly $K_{\text{red}}$) in Proposition IV.1 satisfy
\[ \sum_{j=1}^k \lambda_j(K_{\text{red}}) \leq \min(k, dA - 1), \]
for the non-increasingly ordered eigenvalues of $K_{\text{red}}$ and $K_{\text{red}}$.

Proof: One can argue as in Proposition IV.11 using the fact that a convex combination of matrices leads to more mixed matrices in the sense of majorization [33]. ■

This property can immediately be applied to evaluate the CMC, making use of proposition IV.1 and Weyl’s inequalities [33]. For example, if we consider $dA = dB = d$ and the $K$-Ky-Fan norm $\| \cdot \|_{K_{\text{red}}} = \langle A \rangle/dA$, we can apply the first of Weyl’s inequalities with $i = 1$, and $s = 1, \ldots, d - 1$, to conclude that
\[ \| A - K_{\text{red}} \|_{K_{\text{red}}} = \sum_{j=1}^k \lambda_j(A - K_{\text{red}}) \]
\begin{align*}
&\leq \sum_{j=1}^k \lambda_1(A) + \sum_{j=1}^k \lambda_j(-K_{\text{red}}) \\
&= (d^2 - d + 1 + s)\| A \| \\
&\leq \sum_{j=d^2-k+1}^{d^2} \lambda_j(K_{\text{red}}),
\end{align*}
where $\| A \|$ denotes the spectral norm of $A$. Using that $K_{\text{red}}$ will be more mixed in the sense of majorization than $\| \cdot \|_{K_{\text{red}}}$, one hence arrives at the observation that any separable state $\rho$ on a bipartite Hilbert space satisfies
\[ \langle (d^2 - d + 1 + s)\| A \| - s \rangle - \| C \|_{K_{\text{red}}}^2 \geq 0. \]
It is an interesting open question whether more sophisticated uses of the knowledge of spectral properties of $K_{\text{red}}$ and $K_{\text{red}}$ can be employed the further sharpen the evaluation of the CMC.

B. Evaluation of the CMC via traces of submatrices

Let us first prove a simple condition on the traces of $A$, $B$, and $C$, which follows from the CMC. In the following, we always assume that $dA \leq dB$. Sometimes we assume that the dimensions are the same, meaning that $d = dA = dB$.

Proposition IV.8 (CMC evaluated from traces). Let
\[ \gamma = \begin{pmatrix} A & C \\ C^T & B \end{pmatrix} \]
be the symmetric CM of a state $\rho$ and let $J = \{j_1, \ldots, j_d\} \subset \{1, \ldots, d^2 \}$ be a subset of $d^2$ pairwise different indices. Then if $\rho$ is separable, we have
\[ 2\sum_{i=1}^{d^2} \sum_{j \in J} |C_{i,j}| \leq \left( \sum_{i=1}^{d^2} A_{i,i} - dA + 1 \right) + \left( \sum_{i=1}^{d^2} B_{i,i} - dB + 1 \right) = [1 - \text{tr}(\rho_A^2)] + [1 - \text{tr}(\rho_B^2)], \]
If this inequality is violated, then $\rho$ must be entangled.
**Proof:** First, note that a necessary condition for a $2 \times 2$ matrix

$$X = \begin{pmatrix} a & c \\ c & b \end{pmatrix}$$

(56)

to be positive semidefinite is that $2|c| \leq a + b$. If $\rho$ is separable, then by the CMC we have $Y = \gamma - \kappa_A \oplus \kappa_B \geq 0$. This implies that all $2 \times 2$ minor submatrices of $Y$ have to be positive semidefinite as well. Hence for all $i, j$ we have

$$2|C_{i,j}| \leq A_{i,i} + B_{j,j} - (\kappa_A)_{i,i} - (\kappa_B)_{j,j}.$$  (57)

Summing over $i, j$ and using Corollary 11.9 proves the claim. 

We will use this Proposition mainly for the case that $d_A = d_B$ and where we sum over the diagonal entries of $C$. In this case, it just gives the condition that for separable states, $2\text{tr}(C) \leq 2 - \text{tr}(\rho_A^2) - \text{tr}(\rho_B^2)$. This is a quadratic polynomial in the entries of the state, and may be viewed as a suitable entanglement witness on two specimens on a state. In the light of this fact, the criterion evaluated in this fashion is surprisingly strong. It is also worth mentioning here that one can improve Proposition IV.8 by taking $4 \times 4$ minor submatrices for evaluation. Then, however, also off diagonal terms of $\kappa_{A/B}$ will occur, for which not many properties are known. This makes the resulting conditions difficult to evaluate.

Physically, Proposition IV.8 says that if the correlations $C_{i,j}$ are sufficiently large, then $\rho$ must be entangled. The question arises, how to find the observables, for which the $C_{i,j}$ are large. There are several ways of doing this. A first result is the following:

**Proposition IV.9 (Criterion in Proposition IV.8 and diagonal block matrices).** The criterion in Proposition IV.8 detects most states if the observables are chosen in such a way that $C$ is diagonal. For any state there exist a choice of observables that this can be achieved. However, even with this optimal choice of observables Proposition IV.8 delivers a strictly weaker separability criterion than Proposition IV.2.

**Proof:** It is clear that the criterion is optimal, if the trace of $C$ is maximal, which is the case if it is brought into the singular value diagonal form \[21, 22\]. This can always be achieved [see Eq. (37)]. The fact that Proposition IV.2 is stronger, was in a different language proven in Ref. \[20\].

Interestingly, the fact that Proposition IV.8 is weaker than Proposition IV.2 can also be seen from Eq. (100) from the alternative proof of Lemma IV.1. If $C$ is chosen to be diagonal, then Proposition IV.8 reduces to this equation with $\alpha = \beta$. Clearly, allowing $\alpha$ and $\beta$ to be different, improves the criterion. 

In the following, however, we will consider two different strategies: Firstly, we use the Schmidt decomposition in operator space of the density matrix \[37\]. This will lead to a natural choice of the observables \{A\_l\} and \{B\_l\}, and will further connect the CMC to the CCNR criterion.

Secondly, we will consider appropriate local filterings of the state \[38, 39, 40, 41\]. These are active transformations of the state, which, however, do not change the entanglement properties. Under this transformations, the state can be transformed into what is called its standard form in Ref. \[38\]. In this standard form, the CMC becomes very strong and even necessary and sufficient for two qubits.

### C. Schmidt decomposition and the CMC

We will first remind ourselves of what is called the Schmidt decomposition in operator space. It is the same construction as the ordinary Schmidt decomposition in the vector space now equipped with the Hilbert-Schmidt scalar product. A general density matrix of a composite system can be written as

$$\rho = \sum_{k=1}^{d_A} \sum_{l=1}^{d_B} \xi_{k,l} \hat{G}^A_k \otimes \hat{G}^B_l,$$  (58)

with real $\xi_{k,l}$ and the \{\hat{G}^A_k\} (respectively, \{\hat{G}^B_l\}) form an orthonormal Hermitian basis of observables. The Schmidt decomposition can now be achieved by diagonalizing the above expression using the singular value decomposition of the matrix $\xi$,

$$\rho = \sum_{k=1}^{d_A} \lambda_k G^A_k \otimes G^B_k,$$  (59)

where we made the assumption that $d_A \leq d_B$. Clearly, the Schmidt coefficients $\lambda_k$ are real and non-negative. Using the new basis observables \{\hat{G}^A_k\} and \{\hat{G}^B_l\} as observables for the construction of the symmetric block CM, we have a normal form of the CMC, which we will call the Schmidt CMC.

**Proposition IV.10** (Schmidt CMC). If $\rho$ is separable, then

$$2 \sum_i |\lambda_i - \lambda_i^2 g_i^A g_i^B| \leq 2 - \sum_i \lambda_i^2 [(g_i^A)^2 + (g_i^B)^2],$$  (60)

where we defined $g_i^A = \text{tr}(G_i^A)$ and $g_i^B = \text{tr}(G_i^B)$. If this condition is violated, the state must be entangled.

**Proof:** Using the orthonormality of the \{\hat{G}^{A(B)}_k\}, it is not difficult to see that with the observables from the Schmidt decomposition $C_{i,j} = \lambda_i \delta_{i,j} - \lambda_i \lambda_j g_i^A g_j^B$ holds. In addition, we have $\text{tr}(\rho_A^2) = \sum_i \lambda_i^2 (g_i^B)^2$. Together with Proposition IV.8, this proves the claim.

Interestingly, this Proposition includes the CCNR criterion as a corollary. This shows that the CMC, even without filtering, and evaluated merely via the trace of the blocks, once the matrix is brought to Schmidt form, is stronger than the CCNR, which it implies as a corollary.
Corollary IV.11 (CMC and CCNR). If a state $\rho$ is separable, then in the Schmidt decomposition
\begin{equation}
\sum_k \lambda_k \leq 1
\end{equation}
has to hold. This condition is just the CCNR criterion, hence the CCNR criterion is a corollary of the CMC.

Proof: Using the relations $|a - b| \geq |a| - |b|$ and $a^2 + b^2 \geq 2|ab|$ we have $2 \sum \lambda_i - \lambda_i^2 g_i A g_i B \geq 2 \sum \lambda_i - 2 \sum \lambda_i^2 |g_i A|^2 |g_i B|^2$ and $2 - \sum \lambda_i^2 |g_i A|^2 + |g_i B|^2 \leq 2(1 - \sum \lambda_i^2 |g_i A|^2 |g_i B|^2)$, which, due to the Proposition IV.10 proves the claim.

D. Filtering and the CMC

Let us now consider local filtering operations or SLOCC (stochastic local operations assisted by classical communication) \[41\] of the form
\begin{equation}
\rho \mapsto \hat{\rho} = (F_A \otimes F_B)\rho(F_A \otimes F_B)^†,
\end{equation}
where and $F_A \in SL(d_A, \mathbb{C})$ and $F_B \in SL(d_B, \mathbb{C})$ are invertible matrices on the respective Hilbert spaces. Clearly, such operations cannot map a separable state into an entangled one (although they might increase entanglement measures). Also, since $F_A$ and $F_B$ are invertible, they will also not destroy any entanglement that may be present in the state. In other words, $\rho$ is entangled if and only if $\hat{\rho}$ is entangled.

As has been shown in Refs. \[38,41\] we can bring any state of full rank (i.e., $\rho > 0$) by such filtering operations in its standard form which is given by
\begin{equation}
\hat{\rho} = \frac{1}{d_A d_B} \left( I + \sum_{k=1}^{d_A^2 - 1} \xi_k \hat{G}_k^A \otimes \hat{G}_k^B \right)
\end{equation}
where the $\{\hat{G}_k^A\}, \{\hat{G}_k^B\}$ are traceless orthogonal observables. Here, we again assumed that $d_A \leq d_B$.

The idea now is to first apply a filtering operation and bring the state into its normal form. Then, the new separability criteria are applied afterwards. Note that the reduction to the normal form is always possible. The merits of this approach are twofold: Firstly, the normal form reduces the number of relevant parameters, while still encoding all information about entanglement and separability. Secondly, the normal form is in a certain sense “more entangled” than the original state, as it was shown in Ref. \[40\]:

Remark IV.12 (Extremality of states in normal form). The local filtering operations bringing a mixed state into its normal form are those operations which maximize all entanglement monotones that remain invariant under determinant 1 SLOCC operations.

Therefore, it may be expected that many separability criteria become stronger if we first bring the state into its normal form. Note, however, that this does not hold for the PPT criterion, as local filtering leaves this criterion invariant.

Following Ref. \[38\], let us explain briefly an algorithm for transforming a state of a form as in Eq. (65) to its normal form in Eq. (66). As a starting point, one considers the compact space $D_A \otimes D_B$ of all normalized product density matrices $\rho_A \otimes \rho_B$. For any given density matrix $\rho$ one can define a function $f$ of $\rho_A$ and $\rho_B$ via
\begin{equation}
f_\rho(\rho_A, \rho_B) = \frac{\text{tr} [\rho(\rho_A \otimes \rho_B)]}{(\det \rho_A)^{1/d_A} (\det \rho_B)^{1/d_B}}.
\end{equation}

$f_\rho(\rho_A, \rho_B)$ is a family of positive well defined functions on the interior of $D_A \otimes D_B$, where the reduced density matrices both have full rank. Since $\rho$ has also full rank, we have $\text{tr} [\rho(\rho_A \otimes \rho_B)] > 0$ and because of compactness of $D_A \otimes D_B$ one has even stronger $\text{tr} [\rho(\rho_A \otimes \rho_B)] \geq c_\rho > 0$. Divergence of $f_\rho(\rho_A, \rho_B)$ on the boundary implies that it has a positive minimum on the interior of $D_A \otimes D_B$.

Minimization of the function $f_\rho$ will, as proven in Ref. \[38\], yield the filtering operations needed. Suppose the minimum value for $f_\rho$ attained for some product density matrix $\tau_A \otimes \tau_B$ with $\text{det} \tau_A > 0$, $\text{det} \tau_B > 0$. Each of them can be decomposed as (see Eq. (66) in Ref. \[38\])
\begin{equation}
\tau_A = T_A^\dagger T_A, \quad \tau_B = T_B^\dagger T_B, \quad T_{A/B} \in SL(d_{A/B}, \mathbb{C}) \quad (65)
\end{equation}
where the $T_A$ and $T_B$ are desired local filtering operations. Normalization factors have been ignored.

Using this filtering operations one obtains the new state $\hat{\rho}$ which has a form
\begin{equation}
\hat{\rho} = \frac{1}{d_A d_B} \left( I + \sum_{i=1}^{d_A^2 - 1} \sum_{k=1}^{d_B^2 - 1} \xi_{ik} \hat{G}_{ik}^A \otimes \hat{G}_{ik}^B \right)
\end{equation}
The final step involves a standard singular value decomposition of $\xi_{ik}$, which leads to Eq. (63). A priori, it is not clear whether the normal form is in some sense unique or not. However, it is easy to see that if we start from a given state and convert it into two different states in a normal form, then these two normal forms have to be connected by a local filtering operation. Using the fact that the reduced states of a state in the normal form are maximally mixed, one can further conclude that two different normal forms can only differ by a local unitary transformation.

In practice, the minimization of $f_\rho(\rho_A, \rho_B)$ in Eq. (64) can be performed by an iteration as follows: let us fix $\rho_B$ and consider only the minimization over $\rho_A$. This minimization can further be split into a minimization over the spectrum of $\rho_A$ and a local unitary transformation. If the spectrum is fixed, the optimal unitary is constructed such that $\rho_A$ and $X = \text{tr}_B[\rho(I \otimes \rho_B)]$ are diagonal in the same basis where the maximal eigenvalue of $X$ has the same eigenvector as the minimal eigenvalue of $\rho_A$ and the second largest eigenvalue of $X$ has the same eigenvector as
the second smallest eigenvalue of \( \rho_A \) etc. If the basis is fixed, and \( \lambda_k (\mu_k) \) are the eigenvalues of \( \rho_A (X) \) then a simple calculation using Lagrange multipliers shows that the optimal \( \lambda_k \) fulfill
\[
\lambda_k \sim \left[ \sum_{i \neq k} \mu_i \lambda_i / (\prod_{i \neq k} \lambda_i) \right]^{1/2},
\]
which can be used for an iterative determination of the optimal \( \lambda_k \). In this way, the optimization can be iterated, converging to a minimum. Note while it is known that every state can be brought into this normal form, the above procedure of Ref. \[38\] is not known to be strictly efficient in the physical dimension \( d \). Yet, for “reasonable physical dimensions”, the method in practice converges quickly. Moreover, and importantly, at the end of the procedure, one can easily (and efficiently) check via direct inspection whether the obtained filters map the state onto the normal form or not. Global optimality can hence be easily certified.

As one can directly calculate, for a state in the normal form the CM takes a really simple form, namely
\[
\gamma = \frac{1}{d_A d_B} \left( \text{diag}(0,d_B,d_B,\ldots) \text{diag}(0,\xi_1,\xi_2,\ldots) \right).
\]
Using this form we obtain the following strong separability criterion, which we call the filter CMC.

**Proposition IV.13 (Filter CMC).** If \( d = d_A = d_B \) and \( \rho \) is separable, then the coefficients in the filter normal form fulfill
\[
\sum_i \xi_i \leq d^2 - d.
\]

**Proof:** The claim obviously follows from Proposition IV.8 and the form of the CM for the normal form of the state.

Interestingly, for two qubits we have:

**Remark IV.14 (Filter CMC for two qubits).** For two qubits, the filter CMC in Proposition IV.13 is a necessary and sufficient criterion for separability.

**Proof:** If a two-qubit state is of full rank, the normal form reads
\[
\hat{\rho} = \frac{1}{4} \left( \mathbf{1} + \sum_{k=1}^{3} \xi_k \sigma_k^{A} \otimes \sigma_k^{B} \right),
\]
where \( \{ \sigma_k^{A/B} \} \) are the Pauli matrices \[38\]. Such states are diagonal in the Bell basis, and it is known that for these states \( \sum_{k=1}^{3} \xi_k \leq 2 \) is necessary and sufficient for separability \[38, 45\]. Note also that the filter normal form can be explicitly stated for two-qubit systems.

If an entangled (or separable) state is not of full rank, it can, as explicitly shown in Ref. \[39\], be brought by filtering operations arbitrarily close to a Bell diagonal state with finite (or vanishing) concurrence. Such a state will also be detected by the CMC (or not).

Direct comparison of this result with the discussion in Section II and Fig. 1 (and later the result of Proposition IV.2) might be confusing at this point, since we know already that the CMC itself cannot be necessary and sufficient for two qubits. This can be resolved in the following way: We have already learned that filtering brings the state in the form which in a certain sense contains the maximum amount of entanglement (it maximizes all monotones). This indeed shows that the filter CMC is sometimes a real improvement of the “bare” CMC, and filtering is more than just an appropriate choice of the observables.

Let us now consider the asymmetric case, when \( d_A < d_B \). We can formulate for this case following statement:

**Proposition IV.15 (Separability criterion for uneven local dimension).** If \( \rho \) is separable, then the following inequalities hold
\[
\sum_i \xi_i \leq \frac{d_A d_B}{2} \left[ 1 - \frac{1}{d_A} + \frac{1}{d_B} \right] + \min(0, -(d_A - 1) + (d_B^2 - d_A^2) \frac{1}{d_B})
\]
and
\[
\sum_i \xi_i \leq [d_A d_B(d_A - 1)(d_B - 1)]^{1/2}.
\]

holds. If one of these inequalities is violated, the state must be entangled.

**Proof:** Eq. (72) is nothing but an application of Proposition IV.3 (or IV.2), it has already been derived in Ref. 16. Concerning Eq. (71), we will again apply Proposition IV.8 but with two modifications. First, when carrying out the sum over \( 2|C_{i,j}| \leq A_{i,i} + B_{j,j} - \kappa_{A,i,i} - \kappa_{B,j,j} \) (see Eq. 67) in Proposition IV.8, we do not sum over all \( B_{i,i} \). But then, we cannot subtract all of the \( \kappa_{B,j,j} \) anymore, since \( d_B^2 - d_A^2 \) diagonal elements of \( \kappa_B \) do not occur in the sum.

As a first approach, we can drop completely the summation over all \( \kappa_{B,j,j} \), since they are positive anyway. This gives
\[
\frac{2}{d_A d_B} \sum_{i=1}^{d_A^2} \xi_i \leq 1 - \frac{1}{d_A} + \frac{d_A^2 - 1}{d_B},
\]
justifying one part of Eq. (71).

In a second approach, we estimate \( \sum_{i=1}^{d_A^2} \kappa_{B,i,i} \). As one can see by direct inspection, the non-vanishing elements of \( \gamma \) in Eq. 68 originate only from the linear part of CM (in the spirit of Proposition IV.3 this linear part is denoted by \( \mathfrak{g} \)). But as we have seen in the proof of Proposition 11.12 that this linear part \( \mathfrak{g} \) is just the same as the linear part of the direct sum of \( \kappa_A \oplus \kappa_B \) (denoted by \( \mathfrak{t}_A \oplus \mathfrak{t}_B \))
for separable states, i.e. \( \mathbf{g} = t_A \oplus t_B \), hence \( B = \mathcal{B} = t_B \).

This implies that for the diagonal elements of \( \kappa_B \) the relation \( \kappa_{B,i,i} \leq \mathcal{B}_{i,i} = 1/d_B \) holds, leading to

\[
\sum_{i=1}^{d_B} \kappa_{B,i,i} = d_B - 1 - \sum_{i=d_B+1}^{d_A} \kappa_{B,i,i} \geq d_B - 1 - (d_B^2 - d_A^2) \frac{1}{d_B}.
\]

(74)

This proves the second part of Eq. (74).

V. CONNECTION TO LOCAL UNCERTAINTY RELATIONS

In this section we will further analyze the connection of CMC with the separability criterion based on local uncertainty relations (LURs) \[18\]. To start with, we again state the LUR criterion as a reminder:

**Proposition V.1** (Criterion based on local uncertainty relations). Let be \( \hat{A}_k \) and \( \hat{B}_k \) observables in system A and B, respectively, for which some of the variances on single systems is bounded by constants \( U_A, U_B \) such that

\[
\sum_{k} \delta^2(\hat{A}_k) \geq U_A \quad \text{and} \quad \sum_{k} \delta^2(\hat{B}_k) \geq U_B.
\]

(75)

Then, we have for separable states

\[
\sum_{k} \delta^2(\hat{A}_k \otimes 1 + 1 \otimes \hat{B}_k) \geq U_A + U_B
\]

(76)

and violation implies the presence of entanglement.

Physically, the LURs state that separable states inherit the uncertainty relations from their reduced states, which is not the case for entangled states. Due to this observation the LURs have attracted a considerable interest, and a number of interesting properties have been discovered: LURs can detect bound entangled states \[42\] and can be used to estimate the concurrence \[43\]. They discovered: LURs can detect bound entangled states \[42\], while for the LURs the appropriate observables have to be identified. Moreover, we can state:

**Corollary V.3** (Insufficiency of LUR to detect all entangled states). There exist entangled two qubit states which can not be detected by a LUR, hence LURs are not a necessary and sufficient criterion for separability.

**Proof:** In the Section \[11\] we have already constructed a family of states \( \rho_\gamma \) which cannot be detected by the CMC, as their symmetric block CM is compatible with a separable as well as an entangled state. This proves the claim.

VI. THE CMC FOR TWO QUBITS

After the previous discussion of the situation of Hilbert spaces of arbitrary finite dimension, we now turn to the important simple case of a \( 2 \times 2 \)-system – two qubits – in some more detail. We take as observables the set \( \{ A_k \} = \{ B_k \} = \{ 1/\sqrt{2}, \sigma^x/\sqrt{2}, \sigma^y/\sqrt{2}, \sigma^z/\sqrt{2} \} \) as in Eq. (8).

Since these observables contain the identity, one can easily check that many terms in the symmetric block CM vanish. Effectively, \( \gamma \) is actually a \( 6 \times 6 \) matrix (denoted by \( \gamma^{\text{eff}} \)) originating only from the \( \{ A_k \} \) with \( k = 1, 2, 3 \) which are not proportional to the identity, and not by an \( 8 \times 8 \) as one could guess from the general theory.

To characterize the \( \kappa_A \) in the CMC, note that for a pure state \( \psi \) on system A we find, according to Proposition \[11\] the following properties of the \( 4 \times 4 \) matrix \( \gamma^{\text{eff}}(\psi) \):

(i) \( \text{Rank}(\gamma) = 2 \).

(ii) The nonzero eigenvalues of \( \gamma \) are equal to \( 1/2 \) in a suitable basis.

We also know that in the chosen basis, the first row as well as the first column of \( \gamma(\psi) \) vanish, and we have

\[
\gamma(\psi) = \mathcal{O}_1 \oplus \gamma(\psi)^{\text{eff}}
\]

(77)

where \( \gamma^{\text{eff}} \) is the effective \( 3 \times 3 \) CM as above. This has to be of rank two with eigenvalues 1/2. This implies that \( \gamma(\psi)^{\text{eff}} \) can be written as

\[
\tilde{\gamma}(\psi) = \frac{1}{2}(1 - \phi_A \langle \phi_A \rangle),
\]

(78)

where \( \mathcal{I}_3 \) denotes a \( 3 \times 3 \) identity matrix, and \( \phi_A \in \mathbb{R}^3 \). In fact, any matrix of this form is a valid CM:

**Lemma VI.1.** For any vector \( \phi \in \mathbb{R}^3 \) a matrix of the form \( \mathcal{I}_3 - |\phi_A \rangle \langle \phi_A | / 2 \), is a valid CM of some two qubit state. Consequently, the set of valid \( \kappa_A \) is given by all matrices of the form

\[
\kappa_A = \frac{1}{2}(\mathcal{I}_3 - \rho_A)
\]

(79)

where \( \rho_A \) is a real \( 3 \times 3 \) matrix with trace one and positive eigenvalues.
Let $\rho$ solution to the dual problem with primal duality holds, meaning that a pair $(x^*, Z^*)$ exists such that $c^T x^* + \text{tr}(F_0 Z^*) = 0$ holds. See also Ref. [17] for an extensive treatment of the subject.

For the evaluation of the CMC, we can formulate the problem differently, such that if the primal problem detects the state as entangled, then from the solution of the dual problem local operators can be extracted which allow for the detection of the state with LURs. This is similar in spirit as the solution in the continuous variable case [34].

Explicitly, we formulate the primal problem as

$$
\begin{align*}
& \text{min} & & -\lambda \\
& \text{subject to} & & \gamma^{\text{eff}} - \kappa_A \oplus \kappa_B \geq 0 \\
& & & \kappa_{A,B} = \frac{1}{2} \left[ (1 + \lambda) \mathbb{I}_3 - \rho_{A,B} \right] \geq 0 \\
& & & \text{tr} (\rho_{A,B}) = 1 + \lambda.
\end{align*}
$$

(84)

In this formulation, the matrices $\kappa_{A,B}$ are positive and have trace $1 + \lambda$. If the constraints can be fulfilled for $\lambda < 0$ only, then the state corresponding to $\gamma^{\text{eff}}$ is entangled. The SDP can be formulated with block-diagonal matrices $\{F_i\}$ collecting all the constraints. For instance, by inserting the definition of $\kappa_{A,B}$ into the first constraint and expressing the equality constraints by a ‘$\geq$’ and a ‘$\leq$’ constraint, we can write $F_0$ as

$$
F_0 = \left( \gamma^{\text{eff}} - \frac{1}{2} \mathbb{I}_6 \right) \oplus \frac{1}{2} \mathbb{I}_3 \oplus \frac{1}{2} \mathbb{I}_3 \oplus (-1) \oplus 1 \oplus (-1) \oplus 1,
$$

(85)

and the matrices $F_i$ accordingly by choosing a basis for real, symmetric matrices for the blocks. Without loss of generality, the matrix $Z$ can be chosen block-diagonal accordingly. In the order from above we have $Z = Z_1 \oplus Z_2^A \oplus Z_2^B \oplus Z_3^{A1} \oplus Z_3^{A2} \oplus Z_3^{B1} \oplus Z_3^{B2}$, where $Z_1$ is a $6 \times 6$ matrix, $Z_2^{A,B}$ are of dimension $3 \times 3$, and $Z_3^{A,B,1,2}$ are scalar. The dual problem can then be formulated as

$$
\begin{align*}
& \text{max} & & -\text{tr}(\gamma^{\text{eff}} Z_1) - 1 \\
& \text{subject to} & & -\frac{1}{2} [\text{tr}(Z_1) - \text{tr}(Z_A^1) - \text{tr}(Z_B^1)] \\
& & & = Z_3^{A1} - Z_3^{A2} + Z_3^{B1} - Z_3^{B2} - 1 \\
& & & = -2(Z_3^{A,B})_{i < j} - 2(Z_3^{A,B})_{i = j} \\
& & & = (Z_3^{A,B})_{i = j} - (Z_3^{A,B})_{i < j},
\end{align*}
$$

(86)

where $Z_3^{A,B}$ are the single-particle subblocks of system $A$ and $B$, respectively, and $i$ and $j$ run from 1 to 3. It turns out that $Z_1$ has the properties of an entanglement witness in the space of covariance matrices (CM-witness) as in the continuous-variables case [34]:

**Proposition VI.3** (CM-Witness from dual program). For every feasible solution $Z$ to the dual program formulated above, the matrix $Z_1$ is a CM-witness in the sense that it fulfills $\text{tr}(\gamma^{\text{eff}} Z_1) \geq 1$ for all CMs $\gamma^{\text{eff}}$ from separable states. Hence if $\text{tr}(\gamma^{\text{eff}} Z_1) < 1$ then the corresponding state is entangled. Further, it is optimal in the sense that $\text{tr}(\gamma^{\text{eff}} Z_1)$ is the minimal value of $\text{tr}(\gamma^{\text{eff}} X)$ for any $X \geq 0$ of the same dimensions.
Proof: It follows from weak duality that \( \text{tr}(\gamma^\text{eff}Z_1) \geq 1 + \lambda \), hence \( \text{tr}(\gamma^\text{eff}_S Z_1) \geq 1 \) holds for all \( \gamma^\text{eff}_S \) from separable states. In this case, strong duality holds, which we prove by providing an example:

\[
Z = \frac{3}{2} \mathbb{I}_6 \oplus \mathbb{I}_3 \oplus \mathbb{I}_3 \oplus \frac{3}{4} \oplus \frac{3}{4} \oplus 1 > 0
\]  

fulfills all constraints. Hence there exist \((\lambda^*, Z^*)\) such that \( \text{tr}(\gamma^\text{eff}_S Z_1^*) = 1 + \lambda^* \) holds, and the dual program reaches the minimal value of \( \text{tr}(\gamma^\text{eff}_S Z_1) \).

If the entanglement of a state is detected by a CW-witness \( Z_1 \), then it is possible to write down a LUR detecting the state as well. This is remarkable because it is in general very difficult to find a LUR detecting the entanglement of a given state.

**Proposition VI.4 (LUR observables from witness).**

Given a CM-witness \( Z_1 \), it is possible to define LUR matrices \( \{A_k\} \) and \( \{B_k\} \) from \( Z_1 \) such that

\[
\text{tr}(\gamma^\text{eff}_S Z_1) = \sum_k \delta^2(A_k \otimes I + I \otimes B_k)
\]

holds.

Proof: The LUR corresponding to \( Z_1 \) can be extracted as shown in the proof of Proposition VI.2. In the Appendix: we can spectrally decompose \( Z_1 = \sum_k \lambda_k |\psi_k\rangle \langle \psi_k| =: \sum_k \lambda_k (\alpha(k) \oplus \beta(k)) (\alpha(k) \oplus \beta(k)) \). Defining the local LUR variables \( \hat{A}_k = \sqrt{\lambda_k} \sum_i \alpha_{ik} A_i \) and \( \hat{B}_k = \sqrt{\lambda_k} \sum_i \beta_{ik} B_i \) we have for \( \rho \) that \( \text{tr}(Z_1 \gamma^\text{eff}) = \sum_k \delta^2(\hat{A}_k \otimes I + I \otimes \hat{B}_k) \), where \( \{A_k\} \) and \( \{B_k\} \) are defined in Eq. (80).

VII. EXAMPLES

In this section, we consider bound entangled states of two different types, and investigate the strength of the different criteria discussed in this paper.

In the first example, we take the \( 3 \times 3 \) bound entangled states, called chessboard states, introduced by D. Bruß and A. Peres [48]. They are defined as

\[
\rho = \mathcal{N} \sum_{j=1}^{4} |V_j\rangle \langle V_j|,
\]

where \( \mathcal{N} \) denotes the normalization, and we used the unnormalized vectors

\[
|V_1\rangle = |m, 0, ac/n; 0, n, 0; 0, 0, 0\rangle,
\]

\[
|V_2\rangle = |0, a, 0; b, 0, c; 0, 0, 0\rangle,
\]

\[
|V_3\rangle = |n, 0, 0; 0, -m, 0; ad/m, 0, 0\rangle,
\]

\[
|V_4\rangle = |0, b, 0; -a, 0, 0; 0, d, 0\rangle.
\]

Characterization of the family is done by six real parameters. We tested all criteria, presented in this paper on randomly generated chessboard states, where parameters have been drawn from the normal distribution with zero mean value and standard deviation of two. The results of this test are presented on the Fig. 2.

As one can see from Fig. 2 the most of the states are detected by bringing first the state in its normal form (Proposition VI.13 - 98.86% of all states). The criterion, which uses an estimation of singular values of the offdiagonal block of CM (Proposition VI.2), which was also proposed earlier in [20] detects 22.57%, whereas another criterion proposed in this paper (Proposition VI.9) detects 22.00%. Moreover the criterion, which uses Schmidt decomposition (Proposition IV.10) detects 20.00% which is more or less the same amount as is detected by CCNR criterion - 19.52%. Finally the criterion presented in Proposition VI.1 which was first proposed by de Vicente [16] detects only 8.57% of randomly generated chessboard states.

As the second example, we consider \( 3 \times 3 \) bound entangled states arising from an unextendible product basis [49], mixed with white noise:

\[
|\psi_0\rangle = \frac{1}{\sqrt{2}} (|0\rangle(|0\rangle - |1\rangle)), \quad |\psi_1\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)|2\rangle,
\]

\[
|\psi_2\rangle = \frac{1}{\sqrt{2}}(|1\rangle - |2\rangle), \quad |\psi_3\rangle = \frac{1}{\sqrt{2}}(|1\rangle - |2\rangle)|0\rangle,
\]

\[
|\psi_4\rangle = \frac{1}{3}(|0\rangle + |1\rangle + |2\rangle)(|0\rangle + |1\rangle + |2\rangle),
\]

\[
\rho_{BE} = \frac{1}{4} (I - \sum_{i=0}^{4} |\psi_i\rangle \langle \psi_i|),
\]

\[
\rho_{UP}(p) = p \rho_{BE} + (1 - p) \frac{1}{9}
\]

These states are detected by Proposition VI.13 for \( p \geq 0.8723 \) while the best known positive map detects them only for \( p \geq 0.8744 \) (see [37] and references therein). Besides this we have also tested all other criteria presented in this paper. Criteria of Propositions VI.2, VI.9 both detect these states for \( p \geq 0.8822 \). The criterion derived for
Schmidt decomposed states (Proposition IV.10) detects the states for \( p \geq 0.8834 \), whereas the CCNR criterion detects them for \( p \geq 0.8897 \). Finally Proposition IV.4 detects the states for \( p \geq 0.9493 \).

Finally, let us shortly comment on the efficiency of the implementation of all these criteria. The filtering operation can be implemented quite fast, using the simple algorithm outlined above takes a few seconds on a desktop computer (5 × 5 system: ca. 6 sec., 10 × 10 system: ca. 24 sec., 15 × 15 system: ca. 72 sec.). Then, the trace norm of \( C \) can be quickly computed as the trace norm of the realignment of the matrix \( \rho - \rho_A \otimes \rho_B \) \[21\]. For comparison, only the first step of the semidefinite program of Ref. \[14\] requires already ca. 10 min. for a 4 × 4 system, becoming practically unfeasible for higher dimensions.

VIII. CONCLUSION AND OUTLOOK

In this work, we have further developed the ideas of Ref. \[22\] and investigated the covariance matrix criterion (CMC). We have shown that this is a strong separability criterion, which can be simply evaluated. Combined with filtering it is necessary and sufficient for two qubits and in higher dimensions it detects states where the PPT criterion fails. Moreover, it contains many other separability criteria, which have been proposed to complement the PPT criterion as corollaries.

There are several open problems which deserve a further investigation:

- First, one might study the exact relation between the CMC for symmetric CMs and non-symmetric CMs. In the present paper, we have used only the trace of \( \kappa^{A/B} \) for the evaluation, hence this difference did not become apparent. However, as the non-symmetric CM describes the state completely and encodes therefore all information about the separability properties, this difference might be a way to improve the CMC. In addition, one could investigate the relation between the linear part and the nonlinear part of the CM in some more detail. In the proof of Prop. IV.15 we have seen already that such an investigation may indeed improve the CMC.

- Another interesting open question is to relate the CMC to quantitative statements, such as to the estimation of entanglement measures. One should expect that the program of Ref. \[51\] linking violations to quantitative statements on the entanglement content is applicable to the discussed criteria. Also, similar relations hold for Gaussian states \[52\]. First steps in this direction have already been taken in Refs. \[17, 24, 43\].

- Finally, it would be very interesting to develop a theory similar to ours for entanglement of multiparticle systems. Here, however, a significant amount of work has yet to be done, as it is not even obvious how to identify the object corresponding to the block CM for multipartite systems.

IX. ACKNOWLEDGMENTS

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X. APPENDIX

In this appendix, we present the more technical proofs of our previous statements.

Proof of Proposition IV.15. Let us first explain some properties of the matrix \( \Gamma \). This matrix has entries which are just the basis vectors \( G_i \) written as columns. Moreover, \( \Gamma^\dagger = \Gamma \Gamma^\dagger \), i.e., \( \Gamma \) is a unitary, since

\[
(\Gamma^\dagger \Gamma)_{i,j} = \sum_k \Gamma^\dagger_{ik} \Gamma_{kj} = \sum_{\alpha,\beta} (G_i^{\alpha,\beta})^* G_j^{\alpha,\beta} = \sum_{\alpha,\beta} (G_i^{\beta,\alpha})^* G_j^{\alpha,\beta} = \text{tr}(G_i G_j) = \delta_{i,j},
\]

where we have used the orthogonality and hermiticity of \( G_i \). However \( \Gamma \) is a special unitary, since the columns are orthonormal Hermitian observables. Now we have in Eq. (93)

\[
\sum_j O_{i,j} G_j^{\alpha,\beta} = \sum_j G_j^{\alpha,\beta} (O^T)_{j,i} = (\Gamma O^T)_{\alpha,\beta|i},
\]

where we have used the definition of \( \Gamma \) and the fact that the expression in the middle of Eq. (93) is nothing but \( i \)-th column of \( \Gamma O^T \). Conversely,

\[
(U G_i U^\dagger)_{\alpha,\beta} = U_{\alpha,\delta} G_i^{\delta,\gamma} U_{\gamma,\beta}^\dagger = U_{\alpha,\delta} U_\delta^* \Gamma_{\delta,\gamma|i} = (U \otimes U^*)_{\alpha,\beta,\delta,\gamma} \Gamma_{\delta,\gamma|i} = (U \otimes U^*)_{\alpha,\beta|i},
\]

where we have used the definition of \( \Gamma \) and that \( A_{i,k} \otimes B_{l,m} \equiv (A \otimes B)_{i,l,k,m} \). Therefore we can write

\[
O^T = \Gamma^\dagger (U \otimes U^*) \Gamma = \Gamma^\dagger (U^* \otimes U) \Gamma^\dagger, \\
O = \Gamma^\dagger (U \otimes U^T) \Gamma = \Gamma^\dagger (U^T \otimes U^\dagger) \Gamma^\dagger,
\]

where we have used that \( O \) is real. With these representations, we can finally check the orthogonality of the \( O \) as

\[
O^T O = \Gamma^\dagger (U^* \otimes U) \Gamma^\dagger (U^T \otimes U^\dagger) \Gamma^* = \Gamma^\dagger (U^* \otimes U) \Gamma^\dagger (U^T \otimes U^\dagger) \Gamma^* = \Gamma^\dagger (U^* U^T \otimes U U^\dagger) \Gamma^* = \Gamma^\dagger \Gamma^* = \Gamma.
\]

\[\blacksquare\]
II.14. Let us consider only subsystem $CM$ does not depend on the particular choice of basis in $\gamma$ by use of the commutators

$|v\rangle$ from the singular value decomposition of norms: $A,B$ pressions like $T$ aking the sum over $k$ $\sigma^2=|V\rangle_2^{\otimes k},$ so the symmetry of $CM$ does not depend on the particular choice of basis in observable space.

Therefore we are able to choose the standard basis. Let us consider only subsystem $A$, i.e., left upper block of matrix $\gamma,$ and let us assume that $A=A^T$ holds. As we have showed already, we can obtain $\rho_A$ from the matrix $A$ by use of the commutators $A_{a_{ij}}-A_{i_{ja}}=(M_A^k,M_B^k)$. However, all those commutators vanish for the case $A=A^T$. Since then $(X_{k,l})=(Y_{k,l})=0$ for all $k,l$, it follows that $\rho_A$ is diagonal. The diagonal elements can also be determined as in Prop. II.4 and since also $(Z_{k,l})=0$ for all $k,l$, it follows that $\rho_A=1/d_{A},$ which completes the first part of the proof.

Finally, local unitary transformations are only a subclass of the orthogonal transformations considered before, hence $\gamma=\gamma^T$ cannot be achieved by a local unitary transformation of $\rho$ neither.

Alternative proof of Proposition IV.4 for Ky-Fan norms: For a matrix as in Eq. 38 the following condition has to be fulfilled:

$$\begin{pmatrix} \alpha \\ \beta \end{pmatrix} \begin{pmatrix} A & C \\ CT & B \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \geq 0,$$  

(98)

for all vectors $|\alpha\rangle,|\beta\rangle,$ which implies that $\langle\alpha|A|\alpha\rangle+\langle\beta|B|\beta\rangle \geq 2\alpha\beta|C|\langle\beta|$, where we took $-|\beta\rangle$ instead of $|\beta\rangle$ for convenience. Especially, we can take $|\alpha\rangle=|\psi_k\rangle$ and $|\beta\rangle=|\phi_k\rangle,$ where the vectors $|\psi_k\rangle$ and $|\phi_k\rangle$ are singular vectors from the singular value decomposition of $C$ and $\langle\psi_k|C|\phi_k\rangle=\sigma_k(C)$ is the $k$-th singular value. Hence

$$\alpha^2\langle\psi_k|A|\psi_k\rangle + \beta^2\langle\phi_k|B|\phi_k\rangle \geq 2\alpha\beta\langle\psi_k|C|\phi_k\rangle.$$  

(99)

Note that $\langle\psi_k|A|\psi_k\rangle$ and $\langle\psi_k|A|\psi_k\rangle$ are greater than zero, because $A$ and $B$ are positive semi-definite matrices. Taking the sum over $k$ and noting that for $A$ and $B$ expressions like $\sum_{k=1}^{K} |\psi_k\rangle A |\psi_k\rangle$ are a lower bound on the $K$-th Ky-Fan norm 35 we get

$$\alpha^2||A||_{KF} + \beta^2||B||_{KF} \geq 2\alpha\beta||C||_{KF}.$$  

(100)

The last formula is necessary and sufficient condition for the $2 \times 2$ matrix

$$\begin{pmatrix} ||A||_{KF} & ||C||_{KF} \\ ||C||_{KF} & ||B||_{KF} \end{pmatrix} \geq 0$$  

(101)

to be positive semi-definite and having a non-negative determinant, from which the claim follows.

Proof of Proposition IV.2. The proof is an adaption of a similar proof given in Ref. 29. We will often use the property that CMs can be used to compute variances. Imagine $N=\sum_k \nu_k M_k$ is a linear combination of the $M_k$ with $\nu_k \in \mathbb{R}$, then

$$\delta^2(N) = \sum_{k,l} \nu_k \nu_l ((M_k M_l) - (M_k) (M_l)) = (\nu|\gamma (\{M\})|\nu).$$  

(102)

Let us now assume that $\rho$ violates the LURs and we can find $A_k, B_k, U_A, U_B$ as in Proposition IV.4. We assume that the CMC is fulfilled, i.e., there exist $\kappa_A$ and $\kappa_B$ such that for the CM $\gamma$ we have $\gamma \geq \kappa_A \oplus \kappa_B$. We can write

$$\hat{A}_k = \sum_i \alpha_i^{(k)} A_i$$  $\hat{B}_k = \sum_i \beta_i^{(k)} B_i$$  

(103)

where the $\{A_k\}$ and $\{B_k\}$ are the observables chosen in the definition of $\gamma$. This leads to $\delta^2(\hat{A}_k \otimes 1 + 1 \otimes \hat{B}_k) = \langle\alpha^{(k)}\otimes\beta^{(k)}|\gamma|\alpha^{(k)}\otimes\beta^{(k)}\rangle$. Also, by definition

$$\kappa_A \oplus \kappa_B = \sum_l p_l \gamma (|a_l\rangle \langle a_l|) \oplus \gamma (|b_l\rangle \langle b_l|)$$  

(104)

and hence $\langle\alpha^{(k)}\otimes\beta^{(k)}|\kappa_A \oplus \kappa_B|\alpha^{(k)}\otimes\beta^{(k)}\rangle = \sum_l p_l [\delta^2(\hat{A}_k)|a_l\rangle \langle a_l| + \delta^2(\hat{B}_k)|b_l\rangle \langle b_l|].$ But then summing over $k$ yields

$$\sum_k \delta^2(\hat{A}_k \otimes 1 + 1 \otimes \hat{B}_k)$$  

(105)

$$\geq \sum_{k,l} [\delta^2(\hat{A}_k)|a_k\rangle \langle a_k| + \delta^2(\hat{B}_k)|b_k\rangle \langle b_k|]$$  

$$\geq \min_{|a\rangle} \sum_k [\delta^2(\hat{A}_k)|a\rangle \langle a| + \min_{|b\rangle} \sum_k [\delta^2(\hat{B}_k)|b\rangle \langle b|]$$  

$$\geq U_A + U_B,$$

which is a contradiction to our assumption that $\rho$ violates the LURs.

To show the converse direction, let us assume that $\rho$ violates the CMC. Let us define a set of matrices as $X = \{x|x = \kappa_A \oplus \kappa_B + P$ with $P \geq 0\}$, which geometrically is a closed convex cone. Using this definition, we can formulate the CMC differently, by saying that if $\rho$ is separable, then $\gamma \in X$. As our $\rho$ violates the CMC, we have $\gamma \notin X$.

According to a corollary to the Hahn-Banach theorem 64 for each $\gamma \notin X$ there exist a symmetric matrix $W$ and a number $C$ such that $tr(W \gamma) < C$ while

$$tr(W x) > C \forall x \in X.$$  

(106)

Since $X$ is a non-compact cone, and we can add arbitrary positive operators to the elements of $X$, we can conclude that $tr(W P) \geq 0$ has to hold for all $P \geq 0$, and consequently we have $W \geq 0$. Now let us make
Finally, since the CMC is violated, $\gamma \notin X$ and $\sum_k \delta^2(\hat{A}_k \otimes I + I \otimes \hat{B}_k) = \text{tr}(W \gamma) < C < U_A + U_B$ leading to a violation of the LURs criterion.

Note that in principle this proof also applies to the CMC for non-symmetric CMs. Then, however, the "observables" in the LURs will be non-hermitian, their variance has to be defined as $\delta^2(X) = \langle XX^\dagger \rangle - \langle X \rangle \langle X^\dagger \rangle$ and their physical interpretation is not so clear.

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