

Analyzing Quantum Entanglement with the Schmidt Decomposition in Operator Space

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Characterizing entanglement is central for quantum information science. Special observables which indicate entanglement, so-called entanglement witnesses, are a widely used tool for this task. The construction of these witnesses typically relies on the observation that quantum states with a high fidelity to some entangled target state are entangled, too. We introduce a general method to construct entanglement witnesses based on the Schmidt decomposition of observables. The method works for two-particle and multiparticle systems and is strictly stronger than fidelity-based constructions. The resulting witnesses can also be used to quantify entanglement and to characterize its dimensionality. Finally, we present experimentally relevant examples, where our approach improves entanglement detection significantly.

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Introduction—In recent years, several experimental breakthroughs on different quantum technologies have been achieved. Examples are the demonstration of quantum supremacy with superconducting qubits [1], the implementation of quantum cryptography using a satellite [2] or in a device-independent manner [3,4], and the study of quantum phases using digital quantum simulation [5]. In such experiments large datasets are collected, and the problem arises of how to analyze them and connect them with the underlying quantum phenomena. For instance, if one wishes to reconstruct the density matrix of the quantum state arising in an experiment, methods like compressed sensing [6], matrix-product-state tomography [7], shadow tomography [8,9], and forms of overlapping tomography [10,11] have been designed.

For analyzing quantum correlations in experiments one frequently considers specific inequalities signaling the presence of correlations. The paradigmatic examples are Bell inequalities, whose violation signals the presence of quantum nonlocality [12]. Bell inequalities do not rely on assumptions on the measurement devices, and if knowledge about at least some of the implemented measurements is given, steering inequalities [13] or entanglement witnesses [14–16] are more efficient. In short, an entanglement witness is an observable with a non-negative expectation value on all separable states; hence a negative expectation value signals the presence of entanglement. Clearly, finding all entanglement witnesses is a hard task, as it is equivalent to characterizing all entangled states, which is known to be an NP-hard problem [17]. Still, many constructions exist,

often based on the idea of measuring the fidelity of the experimental state with some target state. If this fidelity is high enough, entanglement must be present.

In this Letter, we present a method to analyze quantum entanglement based on the so-called Schmidt decomposition of operators. The Schmidt decomposition is a ubiquitous tool when analyzing pure two-particle quantum states, but it can also be applied to bipartite observables. Our method leads to novel entanglement witnesses, which outperform fidelity-based witnesses and tolerate significantly more noise when analyzing multiparticle entanglement. Our approach is computationally simple and can also be used to quantify entanglement or its dimensionality.

Entanglement and witnesses—To start, recall that a bipartite quantum state ρ_{AB} shared by two parties, traditionally named Alice and Bob [14,18] is separable if it can be written as $\rho_{AB} = \sum_k p_k |a_k\rangle\langle a_k| \otimes |b_k\rangle\langle b_k|$, where the p_k form a probability distribution. If a state cannot be written in this way, it is entangled, which is, for many quantum tasks, a necessary condition to outperform classical protocols [19,20]. Unless stated otherwise, we assume that the dimensions of Alice’s and Bob’s space are the same, $d_A = d_B = d$.

For characterizing quantum entanglement, in experiments as well as in theory, entanglement witnesses have turned out to be useful [16,21,22], since they do not require full knowledge of the quantum state. As already mentioned, entanglement witnesses have a positive expectation value on separable states, so measuring a negative expectation value proves entanglement. For the construction of witnesses, several methods exist [22–29], and one of the well-known key methods is the use of witnesses based on the fidelity with a given *pure* target state. They are of the form $\mathcal{W} = \alpha \mathbb{1} - |\psi\rangle\langle\psi|$, where $|\psi\rangle$ is some pure entangled target state. This witness expresses the fact that states with a high

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fidelity with $|\psi\rangle$, namely the ones with $F_\psi = \langle \psi | \rho | \psi \rangle > \alpha$ are entangled, too. Three remarks are in order. First, the coefficient α can directly be computed. If $|\psi\rangle = \sum_{i=1}^R s_i |ii\rangle$ is the Schmidt decomposition (with decreasingly ordered Schmidt coefficients $s_i > 0$ and Schmidt rank R), it is given by the maximal squared Schmidt coefficient $\alpha = s_1^2$ [21]. Second, while fidelity-based witnesses are easy to construct, they have the disadvantage that they are not able to detect all entangled states, such as states with a positive partial transpose [30,31]. Still, fidelity-based witnesses have the advantage that they can be extended easily to the multiparticle case by considering the Schmidt decompositions for the different bipartitions [21]; this makes them the standard tool for analyzing entanglement in current experiments [32–34].

The main idea—To introduce our main idea, let us start by pointing out the well-known fact that the Schmidt decomposition does not apply to pure states only, but also to observables. Indeed, one can decompose any operator \mathcal{X} acting on a bipartite space in the operator Schmidt decomposition (OSD) [35,36]

$$\mathcal{X} = \sum_{i=1}^S \mu_i G_i^A \otimes G_i^B. \quad (1)$$

Here, the $\mu_i \geq 0$ are the operator Schmidt coefficients (OSC), chosen to be decreasingly ordered, and if \mathcal{X} is a quantum state, then the largest one μ_1 encodes the maximal correlation between two appropriately normalized observables. Further, the G_i^A (G_i^B , respectively) form an orthonormal basis of Alice’s (Bob’s) operator space. This means that $\text{Tr}(G_i^A G_j^A) = \delta_{ij}$; examples of such bases are the appropriately normalized Pauli or Gell-Mann matrices. In fact, several works used the OSD, for example to analyze entanglement of mixed states [37–40] or dynamics [41]. We now write down our first main result, where we apply the OSD to a general operator \mathcal{X} .

Observation 1—Let \mathcal{X} be an operator with its OSD as in Eq. (1) and μ_1 its largest OSC. Then

$$\mathcal{W} = \mu_1 \mathbb{1} - \mathcal{X} \quad (2)$$

is an entanglement witness for bipartite entanglement.

Note that the choice of the parameter μ_1 guarantees the positivity of the witness on separable states, but for general \mathcal{X} there may be proper witnesses $\mathcal{W} = \alpha \mathbb{1} - \mathcal{X}$ with a smaller $\alpha < \mu_1$. This is in contrast to witnesses based on pure state fidelities, where $\alpha = s_1^2$ is optimal. In order to prove the observation, it suffices to show that the expectation value $\langle a, b | \mathcal{W} | a, b \rangle$ is non-negative for an arbitrary pure product state $|a, b\rangle$; this implies the statement for general separable states. First, writing \mathcal{X} in its OSD according to Eq. (1) it is clear that $\langle a, b | \mathcal{X} | a, b \rangle \leq \mu_1 \sum_i |\langle a | G_i^A | a \rangle \langle b | G_i^B | b \rangle|$. Then, for $x = a$ and $x = b$ and any orthonormal basis of the operator space one has

$\sum_i \langle x | G_i^X | x \rangle^2 = 1$; this follows from the fact that for $\rho = |x\rangle\langle x|$ the relation $\text{Tr}(\rho^2) = 1$ holds. So, by the Cauchy-Schwarz inequality we have $\langle a, b | \mathcal{X} | a, b \rangle \leq \mu_1$, and Observation 1 follows.

From this simple construction of witnesses, several questions arise: How shall one choose the operator \mathcal{X} to detect a given entangled state ρ ? Which states can be detected by this construction? What about the characterization of high-dimensional entanglement? Can this method be extended to the multiparticle scenario, in order to detect genuine multiparticle entanglement?

In the following, we will answer all these questions. For the moment, we would like to stress that the construction in Eq. (2) contains the pure state fidelity-based witness mentioned in the second paragraph as a special case, but still it is a more general description, so the OSD witnesses are strictly stronger. Indeed, starting from a pure state $|\psi\rangle = \sum_{i=1}^R s_i |ii\rangle$ one can directly calculate the OSD of $\mathcal{X} = |\psi\rangle\langle\psi|$. One finds R^2 nonzero operator Schmidt coefficients of the type $\{\mu_i\} = \{s_\alpha s_\beta\}$, and the largest one is hence given by $\mu_1 = s_1^2$. Thus, the pure state fidelity-based witness is indeed a special case of Eq. (2).

Schmidt number witnesses—Let us now explain how the method of OSD witnesses can be used to characterize the dimensionality of entanglement, as characterized by the Schmidt number. Given the Schmidt decomposition of a pure state as above, the number R of nonzero Schmidt coefficients is called the Schmidt rank, and is known to be an entanglement monotone characterizing the dimensionality of entanglement [42]. It can be generalized to mixed states as follows. If a mixed state cannot be written as a convex decomposition into pure states with Schmidt rank k , then the mixed state has Schmidt number (SN) $k + 1$ [43]. Note that in this classification, mixed states with SN 1 are just the separable states, while entangled states have at least an SN of 2.

Similar to entanglement witnesses, one can define Schmidt number witnesses as observables whose expectation values are positive for all states with SN $k - 1$ such that a negative result indicates at least SN k [44]. In our scheme, these witnesses may be constructed analogously to Eq. (2), where the prefactor μ_1 is replaced by a different number λ_k , which is a not necessarily optimal bound on the overlap of pure Schmidt-rank $k - 1$ states with the operator \mathcal{X} . It turns out that these λ_k are simply given by the solution of a $(k - 1)$ th order polynomial equation in the OSC of \mathcal{X} . For example, for SN $k = 3$ we find $\lambda_3 = [\mu_1 + \mu_4 + \sqrt{(\mu_1 - \mu_4)^2 + (\mu_2 + \mu_3)^2}] / 2$. Then the witness $\mathcal{W} = \lambda_3 \mathbb{1} - \mathcal{X}$ detects only three-dimensional entanglement. However, for SNs greater than 3, the prefactor is not so compact anymore; details on the computation of λ_3 and the prefactors for higher SN are given in Appendix A in the Supplemental Material [45]. These witnesses can be seen as a generalization of the computable cross norm or realignment (CCNR) criterion for detecting the Schmidt number

(see also Observation 2 below), similar to the one in Ref. [58]. But one can choose \mathcal{X} such that it certifies the SN of states, for which the CCNR extension [58] fails; see also Appendix A [45].

Estimating bipartite entanglement monotones—In many cases, one is not only interested in detecting quantum entanglement, but also wishes to quantify it and its resource character. For this quantification, many entanglement monotones have been proposed [59–75]. A frequently used monotone is the concurrence [64–69], defined for pure states as $C(|\psi\rangle) = \sqrt{2[1 - \text{Tr}(q_A^2)]}$ and for mixed states via the so-called convex roof construction (see Appendix B in the Supplemental Material for details [45]). This quantity is notoriously difficult to compute, but with the OSD witness, it can be directly estimated. Indeed, one can show that

$$C(q) \geq \sqrt{\frac{2}{d(d-1)}}(S-1) \quad (3)$$

where $S = \max\{\text{Tr}(q\mathcal{X})/\mu_1, 1\}$. Note that Eq. (3) has a similar form of the result in Ref. [76], but interestingly analogous bounds can be derived for other measures, such as the convex-roof extended negativity [63], the G concurrence [70–72], and the geometric measure of entanglement [73–75]; details are given in Appendix B of the Supplemental Material [45]. Moreover, they can finally be extended to the multiparticle case.

Optimization of OSD witnesses—Having established basic properties of the OSD witness, we can now ask how to choose the observable \mathcal{X} in an optimal manner. Consider an entangled state q that is detected by a witness as in Eq. (2) with the \mathcal{X} as in Eq. (1). Since we want to minimize the expectation value of the witness we can, without loss of generality, consider a witness where the expectation values $\langle G_i^A \otimes G_i^B \rangle$ are positive for the given state and the μ_i are positive. In addition, the witness may be renormalized to achieve $\mu_1 = 1$. But then it is clear that the optimal choice of the other μ_i is to take $\mu_i = 1$, too.

So, an entangled quantum state is detected by a witness from Eq. (2) if and only if it can be detected by a witness of the form $\mathcal{W}_{\text{CCNR}} = 1 - \sum_{i=1}^S G_i^A \otimes G_i^B$. These witnesses, however, are characteristic for the CCNR criterion [25,77,78], and we have the following.

Observation 2—A bipartite quantum state can be detected by an OSD witness as in Eq. (2) if and only if it can be detected by the CCNR criterion.

The critical reader may ask at this point, why we have defined the OSD witnesses in the general form of Eq. (2) although the simpler subclass of CCNR witnesses contains all the relevant cases already. There are two reasons for that: First, as stressed above, the direct connection to the CCNR criterion does not hold for witnesses for a higher Schmidt number. Second, the form of the witness in Eq. (2) is the key for the generalization to multiparticle entanglement.

There, we will search for multiparticle witnesses, which have the form as in Eq. (2) for any bipartition. Restricting then the attention to specific optimal witnesses for each bipartition does not lead to strong witnesses for the entire system [79], and there is a trade-off between the optimality of the bipartite witness and the efficiency for multiparticle entanglement detection.

So, let us discuss how a given OSD witness can be gradually optimized; this will be central for the discussion of multiparticle entanglement later. We consider an entangled state q (e.g., some pure state) which is affected by some separable noise σ (e.g., the maximally mixed state $1/d^2$). So, the total state is of the form $\eta(p) = pq + (1-p)\sigma$, and one can ask for the minimum of the required visibility p_{crit} , such that all states with $p > p_{\text{crit}}$ are detected by the OSD witness.

A given OSD witness can be optimized in two directions. First, one may alter the coefficients μ_i in Eq. (1), and second, one may change the operators G_i^X in the Schmidt decomposition. Let us first discuss the optimization of the OSC. For a given OSD witness, one can directly compute the p_{crit} and, leaving all other quantities fixed, this is a function of the parameters $\{\mu_i\}$. Then, one can compute the gradient $\nabla p_{\text{crit}}(\{\mu_i\})$ and minimize p_{crit} with some steepest descent algorithm (see Appendix C in the Supplemental Material for details [45]). We stress that after adjusting the $\{\mu_i\}$ in one iteration step one can calculate the updated $\tilde{\mu}_1$ in order to guarantee that the updated $\tilde{\mathcal{W}}$ is indeed a proper witness, so no fake entanglement detection can arise from this procedure.

Second, we explain the optimization of the Schmidt operators G_i^A while keeping the $\{\mu_i\}$ and $\{G_i^B\}$ fixed. Since the G_i^A form an orthonormal basis, one can consider an infinitesimal rotation $G_i^A \rightarrow \tilde{G}_i^A = \sum_k O_{ik} G_k$ with O_{ik} being an infinitesimal rotation matrix of the form

$$O = 1 + \sum_l \epsilon^{(l)} g^{(l)}, \quad (4)$$

with $g^{(l)}$ being the generator matrices of the $\text{SO}(N)$. Finally, one can write p_{crit} as a function of the $\epsilon^{(l)}$ and optimize the G_i^A via a gradient algorithm.

In practice, these two approaches work very well, even if the initial OSD witness was not chosen properly. For instance, for a bound entangled state (the so-called unextendible product basis (UPB) state in 3×3 systems) the procedures directly find a witness that detects it, even if the initial witness was not capable of detecting it. Details on the optimization procedures and on the examples are given in Appendix C of the Supplemental Material [45].

Multiparticle entanglement—Now we are ready to present the extension of OSD witnesses to the multiparticle case. Let us first recall the notion of genuine multiparticle entanglement (GME) [15]. For the case of three particles, a pure state can be fully separable (e.g., $|\psi^{\text{fs}}\rangle = |000\rangle$) or biseparable for some bipartition (e.g., $|\psi^{\text{bs}}\rangle = |\phi\rangle_A \otimes |\psi^-\rangle_{BC}$,

where $|\psi^-\rangle$ is a 2-qubit singlet state). Finally, a pure state is genuine multipartite entangled if it is not biseparable with respect to any bipartition. Well-known examples of genuine multipartite entangled states for 3 qubits are the Greenberger-Horne-Zeilinger (GHZ) state $|GHZ_3\rangle = (|000\rangle + |111\rangle)/\sqrt{2}$ and the W state $|W_3\rangle = (|001\rangle + |010\rangle + |100\rangle)/\sqrt{3}$. Similarly, one can define biseparability and genuine multipartite entanglement of more than three particles.

The generalization to mixed states goes via convex combinations. A mixed state is fully separable, if it can be written as a convex combination of pure fully separable states, that is $\rho = \sum_k p_k |\psi_k^{\text{fs}}\rangle\langle\psi_k^{\text{fs}}|$. A state is biseparable if it can be expressed as a convex combination of pure biseparable states; these pure states may be biseparable with respect to different bipartitions. Finally, mixed states are genuine multipartite entangled, if they are not biseparable.

For the characterization of genuine multipartite entanglement, entanglement witnesses can be directly used again, and a witness for GME is defined by the property that it is non-negative on all biseparable states. The method of OSD witnesses can directly be used to write down GME witnesses: Consider a tripartite operator \mathcal{X}_{ABC} . We can compute the OSD for the three bipartitions $A|BC$, $B|AC$, and $C|AB$, resulting in three maximal Schmidt coefficients $\mu_1^{A|BC}$, $\mu_1^{B|AC}$, and $\mu_1^{C|AB}$. Note that these are asymmetric scenarios for the OSDs, where the dimensions of the two sides are not the same. Then, taking μ as the maximum of these, the operator

$$\mathcal{W} = \mu \mathbb{1} - \mathcal{X}_{ABC} \quad (5)$$

has a positive expectation value on all pure biseparable states; hence it is a witness for genuine multipartite entanglement; the generalization for more particles is described in Appendix E of the Supplemental Material [45].

It is clear that the witness in Eq. (5) is more general than fidelity-based witnesses for multipartite entanglement. Such fidelity-based witnesses have been a standard tool to analyze GME in experiments in the last years, so we will analyze in the following the advantage occurring from the construction in Eq. (5).

Examples of multipartite states—Now we are ready to use our methods to derive stronger witnesses for genuine multipartite entanglement. In the following, we explain our approach for the 3-qubit W state $|W_3\rangle$; the approach for other states is similar. A known witness for genuine multipartite entanglement in the vicinity of the W state is [80]

$$\mathcal{W} = \frac{2}{3} \mathbb{1} - |W_3\rangle\langle W_3|. \quad (6)$$

This can be viewed as an OSD witness from Eq. (5) with $\mathcal{X}_{ABC} = |W_3\rangle\langle W_3|$. The recipe for its improvement is as

TABLE I. Improvement of the noise robustness of entanglement detection for various multiqubit states. For five different states, the required visibility p_{fid} for the fidelity-based witness and p_{OSD} for the OSD witness are shown. Look at the text for further details.

State	Visibility p_{fid}	Visibility p_{OSD}
$ W_3\rangle$	$13/21 \approx 0.619$	0.556
$ H_3\rangle$	$5/7 \approx 0.714$	0.545
$ W_4\rangle$	$11/15 \approx 0.733$	0.714
$ D_4\rangle$	$29/45 \approx 0.644$	0.540
$ \Psi_4\rangle$	$11/15 \approx 0.733$	0.572

follows. We consider $\rho = |W_3\rangle\langle W_3|$ as an entangled target state and wish to maximize the robustness for the separable noise given by $\sigma = \mathbb{1}/8$. For a given bipartition one can improve \mathcal{X}_{ABC} by adjusting the Schmidt coefficients or the Schmidt operators as outlined above. We then go through the bipartitions, and for each bipartition we improve the witness by a combination of the two optimization methods. Numerical details of the procedure are given in Appendix C of the Supplemental Material [45].

The starting witness in Eq. (6) requires a visibility of $p_{\text{fid}} \geq 0.620$ in order to detect GME. Already after some iterations of the optimization procedure one arrives at a witness for which the required visibility is reduced to $p_{\text{OSD}} \geq 0.556$, demonstrating the superiority of the OSD witness over the fidelity-based construction.

We have applied the same method to a variety of other multiqubit states. This includes the 3-qubit uniform hypergraph state $|H_3\rangle$ [81] and the 4-qubit W state $|W_4\rangle$, Dicke state $|D_4\rangle$, and singlet state $|\Psi_4\rangle$ [15]. For all these states we found a significantly improved noise robustness; see Table I for concrete values. Detailed forms of the states as well as the results for other states are given in Appendix C of the Supplemental Material [45]. Note that OSD witnesses do not improve the fidelity-based witness $\mathcal{W} = 1/2 - |GHZ_3\rangle\langle GHZ_3|$ for the GHZ state, as this witness is known to be optimal for maximally mixed noise [82].

Analytical approaches—Two analytical approaches are worth mentioning. First, it is also possible to construct the OSD witnesses analytically by starting from a pure high-dimensional quantum state and interpreting this as an operator on a lower-dimensional space. For instance, for the GHZ state $|GHZ\rangle = (1/2) \sum_{i=1}^4 |iii\rangle$ on three four-level systems the vector Schmidt decomposition is directly given. Consequently, taking $\mathcal{X} = \sum_{i=1}^4 \mathcal{G}_i^A \otimes \mathcal{G}_i^B \otimes \mathcal{G}_i^C$ for arbitrary orthonormal bases \mathcal{G}_i^X , ($X = A, B, C$) on 3 qubits will always result in an entanglement witness $\mathcal{W} = \mathbb{1} - \mathcal{X}$. This ansatz can be generalized using arbitrary highly entangled pure states. Most importantly, given such a witness with a fixed structure, one can optimize the operators \mathcal{G}_i^X for given states by an iteration of purely analytical steps, which is indeed more general than a simple

optimization over local unitary transformations. Details and examples are given in Appendix D of the Supplemental Material [45]. Second, note that the operators \mathcal{G}_i^x are actually local orthogonal observables. Thus we can use the results from Ref. [83] to define the OSD witnesses for continuous variable systems, too.

Multipartite entanglement measures—Again, the novel multipartite witnesses can be made quantitative and be used to estimate monotonies for genuine multipartite entanglement. One possibility to build such monotonies is to start with an entanglement monotone E for pure two-particle states. Then, one can define for a multipartite state the global entanglement E_{GME} as the minimum of E for all bipartitions. Finally, one extends this to mixed states via the convex roof construction.

Such entanglement monotonies can be directly estimated from the expectation value of the witness in Eq. (5). For instance, one may consider the multipartite version of the concurrence. Then, one finds $C_{\text{GME}} \geq \sqrt{2/[m(m-1)]}(S-1)$ where $S = \max\{\text{Tr}(\rho \mathcal{X}_{ABC})/\mu, 1\}$ and m is, for the special case of tripartite systems the maximum of dimensions of Alice, Bob, and Charlie. This approach can be generalized to other measures and more particles; details are given in Appendix E of the Supplemental Material [45].

Conclusion—We have introduced a novel method to characterize entanglement for quantum systems of two or more particles. The resulting entanglement witnesses are strictly stronger than the widely used fidelity-based witness and can improve entanglement detection in realistic scenarios significantly. On the technical level, the approach does not involve advanced numerical tools such as semi-definite programming. The method can be seen as an extension of the CCNR criterion of separability to the multipartite case, in the same sense as Ref. [84] presented an extension of the criterion of the positivity of the partial transpose to the multipartite case.

Several new lines of research emerge from our findings. First, it would be highly desirable to further characterize the resulting witnesses analytically for interesting families of quantum states. Second, entanglement witnesses can also be used to characterize other properties of quantum states, such as the teleportation fidelity [85], the distillability [86], and the multipartite Schmidt vector [87,88], so it is relevant to apply our methods to these cases. Third, the statistical analysis of entanglement tests from finite data has become essential in the last years [89], so our approaches also need to be analyzed from this viewpoint. Fourth, thinking of experimental implementations, it is desirable to give an estimation of the errors occurring when assuming small deviations of the desired measurements. In fact, for a special case of two-particle OSD witnesses this was recently discussed [90], but it remains open to generalize this approach further and apply it to the multipartite case. Finally, in general, as fidelity-based entanglement witnesses

have been used for many experiments, the presented improvement may allow for novel and exciting experiments.

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