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Entanglement and correlations in composite quantum systems

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Abstract

Entanglement is a key feature of quantum theory which has no classical analogue. Due to this feature it is no longer accurate to regard composite systems as a mere combination of independently describable subsystems. Instead there are quantum states which are inseparable with respect to the individual parts of the system. Initially regarded as an artifact of the theory, numerous experiments performed in the last decades have provided evidence of the existence of entanglement in nature. The consequences of entanglement are far-reaching. On a fundamental level, it allows to demonstrate that there is no local-realistic alternative to quantum theory. In addition, entanglement also serves as a resource for novel information processing technologies such as quantum cryptography, dense coding, quantum teleportation and quantum computing. Despite extensive research in recent years, several questions concerning entanglement and its manifestations still remain open — especially in complex many-body systems.

The aim of this dissertation is to investigate entanglement and non-local-realistic correlations in composite finite-dimensional quantum systems (i.e. multipartite qudits). In order to simplify the analysis of those systems, we present new mathematical tools such as convenient parameterizations for unitary groups, density matrices and subspaces. We study the structure of entanglement in multipartite systems and introduce a precise characterization of multilevel-multipartite entanglement. We consider methods for entanglement detection and discuss their implementation in experiments. Another problem treated in this thesis concerns the quantification of entanglement. Here, we introduce a useful measure of multipartite entanglement and derive computable lower bounds. Moreover, the classification of multipartite entanglement is also addressed, where a systematic approach for discriminating between different classes is given. The last part of this work deals with relations between entanglement and other foundational aspects of quantum theory. Specifically, we establish a link between complementarity and the separability problem. Particular attention is also devoted to the connection between entanglement and non-local-realistic correlations. Here, we exploit a geometric structure underlying discrete composite systems to illustrate their dissimilarities.

Kurzfassung

Verschränkung ist eine der wichtigsten Besonderheiten der Quantentheorie, welche kein klassisches Analogon besitzt. Aufgrund dieser ist es nicht länger angemessen zusammengesetzte Systeme lediglich als eine Kombination von unabhängig voneinander beschreibbaren Subsystemen zu betrachten. Anstatt dessen gibt es Quantenzustände die inseparabel bezüglich der einzelnen Bestandteile des Systems sind. Wohingegen Verschränkung zunächst als eine Art künstlicher Fehler der Theorie angesehen wurde, hat sich deren Existenz mittlerweile durch zahlreiche Experimente bestätigt. Diese Gegebenheit hat weitreichende Konsequenzen. Auf einer fundamentalen Ebene lässt sich hiermit zeigen, daß es keine lokal-realistische Alternative zur Quantentheorie gibt. Zusätzlich stellt Verschränkung eine Ressource für neue Technologien der Informationsverarbeitung dar, wie z.B. Quantenkryptographie, Dense Coding, Quantenteleportation oder der Quantencomputer. Trotz intensiver Forschung in den letzten Jahrzehnten gibt es noch viele offene Fragen bezüglich Verschränkung und deren Manifestationen. Dies gilt insbesondere für Verschränkung in komplexen Vielteilchensystemen.

Gegenstand dieser Dissertation ist es Verschränkung und nicht-lokal-realitsche Korrelationen in zusammengesetzten endlich-dimensionalen Quantensystemen (Multipartite Qudits) zu untersuchen und zu verstehen. Um die Analyse solcher Systeme zu erleichtern, werden neue mathematische Hilfsmittel, wie zum Beispiel praktische Parameterisierungen von unitären Gruppen, Dichtematrizen und Unterräumen vorgestellt. Die Struktur von Verschränkung in Vielteilchensystemen wird betrachtet, und eine exakte Charakterisierung von Multilevel-Vielteilchenverschränkung wird eingeführt. Es werden Methoden zur Verschränkungsdetektion angegeben, und deren experimentelle Implementierung diskutiert. Ein weiteres Thema ist die Quantifizierung von Verschränkung. In diesem Zusammenhang wird ein nützliches Maß für Vielteilchenverschränkung vorgestellt. Darüber hinaus wird auch die Klassifizierung von Vielteilchenverschränkung thematisiert, und ein systematischer Ansatz zur Unterscheidung verschiedener Klassen angegeben. Der letzte Teil dieser Arbeit beschäftigt sich mit Relationen zwischen Verschränkung und anderen fundamentalen Aspekten der Quantentheorie. Insbesondere wird eine Verbindung zwischen dem Komplementaritätsprinzip und dem Separabilitätsproblem hergestellt. Besondere Aufmerksamkeit gilt auch dem Zusammenhang zwischen Verschränkung und nicht-lokal-realitischen Korrelationen. Hier wird eine geometrische Struktur, welche diskreten zusammengesetzten Systemen zugrunde liegt, verwendet, um deren Verschiedenartigkeit veranschaulichen zu können.

List of journal publications

[P1] C. Spengler, M. Huber, and B. C. Hiesmayr,
A composite parameterization of unitary groups, density matrices and subspaces,
J. Phys. A: Math. Theor. **43**, 385306 (2010).

[P2] C. Spengler, M. Huber, and B. C. Hiesmayr,
Composite parameterization and Haar measure for all unitary and special unitary groups,
J. Math. Phys. **53**, 013501 (2012).

[P3] C. Spengler, M. Huber, A. Gabriel, and B. C. Hiesmayr,
Examining the dimensionality of genuine multipartite entanglement,
Quantum Inf. Process., DOI: 10.1007/s11128-012-0369-8 (2012).

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[P7] C. Spengler, M. Huber, and B. C. Hiesmayr,
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Lorentz invariance of entanglement classes in multipartite systems,
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[P9] A. Di Domenico, A. Gabriel, B. C. Hiesmayr, F. Hipp, M. Huber,
G. Krizek, K. Mühlbacher, S. Radic, C. Spengler, and L. Theussl,
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Phys. Rev. A **78**, 042327 (2008).

Contents

Introduction

A theory becomes interesting when it makes predictions that we do not directly observe in everyday life. It is due to this very reason why quantum physics is so fascinating, as it is particularly counterintuitive from the point of view of common sense. A central feature that essentially contributes to the peculiarity of quantum theory is *entanglement*. It refers to the fact that there exist definite states for composite quantum systems (i.e. systems consisting of more than one object/subsystem/particle) where the individual states of the separate subsystems remain indefinite. This implies that there are situations where it is impossible to make statements about the subsystems, even though the overall state of the entire system is known. According to our intuition this is rather confusing: How should it be possible to have best possible knowledge of the whole without having best possible knowledge of its parts? From the perspective of classical physics this is simply untenable! Entanglement furthermore entails the existence of peculiar correlations among spatially separated objects, which are in conflict with rational interpretations of locality and reality. In the early years of quantum physics (1935), these correlations served as an argument to show that quantum theory is in a sense incomplete [1, 2]. Hence, it was conjectured that there exists a more fundamental theory which resolves entanglement and its curious consequences.

In recent decades, however, the view on entanglement has changed tremendously: It was realized that the manifestations of entanglement can be tested experimentally [3, 4]. In experiments, it was found that the predictions of quantum theory are indeed correct (see e.g. Refs. [5, 6]), such that there is currently no doubt about the existence of entanglement in nature. Furthermore, it was recognized that entanglement does not only provide fundamental insights into physics, but also has applications in a new kind of information processing on the quantum level. Research in this direction has led to new technologies such as quantum cryptography [7], dense coding [8], quantum teleportation [9] and quantum computing [10].

Despite these achievements, there are still many open questions regarding the theory of entanglement. While entanglement is relatively easy to comprehend and characterize in simple systems such as bipartite two-level systems, the situation becomes more and more complicated the more subsystems and more degrees of freedom are involved. Besides the fact that complex systems are hard to analyze mathematically because of the increasing dimensionality of the Hilbert space, entanglement in multilevel and multipartite systems also has a rich structure which is not yet fully understood. Moreover, research on the significance of entanglement and its relations to other features such as complementarity and non-locality is still ongoing. The main objective of this thesis is to contribute to the solution of these issues, i.e. the focus of this work is on open problems in *entanglement theory*.

This doctoral thesis is a cumulative dissertation that consists of seven journal publications [P1]–[P7]. The following Sections 1, 2 and 3 are to be regarded as a guide to these papers providing additional introductory information. The reader is directed to the enclosed publications at the end of a subsection. The content is organized as follows:

In Section 1, we begin with an introduction to the mathematical formalism and terminology of quantum information. Here, special attention is given to quantum states of finite-dimensional composite systems and their transformations. After a survey on the basics, we focus on parameterizations of density matrices and unitary

transformations. Parameterizations are quite useful in the analysis of entanglement properties as they can simplify calculations, or lead to more accurate representations. In general, it is advantageous to have various different parameterizations for the same object — in this case, we may simply use the one which is most convenient for the particular problem. Having in mind a variety of (numerical) optimization problems that arise in quantum information, we introduce a novel parameterization of the unitary group $\mathcal{U}(d)$ and the special unitary group $\mathcal{SU}(d)$. This parameterization is not only very intuitive as it is composed of elementary operations such as rotations and phase shifts, but additionally enables a simple identification of redundant parameters when it is used for the description of density matrices, orthonormal bases and subspaces. For all these objects we obtain representations containing the minimum number of parameters. This in turn reduces the computational effort of optimization problems where these objects are to be varied.

In Section 2, the focus is on the structure of entanglement in bipartite and multipartite discrete-level systems. We define the distinction between separable and entangled states, and explain the concept of k-separability in multipartite systems. After that, we show how entanglement can be characterized in terms of the Schmidt rank and its generalizations. Here, we introduce a precise characterization of multilevel entanglement in multipartite systems. Subsequently, we turn our attention to the separability problem, i.e. we discuss the difficulty of distinguishing separable and entangled (mixed) states. Established methods for the detection of entanglement are reviewed – such as the PPT criterion, positive maps and entanglement witnesses. Moreover, a recently developed method based on relations between density matrix elements is also reviewed. Using this approach, we construct strong criteria for the verification of multilevel entanglement in multipartite systems. These are shown to have a remarkable detection strength for certain types of mixed states.

Besides the detection of entanglement, a major problem in entanglement theory concerns the quantification of entanglement. That is, if a state is entangled we might also want to know *"how much"*? Subsequent to a thorough discussion of the requirements on measures of entanglement, we focus on a specific entanglement measure for bipartite systems: the concurrence. In this context, we present two results. First, we describe a method for computing and optimizing lower bounds on the concurrence. Second, we look at the extension to multipartite systems. In this way, a functional measure of genuine multipartite entanglement (i.e. non-2-separability) including a lower bound is obtained.

A central feature of multipartite systems is that entanglement can have various forms. In order to discriminate different types, one can introduce entanglement classes. One way of defining classes is via invertible local operations. For three qubits this leads to 4 different types of states (only two of them are genuinely multipartite entangled), and for four qubits there are 9 distinct families. Beyond this, it is unclear how many such classes there are and how their representatives look like. In order to have the possibility to formulate and discriminate different types of states for more complex systems (including mixed states), we introduce an alternative classification scheme based on equivalences with respect to unitaries and permutations. Moreover, for exemplary classes formulated in this way, we provide computable criteria for distinguishing between them.

The last part of this section is devoted to the distillability problem. The purpose of a distillation protocol is to transform a larger number of copies of a weakly entangled mixed state into a smaller number of highly entangled states. There are

various such protocols available nowadays, such that one can optimize the distillation rate concerning the given input state and associated noise. Nonetheless, it turns out that there are entangled states that cannot be distilled, regardless of which protocol is used. Those states are called bound entangled. Here, we consider necessary and sufficient conditions for (non-)distillability, and show how the previously introduced parameterization (applied to subspaces) may help in examining these.

In Section 3, we investigate relations between entanglement and other foundational features of quantum theory. First, we consider the uncertainty principle. This principle is at the heart of quantum theory and refers to the fact that there are pairs of observables that cannot simultaneously have definite values. In the mathematical formalism of quantum information, this means that these observables do not share a common eigenbasis. The uncertainty reaches its maximum for complementary observables, which is when all (normalized) eigenvectors of one observable have the same overlap with all eigenvectors of the other observable. In this case, the eigenbases are also referred to as mutually unbiased. The question of how many such bases exist for a given Hilbert space has been a lively topic of research. In this thesis, we establish a link between complementary observables and the separability problem. Specifically, using complementary observables for entanglement detection, we confirm an upper bound on the number of mutually unbiased bases via the separability boundary.

Finally, we compare entanglement with non-local-realistic correlations. These correlations manifest themselves through the violation of a Bell inequality. Although non-local-realism of quantum theory is a consequence of entanglement, it becomes apparent that not all entangled states give rise to a violation of a Bell inequality. Thus, instead of a one-to-one correspondence one finds that the relation between entanglement and non-local-realistic correlations is rather intricate. In the last part of this thesis, we compare both properties in a geometric context, i.e. we consider a regular simplex of bipartite quantum states. In this way, we are able to graphically illustrate the differences of both features.

1 Mathematical formalism

1.1 Quantum systems and quantum states

The central object of a quantum system is its underlying Hilbert space. This is a vector space equipped with an inner product and an associated norm and metric. In this thesis we restrict ourselves to systems where measurements yield finitely many distinguishable outcomes. Hence, we focus on Hilbert spaces $\mathcal{H} = \mathbb{C}^d$, where $d = 2, 3, 4, \ldots$ corresponds to the number of discrete measurement results. In quantum information, such d-level systems are commonly called *qudits* – a term that generalizes qubits ($d = 2$) and qutrits ($d = 3$) to arbitrary d. The elements of $\mathcal{H} = \mathbb{C}^d$ are written in Dirac notation, i.e. vectors are denoted by the symbol $|\psi\rangle$ (ket-vector) and their adjoints by $\langle\psi|$ (bra-vector). Thus, the inner (scalar) product of two vectors $|\psi_1\rangle$ and $|\psi_2\rangle$ reads $\langle\psi_1\,|\psi_2\rangle \in \mathbb{C}$, and $\| \, |\psi\rangle \, \| = \sqrt{\langle\psi\,|\psi\rangle} \geq 0$ will be our standard norm. Vector transformations $|\psi\rangle \mapsto |\psi'\rangle$ are realized through linear operators acting on the Hilbert space. In our case, these operators can be expressed through complex matrices. In terms of an arbitrary basis $\{|0\rangle, \ldots, |d-1\rangle\}$ of $\mathcal{H} = \mathbb{C}^d$, we can write an operator A in the form $A = \sum_{i,j=0}^{d-1} A_{i,j} \, |i\rangle \langle j|$ where $A_{i,j} \in \mathbb{C}$. The adjoint of A is denoted by $A^\dagger = \sum_{i,j=0}^{d-1} A_{i,j}^* \, |j\rangle \langle i|$. Introducing the Hilbert-Schmidt inner product $\langle A|B\rangle_{HS} = \mathrm{Tr}\left(A^\dagger B\right)$ for a pair of operators (A and B), we can define an operator norm $\|A\|_{HS} = \sqrt{\langle A|A\rangle_{HS}}$, and a distance $\mathcal{D}(A, B) = \|A - B\|_{HS}$.

Pure quantum states are represented (up to an irrelevant global phase $e^{i\varphi}$) by normalized vectors, i.e. $|\psi\rangle \in \mathbb{C}^d$ with $\| \, |\psi\rangle \, \| = 1$. Mixed states are formulated in terms of density matrices ρ. These are operators on $\mathcal{H}$ which are convex combinations $\rho = \sum_i p_i \, |\psi_i\rangle \langle\psi_i|$ of state vectors $|\psi_i\rangle$ where $p_i \geq 0$ and $\sum_i p_i = 1$. Thus, they are hermitian, positive-semidefinite and normalized ($\mathrm{Tr}\,(\rho) = 1$). The mixedness of a given density matrix can be determined straightforwardly via $\mathrm{Tr}\,(\rho^2)$, which scales between $\frac{1}{d}$ for maximally mixed states and 1 for pure states. An observable is represented through a hermitian operator $A = A^\dagger$ whose eigenvalues $\{\lambda_i\}$ correspond to measurable quantities such as, for instance, position, momentum, energy or spin. As we work with discrete systems, the d possible measurement outcomes will be labeled by integers $0, \ldots, d-1$. Similarly, the associated (normalized) eigenvectors of A are labeled by $|i_A\rangle$ with $i \in \{0, \ldots, d-1\}$, and thus the probability of obtaining output i when measuring A is $P(A = i) = \mathrm{Tr}\,(\rho \, |i_A\rangle \langle i_A|)$.

The main objective of this thesis is to investigate composite quantum systems. These are systems that are composed of several subsystems. A system consisting of n qudits is described by a Hilbert space $\mathcal{H} = \bigotimes_{m=1}^n \mathcal{H}_m = \mathbb{C}^{d_1} \otimes \cdots \otimes \mathbb{C}^{d_n}$, where d_k refers to the dimension of qudit k and $\otimes$ denotes the tensor product. Mathematically, this Hilbert space is equivalent to $\mathcal{H} = \mathbb{C}^{d_1 \cdot \ldots \cdot d_n}$. From the perspective of physics, however, we must take the tensor product structure seriously as quantum state transformations are generally related to physical operations on single qudits or interactions between them. Finally, note that product basis vectors $|i\rangle \otimes |j\rangle \otimes \cdots \otimes |k\rangle \in \mathcal{H} = \bigotimes_{m=1}^n \mathcal{H}_m$ are commonly written in the short form $|i\rangle \, |j\rangle \ldots |k\rangle$ or $|ij \ldots k\rangle$ where the tensor product symbol is omitted.

1.2 Quantum operations

Quantum operations are the union of all physical operations transforming a density matrix ρ on $\mathcal{H}$ into another density matrix ρ' on $\mathcal{H}'$. Here, $\mathcal{H}$ and $\mathcal{H}'$ are not necessarily equal, meaning that these operations include reductions and enlargements of the system. According to quantum theory we can perform the following four elementary maps Λ:

- **Unitary transformations**

$$\Lambda_1(\rho) = U\rho U^\dagger \ , \tag{1.1}$$

  where U is a unitary operator, i.e. $U^{-1} = U^\dagger$. These operations arise from the dynamics of closed quantum systems $U = \exp(-\mathbb{i}\int_{t_0}^{t} H(\tau)d\tau)$ through the Hamiltonian $H(\tau)$. A change between different orthonormal bases of the system also realizes such a transformation.

- **Projective (von Neumann) measurements**

$$\Lambda_2(\rho) = \frac{\sum_{i\in\mathcal{M}} P_i\rho P_i^\dagger}{\mathrm{Tr}\left(\sum_{i\in\mathcal{M}} P_i\rho P_i^\dagger\right)} \ , \tag{1.2}$$

  where $\{P_i\}$ are the projectors $P_i = |i_A\rangle\langle i_A|$ defined by the eigenvectors of the measured observable A. We speak of a *non-selective measurement* when we do not filter out particular eigenstates, i.e. $\mathcal{M} = \{0,\ldots,d-1\}$. On the other hand, we speak of a *selective measurement* when $\mathcal{M} \subsetneq \{0,\ldots,d-1\}$, that is when some eigenstates are discarded.

- **Adding an ancilla**

$$\Lambda_3(\rho) = \rho\otimes\sigma \ . \tag{1.3}$$

  Here, the system is enlarged through an additional system in the state σ. This operation also includes the use of several copies of a state $\rho^{\otimes m}$.

- **Discarding subsystems**

$$\Lambda_4(\rho) = \mathrm{Tr}_m\rho \ . \tag{1.4}$$

  Here, the system is reduced to a smaller one by performing a partial trace over subsystem m.

Any map composed of these four operations is completely positive (see Ref. [11] and Section 2.3) and trace preserving. Such a map may be written as

$$\Lambda(\rho) = \frac{\sum_i K_i\rho K_i^\dagger}{\mathrm{Tr}\left(\sum_i K_i\rho K_i^\dagger\right)} \ , \tag{1.5}$$

using so-called Kraus operators $\{K_i\}$ satisfying $\sum_i K_i^\dagger K_i \leq \mathbb{1}$. This form can be used to describe all types of physical dynamics including decoherence and generalized measurements (POVMs). Note that because of possible reductions and extensions of the Hilbert space, the Kraus operators $\{K_i\}$ are not necessarily quadratic.

In quantum information processing an important class of quantum operations are *local operations and classical communication* (LOCC). For an n-partite quantum system a *local operation* can be written as

$$\Lambda_{LO}(\rho) = \frac{(K_1 \otimes \cdots \otimes K_n)\rho(K_1 \otimes \cdots \otimes K_n)^\dagger}{\mathrm{Tr}\left((K_1 \otimes \cdots \otimes K_n)\rho(K_1 \otimes \cdots \otimes K_n)^\dagger\right)} , \tag{1.6}$$

where $K = K_1 \otimes \cdots \otimes K_n$ only acts *locally* on single qudits according to the tensor product structure. In addition, *classical communication* allows for classically correlated actions, i.e. in this case the n parties can arrange their local operations. Hence, LOCCs have the form

$$\Lambda_{LOCC}(\rho) = \frac{\sum_i (K_{1,i} \otimes \cdots \otimes K_{n,i})\rho(K_{1,i} \otimes \cdots \otimes K_{n,i})^\dagger}{\mathrm{Tr}\left(\sum_i (K_{1,i} \otimes \cdots \otimes K_{n,i})\rho(K_{1,i} \otimes \cdots \otimes K_{n,i})^\dagger\right)} . \tag{1.7}$$

To be precise, note that there are further nontrivial constraints on the set of Kraus operators $\{K_{1,i} \otimes \cdots \otimes K_{n,i}\}$ besides the product form. These depend on which and how (one-way, two-way, etc.) the different parties can communicate with one another (see e.g. Ref. [12]). When these constraints are relaxed, we call the transformation (1.7) a *separable operation*. More general transformations which cannot be decomposed into local operations are called *non-local* or *global*. Those arise form interactions between two or several qudits.

1.3 Unitary groups and Haar measure

The unitary group $\mathcal{U}(d)$ is defined by the set of all unitary operators on $\mathbb{C}^d$

$$\left\{ U = \sum_{i,j=0}^{d-1} U_{i,j} |i\rangle \langle j| \;\middle|\; U^\dagger U = U U^\dagger = \mathbb{1}_d \right\} , \tag{1.8}$$

with the matrix multiplication as the group operation. An important subgroup of $\mathcal{U}(d)$ is the so-called special unitary group $\mathcal{SU}(d)$ whose elements in addition have determinant one, i.e.

$$\left\{ U = \sum_{i,j=0}^{d-1} U_{i,j} |i\rangle \langle j| \;\middle|\; U^\dagger U = U U^\dagger = \mathbb{1}_d \text{ and } \det(U) = 1 \right\} . \tag{1.9}$$

A part of this thesis is devoted to parameterizations of these groups and their applications in the theory of quantum entanglement. First, recall that $\mathcal{U}(d)$ and $\mathcal{SU}(d)$ are compact connected real Lie groups [19]. Hence, every group element can be written in the form

$$U = \exp(\mathbb{i} \sum_k G_k \lambda_k) , \tag{1.10}$$

using a finite set of *infinitesimal generators* $\{G_k\}$ and real parameters $\{\lambda_k\}$. Generators of a Lie group form a *Lie algebra* satisfying

$$[G_k, G_l] = \mathbb{i} \sum_m f_{klm} G_m , \tag{1.11}$$

wherein $[G_k, G_l] = G_k G_l - G_l G_k$ is the commutator, and the constants f_{klm} are called *structure constants*. The structure constants of a Lie algebra in general depend

on the particular choice of generators. However, the central property is that the commutator of any two generators must be a linear combination of the members of the Lie algebra.

Let us determine the number of generators for $\mathcal{U}(d)$ and $\mathcal{SU}(d)$. An arbitrary complex matrix of dimension $d \times d$ can be expressed in terms of $2d^2$ real parameters. Since unitarity imposes d^2 constraints on these parameters (row and column vectors have to be orthonormal), it follows that $\mathcal{U}(d)$ is a d^2-parameter group. Consequently, there exist d^2 infinitesimal generators. Accordingly, $\mathcal{SU}(d)$ has $d^2 - 1$ infinitesimal generators because of the additional constraint 'determinant one'. The standard generators of $\mathcal{SU}(d)$ are the $d^2 - 1$ *generalized Gell-Mann matrices* (GGM):

- $d(d-1)/2$ symmetric matrices:

$$G_{j^2+2i} = |i\rangle\langle j| + |j\rangle\langle i| \qquad 0 \leq i < j \leq d-1 \tag{1.12}$$

- $d(d-1)/2$ antisymmetric matrices:

$$G_{j^2+2i+1} = -\mathbb{i}\,|i\rangle\langle j| + \mathbb{i}\,|j\rangle\langle i| \qquad 0 \leq i < j \leq d-1 \tag{1.13}$$

- $d-1$ diagonal matrices:

$$G_{(j+1)^2-1} = \sqrt{\frac{2}{j(j+1)}}\left(\sum_{i=0}^{j-1} |i\rangle\langle i| - j\,|j\rangle\langle j|\right) \qquad 1 \leq j \leq d-1\ . \tag{1.14}$$

Note that this construction contains the Pauli matrices $\sigma_1 = G_1 = |0\rangle\langle 1| + |1\rangle\langle 0|$, $\sigma_2 = G_2 = -\mathbb{i}\,|0\rangle\langle 1| + \mathbb{i}\,|1\rangle\langle 0|$ and $\sigma_3 = G_3 = |0\rangle\langle 0| - |1\rangle\langle 1|$ as the special case $d = 2$. Note furthermore that the definitions (1.12)–(1.14) imply that all Gell-Mann matrices are hermitian, traceless and mutually orthogonal $\mathrm{Tr}\,(G_k G_l) = 2\delta_{kl}$ (for more details see Ref. [13]). The corresponding structure constants are

$$f_{klm} = -\frac{\mathbb{i}}{2}\mathrm{Tr}\,([G_k, G_l]G_m)\ . \tag{1.15}$$

The Gell-Mann matrices together with relation (1.10) provide a simple parameterization of the special unitary group $\mathcal{SU}(d)$. Likewise, a parameterization of the unitary group $\mathcal{U}(d)$ can be obtained by adding $G_0 = \mathbb{1}_d$ to the set $\{G_1, \ldots, G_{d^2-1}\}$ of Gell-Mann generators. We refer to these as *canonical parameterizations*.

The canonical approach based on the correspondence (1.10) between Lie groups and Lie algebras is not the only possible way to obtain parameterizations of $\mathcal{SU}(d)$ and $\mathcal{U}(d)$. There also exist alternatives that do not (or only indirectly) rely on this connection. Different such *non-canonical parameterizations* have been introduced (see e.g. Refs. [14, 15, 16, 17]), each of which exploits different theoretical relations and features of unitary groups.

Research contribution(s): In practice, the choice of the parameterization depends on the given problem. The aim of our papers **[P1]** and **[P2]** was to develop a parameterization that is suitable for a broad range of problems arising in quantum information. Therein, we show that $\mathcal{U}(d)$ can be parameterized as[1]

$$U = \left[\prod_{m=0}^{d-2}\left(\prod_{n=m+1}^{d-1}\exp\left(\mathbb{i}P_n\lambda_{n,m}\right)\exp\left(\mathbb{i}Y_{m,n}\lambda_{m,n}\right)\right)\right]\cdot\left[\prod_{l=0}^{d-1}\exp(\mathbb{i}P_l\lambda_{l,l})\right]\ , \tag{1.16}$$

[1] Note that in contrast to the papers **[P1]** and **[P2]**, here all labels run from 0 to $d-1$ instead of 1 to d.

via real parameters $\lambda_{m,n}$, one-dimensional projectors $P_l = |l\rangle\langle l|$ and anti-symmetric matrices $Y_{m,n} = -\mathbb{i}\,|m\rangle\langle n| + \mathbb{i}\,|n\rangle\langle m|$. Likewise, we show that $\mathcal{SU}(d)$ can be parameterized as

$$U = \left[\prod_{m=0}^{d-2}\left(\prod_{n=m+1}^{d-1}\exp\left(\mathbb{i}Z_{m,n}\lambda_{n,m}\right)\exp\left(\mathbb{i}Y_{m,n}\lambda_{m,n}\right)\right)\right]\cdot\left[\prod_{l=0}^{d-2}\exp(\mathbb{i}Z_{l,d-1}\lambda_{l,l})\right] , \tag{1.17}$$

using the rank-2 operators $Y_{m,n} = -\mathbb{i}\,|m\rangle\langle n| + \mathbb{i}\,|n\rangle\langle m|$ and $Z_{m,n} = |m\rangle\langle m| - |n\rangle\langle n|$.

We also discuss structural and numerical advantages of this parameterization and give several example applications. Throughout this thesis, this parameterization (we call it the *composite parameterization*) will repeatedly appear as a mathematical tool in various contexts. Due to its usefulness, we also provide corresponding codes for Matlab and Mathematica, which can be found in the Appendix. For the parameters $\lambda_{m,n}$ we use the matrix notation[2]

$$\text{relative phases} \rightarrow \begin{bmatrix} \lambda_{0,0} & \cdots & \lambda_{0,d-1} \\ \vdots & \ddots & \vdots \\ \lambda_{d-1,0} & \cdots & \lambda_{d-1,d-1} \end{bmatrix} \leftarrow \text{rotations} \quad , \tag{1.18}$$

where the lower left entries correspond to relative phase shifts, diagonal entries to global phase shifts and upper right entries to rotations (as explained in the papers). We will use this notation to visualize which parameters are irrelevant in certain applications.

The composite parameterization can also be used to compute group integrals

$$\int_{\mathcal{G}} f(U)dU \ , \tag{1.19}$$

where $\mathcal{G} = \mathcal{U}(d)$ or $\mathcal{G} = \mathcal{SU}(d)$, respectively. In order to do so, we have to find an infinitesimal volume element dU in terms of the parameters $\lambda_{m,n}$. To achieve an evenly weighted (uniform) integration

$$\int_{\mathcal{G}} f(U)dU = \int_{\mathcal{G}} f(U_1U)dU = \int_{\mathcal{G}} f(UU_2)dU \qquad \forall\ U_1, U_2 \in \mathcal{G} \ , \tag{1.20}$$

we require *left and right invariance*, i.e.

$$dU = d(U) = d(U_1U) = d(UU_2) \qquad \forall\ U_1, U_2 \in \mathcal{G} \ . \tag{1.21}$$

A measure of volume on a compact Lie group with this property is called *Haar measure* [18, 19]. In our paper **[P2]**, we present a universal method how such a measure can be obtained given an arbitrary parameterization of $\mathcal{U}(d)$, $\mathcal{SU}(d)$. Herewith, we find for the composite parameterization the concise formula

$$dU = \frac{1}{N_d}\prod_{m=0}^{d-2}\prod_{n=m+1}^{d-1}\sin(\lambda_{m,n})\cos^{2(n-m)-1}(\lambda_{m,n})\prod_{k,l}d\lambda_{k,l} \ . \tag{1.22}$$

Here, normalization $\int_{\mathcal{G}} dU = 1$ is achieved with

$$N_d = \frac{(2\pi)^{d(d+1)/2}}{\prod_{m=1}^{d-1}\prod_{n=m+1}^{d}2(n-m)} \ , \tag{1.23}$$

[2]Note that there is no diagonal element $\lambda_{d-1,d-1}$ for the special unitary group $\mathcal{SU}(d)$.

for $\mathcal{G} = \mathcal{U}(d)$, and

$$N_d = \frac{2^{d-1}\pi^{d(d+1)/2-1}}{\prod_{m=1}^{d-1}\prod_{n=m+1}^{d} 2(n-m)} \ , \tag{1.24}$$

for $\mathcal{G} = \mathcal{SU}(d)$.

1.4 Density matrix representations

As mentioned in Section 1.1, density matrices are operators on the Hilbert space that are hermitian, positive-semidefinite and normalized. For this reason, when working with them, it is often useful to describe them in terms of a set of parameters satisfying these conditions (or at least some of them). In this section, we give an introduction to two important representations of density matrices that play a role in this thesis.

The best known density matrix representation is based on the generators of the special unitary group $\mathcal{SU}(d)$. It is named the *Bloch vector representation* and is defined as follows [22, 23, 24, 13]: Let $\{G_1, \ldots, G_{d^2-1}\}$ be some generators satisfying $G_k = G_k^\dagger$, $\mathrm{Tr}\,(G_k) = 0$ and $\mathrm{Tr}\,(G_k G_l) = 2\delta_{kl}$. Together with the unity $\mathbb{1}_d$ they form a basis of operators acting on $\mathcal{H} = \mathbb{C}^d$. Consequently, any density matrix may be written in the form

$$\rho = \frac{1}{d}\mathbb{1}_d + \frac{1}{2}\sum_{k=1}^{d^2-1} b_k G_k \ , \tag{1.25}$$

where b_k are coefficients, which together constitute the so-called *Bloch vector* $\vec{b} = (b_1, \ldots, b_{d^2-1})$. In this way, ρ is automatically normalized $\mathrm{Tr}\,(\rho) = 1$ as the generators G_k are traceless. In addition, hermiticity is maintained with real coefficients $b_k \in \mathbb{R}$ because the generators G_k are hermitian. Note that in the following, we once again use the generalized Gell-Mann matrices (1.12)–(1.14) as our standard generators.

Since any density matrix must obey $\mathrm{Tr}\,(\rho^2) \leq 1$, it can be shown straightforwardly that the length of the Bloch vector is restricted to $|\vec{b}| \leq \sqrt{2(d-1)/d}$. For qubits this condition is necessary and sufficient for positive-semidefiniteness as in this case $\det(\rho) = \lambda_1 \cdot \lambda_2 = \frac{1}{4}(1 - |\vec{b}|^2) \geq 0$, where at least one eigenvalue λ_1, λ_2 is positive by default because of $\mathrm{Tr}\,(\rho) = \lambda_1 + \lambda_2 = 1$. Hence, the state space of a single qubit can be represented by a three-dimensional unit sphere - the *Bloch sphere*. States on the surface of this sphere $|\vec{b}| = 1$ are pure; states that lie inside $|\vec{b}| < 1$ are mixed. The Bloch sphere is graphically depicted in Figure 1.1.

It turns out that for higher dimensions (qutrits and beyond) there exists no simple characterization of the state space through a sphere, i.e. for higher-dimensional systems the constraint $|\vec{b}| \leq \sqrt{2(d-1)/d}$ on the Bloch vector is necessary, but does not guarantee non-negativity of ρ. Several papers have been devoted to studying the geometric shape of the state space concerning Bloch vectors. It was found that the shape is related to the structure constants f_{klm} (1.11) which for the Gell-Mann matrices and $d \geq 3$ give rise to nontrivial asymmetries between different vector components b_k. A detailed discussion of this issue can be found in Refs. [23, 24, 25, 26, 27].

It should be emphasized, however, that the intricate geometry for multilevel systems does not diminish the importance of the Bloch vector representation in

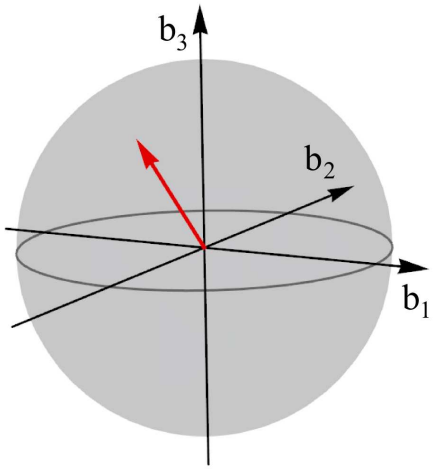

Figure 1.1: Illustration of the single-qubit Bloch sphere (gray) and a randomly chosen Bloch vector $\vec{b}$ (red).

both theory and experiment. First, in experiment, it is directly linked to quantum state tomography [23, 28]: The generators G_k are hermitian and thus observables. Due to $\mathrm{Tr}\,(G_k) = 0$ and $\mathrm{Tr}\,(G_k G_l) = 2\delta_{k,l}$ we have that $b_k = \mathrm{Tr}\,(G_k \rho)$. It can be seen that b_k is simply the expectation value $\langle G_k \rangle$ which can be measured in experiment, and thus the state is reconstructed by

$$\rho = \frac{1}{d}\mathbb{1}_d + \frac{1}{2}\sum_{k=1}^{d^2-1} \langle G_k \rangle G_k \ . \tag{1.26}$$

Second, in theory, the Bloch concept often simplifies calculations and is useful e.g. in the search for constants of motion [29, 30, 31] and the analysis of decaying systems [32, 33]. It furthermore helps in classifying density matrices [27] and studying entanglement [13, 34, 35]. In the latter case, an n-partite qudit extension of the Bloch vector representation is used. Defining the abbreviations

$$F_0 = \frac{1}{d}\mathbb{1}_d \qquad (d = d_1, \ldots, d_n) \ , \tag{1.27}$$

$$F_k = \frac{1}{2}G_k \qquad (k > 0) \ , \tag{1.28}$$

the generalization of (1.25) for $\mathcal{H} = \mathbb{C}^{d_1} \otimes \cdots \otimes \mathbb{C}^{d_n}$ reads

$$\rho = \sum_{k=0}^{d_1^2-1} \cdots \sum_{m=0}^{d_n^2-1} b_{k,\ldots,m} \ F_k \otimes \cdots \otimes F_m \ , \tag{1.29}$$

where $b_{k,\ldots,m}$ are $d_1^2 \times \cdots \times d_n^2$ real coefficients which include the normalization constant $b_{0,\ldots,0} = 1$.

Research contribution(s): Another density matrix representation is the *spectral parameterization* [22, 36, 37, 38]. Because density matrices are hermitian, they can be written as

$$\rho = \sum_{n=0}^{d-1} p_n U \left|n\right\rangle \left\langle n\right| U^\dagger \ , \tag{1.30}$$

where $\{|0\rangle, \ldots, |d-1\rangle\}$ is an arbitrary orthonormal basis and $U \in \mathcal{U}(d)$. This form is simply the spectral representation of ρ with eigenvalues $\{p_n\}$ and normalized eigenvectors $\{U|n\rangle\}$. It enables the parameterization of density matrices through unitary matrices. One of the advantages of the composite parameterization (1.16), (1.17) for this purpose is that it allows to parameterize density matrices of a certain maximum rank with a minimum number of parameters.

Let us first have a look at the eigenvalues p_n. For a rank-k density matrix there are k nonzero eigenvalues p_n summing up to one $\sum_{n=0}^{k-1} p_n = 1$. For e.g. pure states there is only $p_0 = 1$. In the more general case $1 \leq k \leq d$, we can parameterize the non-negative eigenvalues by using $k-1$ real parameters $\theta_1, \ldots, \theta_{k-1} \in [0, \frac{\pi}{2}]$ and

$$p_0 = cos^2\theta_1 \ , \tag{1.31}$$

$$p_n = cos^2\theta_{n+1} \prod_{i=1}^{n} sin^2\theta_i \qquad 0 < n < k-1 \ , \tag{1.32}$$

$$p_{k-1} = \prod_{i=1}^{k-1} sin^2\theta_i \ , \tag{1.33}$$

such that $\sum_{n=0}^{k-1} p_n = 1$. In our papers **[P1]** and **[P2]**, we show that some parameters $\lambda_{m,n}$ of the composite parameterization (1.16), (1.17) are irrelevant for the first k vectors $U|0\rangle, \ldots, U|k-1\rangle$. Namely, in the current application it suffices to use the following nonzero parameters of (1.18)

$$\underbrace{\left[\begin{array}{ccc} 0 & \lambda_{0,1} & \cdots \\ \lambda_{1,0} & \ddots & \ddots \\ \vdots & \ddots & 0 \\ \lambda_{k,0} & \cdots & \lambda_{k,k-1} \\ \vdots & \ddots & \vdots \\ \lambda_{d-1,0} & \cdots & \lambda_{d-1,k-1} \end{array}\right.}_{\text{k}} \underbrace{\left.\begin{array}{ccc} \lambda_{0,k} & \cdots & \lambda_{0,d-1} \\ \vdots & \ddots & \vdots \\ \lambda_{k-1,k} & \cdots & \lambda_{k-1,d-1} \\ 0 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & 0 \end{array}\right]}_{\text{d-k}} \begin{array}{l} \Big\} \text{k} \\ \\ \Big\} \text{d-k} \end{array} \ . \tag{1.34}$$

Counting the number of parameters, we find that density matrices with rank lower equal k require a maximum of $2dk - k^2 - 1$ parameters. In detail, there are $k-1$ parameters θ_i and $k(2d-k-1)$ parameters $\lambda_{m,n}$. This result includes pure states with $2(d-1)$ parameters and full rank density matrices with d^2-1 parameters as special cases. The reduction of parameters for the spectral parameterization (1.30) makes the composite parameterization (1.16), (1.17) particularly interesting for numerical investigations aiming at understanding properties that are related to the rank of the density matrix.

2 Quantum entanglement

2.1 Entanglement and k-separability

Consider a bipartite system $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$. A pure state $|\psi\rangle \in \mathcal{H}$ that can be written as

$$|\Psi\rangle = |\phi\rangle \otimes |\psi\rangle \ , \tag{2.1}$$

with $|\phi\rangle \in \mathcal{H}_1$ and $|\psi\rangle \in \mathcal{H}_2$ is called a *product state*. On the other hand, if it is not possible to assign an individual state vector $|\phi\rangle \in \mathcal{H}_1$ and $|\psi\rangle \in \mathcal{H}_2$ to each of the two subsystems, i.e.

$$|\Psi\rangle \neq |\phi\rangle \otimes |\psi\rangle \ , \tag{2.2}$$

then $|\Psi\rangle$ is called *entangled*. Prominent examples are the four *Bell states*

$$\left|\Psi^{\pm}\right\rangle = \frac{1}{\sqrt{2}} \left(|01\rangle \pm |10\rangle\right) \ , \tag{2.3}$$

$$\left|\Phi^{\pm}\right\rangle = \frac{1}{\sqrt{2}} \left(|00\rangle \pm |11\rangle\right) \ . \tag{2.4}$$

A density matrix ρ is called *separable* if it lies in the convex hull of all possible product states, that is, if it can be written in the form

$$\rho = \sum_i p_i \left|\phi_i\right\rangle \left\langle\phi_i\right| \otimes \left|\psi_i\right\rangle \left\langle\psi_i\right| \ , \tag{2.5}$$

with $p_i \geq 0$ and $\sum_i p_i = 1$. A density matrix for which there exists no decomposition into product states

$$\rho \neq \sum_i p_i \left|\phi_i\right\rangle \left\langle\phi_i\right| \otimes \left|\psi_i\right\rangle \left\langle\psi_i\right| \ , \tag{2.6}$$

is again referred to as *entangled*.

In the multipartite case $\mathcal{H} = \bigotimes_{m=1}^{n} \mathcal{H}_m$ with $n > 2$, the concept of *k-separability* is used (see e.g. Refs. [20, 21, 39]). Let k be the largest integer $1 \leq k \leq n$ for which a given pure state can be written as

$$\left|\Psi^{(k)}\right\rangle = |\psi_1\rangle \otimes \cdots \otimes |\psi_k\rangle = \bigotimes_{m=1}^{k} |\psi_m\rangle \ , \tag{2.7}$$

where each of the k vectors $|\psi_m\rangle$ is an element of a Hilbert space $\mathcal{K}_m$ associated to one or several of the n subsystems, which together form a partition of the entire Hilbert space $\bigotimes_{m=1}^{k} \mathcal{K}_m \cong \mathcal{H}$. This state $\left|\Psi^{(k)}\right\rangle$ is then called a *k-product state*. For mixed states, a density matrix is called *k-separable* if k is the largest integer $1 \leq k \leq n$ for which there exists a pure state decomposition

$$\rho^{(k)} = \sum_i p_i |\Psi_i^{(k')}\rangle\langle\Psi_i^{(k')}| \ , \tag{2.8}$$

into k'-product states $|\Psi_i^{(k')}\rangle$ all satisfying $k' \geq k$. Note that here the involved states $|\Psi_i^{(k')}\rangle$ do not necessarily share a common partition of the Hilbert space.

If a state is n-separable, it contains no entanglement at all. Such a state is also called *fully separable*. States with $1 < k < n$ are *partially entangled*. Finally, the most interesting case is when $k = 1$. In this case, all n parties are involved in the entanglement. We refer to those states as *genuinely multipartite entangled* (GME) [20]. Important representatives for a tripartite system ($n = 3$) are e.g. the Greenberger-Horne-Zeilinger (GHZ) state

$$|\mathrm{GHZ}\rangle = \frac{1}{\sqrt{2}}(|000\rangle + |111\rangle) \ , \tag{2.9}$$

and the W-state

$$|\mathrm{W}\rangle = \frac{1}{\sqrt{3}}(|100\rangle + |010\rangle + |001\rangle) \ . \tag{2.10}$$

2.2 Characterization of entanglement

Bipartite entanglement can be characterized by the *Schmidt rank*. For any pure state $|\Psi\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_2$ there exist orthonormal vectors $\{|0_1\rangle, \ldots, |r-1_1\rangle\} \in \mathcal{H}_1$ and $\{|0_2\rangle, \ldots, |r-1_2\rangle\} \in \mathcal{H}_2$ that allow to write $|\Psi\rangle$ in the form

$$|\Psi\rangle = \sum_{i=0}^{r-1} \lambda_i \, |i_1\rangle \otimes |i_2\rangle \ . \tag{2.11}$$

using strictly positive coefficients $\lambda_i > 0$ satisfying $\sum_{i=0}^{r-1} \lambda_i^2 = 1$ with the convention $\lambda_i \geq \lambda_{i+1}$. This is called the *Schmidt decomposition*, where the minimum number $r \leq \min\{d_1, d_2\}$ of required product vectors $|i_1\rangle \otimes |i_2\rangle$ is called the *Schmidt rank*.

In this terminology, entangled states have Schmidt rank $r \geq 2$. Obviously, the Schmidt rank r provides us with the information of 'how many degrees of freedom' are involved in the entanglement [40, 41]. For instance, if a state has the Schmidt form $|\Psi\rangle = \lambda_0 \, |0_1\rangle \, |0_2\rangle + \lambda_1 \, |1_1\rangle \, |1_2\rangle$ it is entangled in two degrees of freedom $(0, 1)$. For higher-dimensional systems we could also have a state of the form $|\Psi\rangle = \lambda_0 \, |0_1\rangle \, |0_2\rangle + \lambda_1 \, |1_1\rangle \, |1_2\rangle + \lambda_2 \, |2_1\rangle \, |2_2\rangle$, which is entangled in three degrees of freedom $(0, 1, 2)$, and so forth. Note that in literature, there are various terms that refer to this particular characterization, such as *two-level* or *qubit-entanglement* for $r = 2$, as well as *qudit*, *higher-order*, *higher-dimensional* or *multilevel entanglement* for $r > 2$.

We call a state *maximally entangled* if it reaches the upper bound $r = \min\{d_1, d_2\}$ and all Schmidt coefficients are equal $\lambda_0 = \ldots = \lambda_{r-1}$. Those states minimize the locally obtainable information for pure states, in the sense that the result of any local measurement is indeterministic and evenly distributed over $r = \min\{d_1, d_2\}$ outcomes. To see this, observe that the Schmidt coefficients λ_i are simply the square-roots of the non-zero eigenvalues of the reduced density matrices

$$\rho_1 = \mathrm{Tr}_2 \left(|\Psi\rangle \langle\Psi| \right) = \sum_{i=0}^{r-1} \lambda_i^2 \, |i_1\rangle \langle i_1| \ , \tag{2.12}$$

$$\rho_2 = \mathrm{Tr}_1 \left(|\Psi\rangle \langle\Psi| \right) = \sum_{i=0}^{r-1} \lambda_i^2 \, |i_2\rangle \langle i_2| \ . \tag{2.13}$$

Specifically, for two systems of the same dimension $d_1 = d_2 \equiv d$ the reduced density matrix of a maximally entangled state is *maximally mixed* $\rho_1 = \rho_2 = \frac{1}{d} \mathbb{1}_d$. Thus, in

the Schmidt decomposition (2.11) a maximally entangled state reads

$$|\Psi\rangle = \sum_{i=0}^{d-1} \frac{1}{\sqrt{d}} |i_1\rangle \otimes |i_2\rangle \ . \tag{2.14}$$

The Schmidt rank can straightforwardly be extended to density matrices [42]. For a given density matrix the *Schmidt number* r is the smallest integer $1 \leq r \leq d$ for which there exists a decomposition $\rho = \sum_i p_i |\Psi_i\rangle \langle\Psi_i|$ into pure states $|\Psi_i\rangle$ of Schmidt rank $r' \leq r$ for all i. Hence, if the Schmidt number is r, then at least one pure state in any decomposition of ρ has at least Schmidt rank r.

It is ambiguous, how the Schmidt rank/number can be generalized to multipartite systems $\mathcal{H} = \bigotimes_{m=1}^{n} \mathcal{H}_m$. One option is the so-called *tensor rank* [43, 44, 45]. For pure states it is defined as the minimum number ($\equiv t$) of (completely factorized) n-product states (2.7), such that

$$|\Psi\rangle = \sum_{i=0}^{t-1} \lambda_i \bigotimes_{m=1}^{n} |\psi_{m,i}\rangle \ , \tag{2.15}$$

where $\sum_{i=0}^{t-1} |\lambda_i|^2 = 1$. Apparently, the tensor rank is equivalent to the Schmidt rank in case of two parties. Note, however, that for $n > 2$ the coefficients are allowed to be complex numbers $\lambda_i \in \mathbb{C}$. This is because $\lambda_i > 0$ is not always achievable when for all i, the vector $|\psi_{m,i}\rangle$ belongs to an arbitrary but fixed orthonormal basis of $\mathcal{H}_m$ (see e.g. Ref. [46]).

The tensor rank is a useful tool for discriminating between different kinds of multipartite entanglement [47, 48, 49]. For instance, we immediately see that there is a fundamental difference between the GHZ (2.9) and the W-state (2.10) as their tensor ranks ($t = 2$ versus $t = 3$) do not coincide (we will analyze this in more detail in Section 2.5). The tensor rank also allows for characterizing mixed state entanglement. The generalization to density matrices works completely analogous to the Schmidt rank/number [43].

For multipartite qudits, however, it no longer provides information on how many (local) degrees of freedom $(0, 1, 2, \ldots)$ are entangled. This follows from the fact that there is no direct link between the tensor rank, k-separability and multilevel entanglement. For instance, a state with $t = 3$ can be a biseparable state $\left|\Psi^{(2)}\right\rangle = |0\rangle \otimes \frac{1}{\sqrt{3}}(|00\rangle + |11\rangle + |22\rangle)$ containing bipartite three-level entanglement $(0, 1, 2)$, as well as a genuinely multipartite entangled state $|\mathrm{W}\rangle = \frac{1}{\sqrt{3}}(|100\rangle + |010\rangle + |001\rangle)$ which possesses only two-level entanglement $(0, 1)$. Of particular interest are states that are genuinely multipartite entangled in more than two levels. Those states recently got attention in quantum information processing [50, 51, 52, 53, 54, 55] and in the foundations of quantum theory [56, 57, 58, 59, 60]. The simplest example of a multilevel-multipartite entangled state is $|GHZ_3\rangle = \frac{1}{\sqrt{3}}(|000\rangle + |111\rangle + |222\rangle)$, which once more has tensor rank $t = 3$.

Research contribution(s): In our paper **[P3]**, we generalize the Schmidt rank to multipartite systems in a complementary way to the tensor rank. Therein, we propose the following characterization of multilevel-multipartite entanglement: For a pure n-partite state $|\psi\rangle \in \mathcal{H} = \bigotimes_{m=1}^{n} \mathcal{H}_m$ consider the set of all reduced density matrices $\{\rho_A = Tr_B(|\psi\rangle \langle\psi|)\}$ regarding all possible bipartitions $\gamma = \{(A|B)\}$ of the system, i.e. all $\mathcal{K}_A \otimes \mathcal{K}_B \cong \bigotimes_{m=1}^{n} \mathcal{H}_m$. Iff the state $|\psi\rangle$ is fully separable, then the rank of all reduced density matrices ρ_A is 1. On the other hand, the existence of a

reduced density matrix with $\mathrm{rank}(\rho_A) > 1$ implies that $|\psi\rangle$ is entangled. In this case, we know from the Schmidt decomposition that the number of entangled levels equals $\mathrm{rank}(\rho_A)$. Hence, iff $\max\{\mathrm{rank}(\rho_A)\} = f$ with $f \geq 2$ then the state $|\psi\rangle$ contains f-level entanglement. A state is *f-level genuinely multipartite entangled* iff it is at least f-level entangled with respect to *all* bipartitions, i.e. $\min\{\mathrm{rank}(\rho_A)\} = f$. This concept can be extended to mixed states in a natural way: A mixed state $\rho = \sum_i p_i |\psi_i\rangle \langle\psi_i|$ is f-level entangled iff there exists no decomposition $\{p_i, |\psi_i\rangle\}$ into pure state f_i level states $|\psi_i\rangle$ all obeying $f_i < f$, but there exists a decomposition into pure states satisfying $f_i \leq f$ for all i. A mixed state $\rho = \sum_i p_i |\psi_i\rangle \langle\psi_i|$ is f-level GME iff any decomposition $\{p_i, |\psi_i\rangle\}$ of ρ contains at least one pure state $|\psi_i\rangle$ which is at least f-level GME.

Examples of f-level GME states are the generalized GHZ state

$$|GHZ_f\rangle = \frac{1}{\sqrt{f}} \sum_{i=0}^{f-1} |i\rangle^{\otimes n} \ , \tag{2.16}$$

and the generalized *m-Dicke state*

$$|D_f^m\rangle := \frac{1}{\sqrt{(f-1)\binom{n}{m}}} \sum_{l=0}^{f-2} \sum_i \Pi_i |l+1\rangle^{\otimes m} |l\rangle^{\otimes n-m} \ , \tag{2.17}$$

where the inner sum runs over all $\binom{n}{m}$ distinct permutations Π_i between the first m and the last $n-m$ subsystems (see e.g. Refs. [61, 62]). In particular, the 1-Dicke state $|D_f^1\rangle$ is a multilevel generalization of the well-known W-state. For three parties and three levels one obtains, for example,

$$|D_3^1\rangle = \frac{1}{\sqrt{6}}(|100\rangle + |010\rangle + |001\rangle + |211\rangle + |121\rangle + |112\rangle) \ , \tag{2.18}$$

or for $m = 2$ and four qutrits one has, e.g.,

$$\begin{aligned} |D_3^2\rangle = \frac{1}{\sqrt{12}}(&|1100\rangle + |1010\rangle + |1001\rangle + |0110\rangle + |0101\rangle + |0011\rangle \\ &+ |2211\rangle + |2121\rangle + |2112\rangle + |1221\rangle + |1212\rangle + |1122\rangle) \ . \end{aligned} \tag{2.19}$$

2.3 Detection of entanglement

For any given pure state it is simple to tell whether it is separable or entangled, as well as how many parties and levels are involved. We know now from the previous sections that in this case it suffices to look at the reduced density matrices. However, for mixed states the given characterizations of entanglement are not operational. More applicable criteria enabling to verify entanglement are therefore vitally important. In this section, we give an introduction to the techniques of entanglement detection used in this thesis.

Let us start with the bipartite case. Here, one of the best known entanglement criteria is the *positive partial transpose* (PPT) criterion, which was introduced in Refs. [63, 64]. For any bipartite density matrix ρ expressed in the computational product basis

$$\rho = \sum_{i,j,k,l} \langle ik| \rho |jl\rangle |i\rangle \langle j| \otimes |k\rangle \langle l| \ , \tag{2.20}$$

the *partial transpose* is defined as

$$\rho^{T_1} = \sum_{i,j,k,l} \langle ik| \rho |jl\rangle \, (|i\rangle \langle j|)^T \otimes |k\rangle \langle l| = \sum_{i,j,k,l} \langle ik| \rho |jl\rangle \, |j\rangle \langle i| \otimes |k\rangle \langle l| \ , \tag{2.21}$$

$$\rho^{T_2} = \sum_{i,j,k,l} \langle ik| \rho |jl\rangle \, |i\rangle \langle j| \otimes (|k\rangle \langle l|)^T = \sum_{i,j,k,l} \langle ik| \rho |jl\rangle \, |i\rangle \langle j| \otimes |l\rangle \langle k| \ , \tag{2.22}$$

where the index of T denotes in which subsystem the transpose is performed. Here, observe that $\rho^T = (\rho^{T_1})^{T_2}$ and thus $\rho^{T_1} = (\rho^{T_2})^T$. Now, the PPT criterion is based on the observation that the partial transpose of any separable state $\rho = \sum_i p_i \, |\phi_i\rangle \langle\phi_i| \otimes |\psi_i\rangle \langle\psi_i|$ is positive-semidefinite, i.e. $\rho^{T_1} = \sum_i p_i (|\phi_i\rangle \langle\phi_i|)^T \otimes |\psi_i\rangle \langle\psi_i| \geq 0$ which is trivially true since each $(|\phi_i\rangle \langle\phi_i|)^T$ is merely the dyadic product of the complex conjugate state $|\phi_i\rangle^*$. Thus, when ρ^{T_1} (equivalently ρ^{T_2}) has a negative eigenvalue we know that the state must be entangled. Such a state is said to be NPPT which stands for non-positive-semidefinite under partial transpose. For two-qubit systems $\mathcal{H} = \mathbb{C}^2 \otimes \mathbb{C}^2$ and qubit-qutrit systems $\mathcal{H} = \mathbb{C}^2 \otimes \mathbb{C}^3$ it was shown that the PPT criterion is necessary and sufficient for separability [64]. In all other cases, there are entangled states which remain positive-semidefinite under partial transpose [65], meaning that $\rho^{T_1} \geq 0$ is necessary but not sufficient for separability anymore.

It should be mentioned that the PPT criterion is a special case of entanglement detection via *positive maps* [21, 64, 66]: We say that a linear map $\Lambda(\circ)$ is positive iff $\Lambda(A) \geq 0$ holds for all operators $A \geq 0$ on $\mathcal{H}$, i.e. when all positive operators are mapped onto positive operators. It turns out that positive maps are not necessarily also *completely positive*, which is when the extended map $[\Lambda \otimes \mathbb{1}_n](\circ)$ is also positive $[\Lambda \otimes \mathbb{1}_n](A) \geq 0$ for all positive operators $A \geq 0$ on $\mathcal{H} \otimes \mathbb{C}^n$ and any dimension n. Consequently, if a positive map is not completely positive it constitutes a possible candidate for entanglement detection since for any separable state $\rho = \sum_i p_i \, |\phi_i\rangle \langle\phi_i| \otimes |\psi_i\rangle \langle\psi_i|$ on $\mathcal{H}_1 \otimes \mathcal{H}_2$ it is guaranteed that

$$[\Lambda \otimes \mathbb{1}_{d_2}](\rho) = \sum_i p_i \Lambda(|\phi_i\rangle \langle\phi_i|) \otimes |\psi_i\rangle \langle\psi_i| \geq 0 \ , \tag{2.23}$$

whereas if ρ is entangled it can happen that $[\Lambda \otimes \mathbb{1}_{d_2}](\rho) \ngeq 0$. Indeed, it can even be shown that for any entangled state there exists a non-completely positive map detecting it [64]. However, this statement is of no practical use as there is no universal method to track down all relevant maps in a systematic way. Further details on this issue can be found in Refs. [67, 68, 69, 70, 71]. These references also contain important examples of non-completely positive maps inequivalent to the transpose.

Another concept for entanglement detection are *entanglement witnesses*. According to the definition, the set of separable states is closed and convex. From the *Hahn-Banach separation theorem* (HBST) it follows that this set can be fully characterized in terms of half-spaces [72]. In other words, there exist hyperplanes that separate the separable from the entangled states. A hyperplane and its associated half-spaces can be expressed in terms of a normal vector – which in our case is a hermitian operator W. Such an operator W is called an *entanglement witness* iff there are states ρ with

$$\mathrm{Tr}\,(W\rho) < 0 \ , \tag{2.24}$$

and *all* separable density matrices $\sigma = \sum_i p_i \, |\phi_i\rangle \langle\phi_i| \otimes |\psi_i\rangle \langle\psi_i|$ satisfy

$$\mathrm{Tr}\,(W\sigma) \geq 0 \ . \tag{2.25}$$

Obviously, any state with $\mathrm{Tr}\,(W\rho) < 0$ can only be entangled. In fact, for each entangled state ρ there also exists a corresponding entanglement witness with $\mathrm{Tr}\,(W\rho) < 0$ as a consequence of the HBST (see also Refs. [64, 73]).

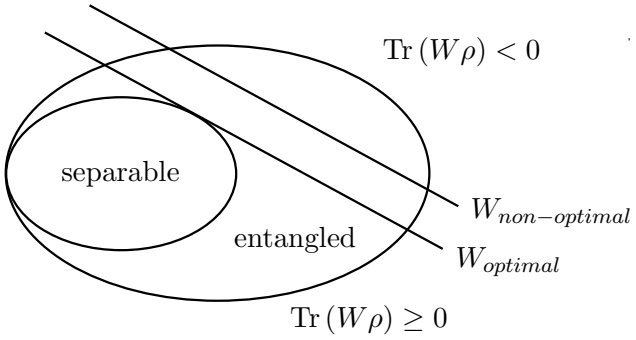

Figure 2.1: Schematic illustration of the convex set of separable states and two entanglement witnesses.

Entanglement witnesses can be compared by their detection strength: For a given W, we denote the set of detected states by $\mathcal{D}(W) = \{\rho \mid \mathrm{Tr}\,(W\rho) < 0\}$. We say the witness W_1 is *finer* than W_2 iff $\mathcal{D}(W_2) \subset \mathcal{D}(W_1)$. A witness for which there exists no finer witness is called *optimal*. An optimal witness W_{opt} is necessarily *tangential* to the set of separable states. That is, there exists at least one separable state σ with $\mathrm{Tr}\,(W_{opt}\sigma) = 0$. The concept of entanglement detection via witnesses is graphically sketched in Figure 2.1.

Besides the fact that entanglement witnesses are conceptually intuitive, they also have the advantage that they are experimentally implementable: Because they are hermitian they correspond to measurable observables. Furthermore, using e.g. the representation (1.29) it is also possible to decompose a witness W into a weighted sum of local hermitian operators

$$W = \sum_{k=0}^{d_1^2-1} \sum_{l=0}^{d_2^2-1} w_{k,l}\ F_k \otimes F_l\ , \tag{2.26}$$

and thus $\mathrm{Tr}\,(W\rho)$ reduces to measuring joint expectation values $\langle F_k \otimes F_l \rangle$. In addition, for many important witnesses only a few of the coefficients $w_{k,l}$ are non-zero, with the consequence that the experimental effort can often be dramatically decreased. In other words, entanglement witnesses generally do not require a full state tomography (which is e.g. needed for the PPT criterion).

Let us now turn to the question of how entanglement witnesses can be constructed. Actually, there is a vast literature on this subject (see Refs. [20, 21] and references therein), and there exist various methods e.g. based on geometric considerations [75, 76], semidefinite programs [77, 78] or positive maps via the Jamiołkowski isomorphism [79, 80, 81, 82]. Here, however, we only discuss a simple approach which can be adapted to the multipartite and multilevel case without any difficulty.

First, note that $\mathrm{Tr}\,(W\rho)$ is linear in the density matrix, and thus to guarantee that $\mathrm{Tr}\,(W\sigma) \geq 0$ holds for all separable states σ it suffices to check $\langle\phi| \otimes \langle\psi|\, W\, |\phi\rangle \otimes |\psi\rangle \geq 0$ for pure product states, which of course simplifies the problem tremendously. Second, for all product states $|\Psi_{prod}\rangle$ there is an upper bound on the overlap with a

given entangled pure state $|\Psi_{ent}\rangle$

$$\alpha = \max_{\{|\Psi_{prod}\rangle\}} |\langle\Psi_{prod}|\Psi_{ent}\rangle|^2 \ . \tag{2.27}$$

It is straightforward to show that α is the square of the largest Schmidt coefficient λ_0 of $|\Psi_{ent}\rangle$ [20, 74]. This observation allows us to write down a so-called *projector-based entanglement witness* (PEW)

$$W = \lambda_0^2 \mathbb{1} - |\Psi_{ent}\rangle\langle\Psi_{ent}| \ , \tag{2.28}$$

using an arbitrary entangled state $|\Psi_{ent}\rangle$.

We can generalize this concept in the following way: Suppose we want to determine the Schmidt number of a bipartite mixed state, i.e. the number of levels $r \geq 2$ that are entangled. For that, we can introduce a *Schmidt number witness* W_r [40, 41] with the property that $\mathrm{Tr}(W_r\rho) < 0$ only if the Schmidt number of ρ is at least r, whereas *all* density matrices σ with a lower Schmidt number satisfy $\mathrm{Tr}(W\sigma) \geq 0$. As before, we can use the maximal overlap between an arbitrary entangled state $|\Psi_{ent}\rangle$ of Schmidt rank greater or equal r, to construct a projector-based Schmidt number witness

$$W_r = \sum_{i=0}^{r-2} \lambda_i^2 \mathbb{1} - |\Psi_{ent}\rangle\langle\Psi_{ent}| \ , \tag{2.29}$$

where we sum over the $r-1$ largest Schmidt coefficients of $|\Psi_{ent}\rangle$.

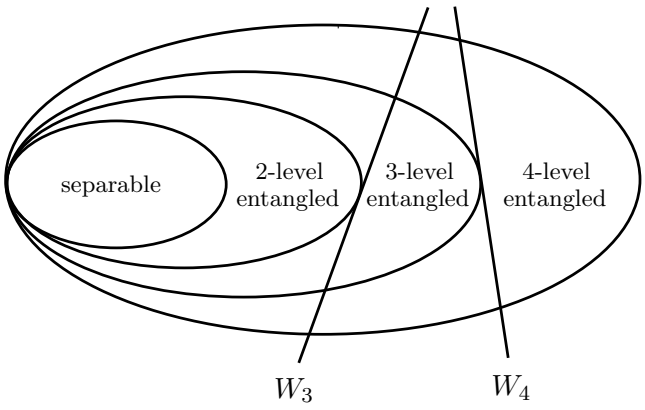

Figure 2.2: Schematic illustration of the convex structure of multilevel entanglement and two Schmidt number witnesses W_3, W_4.

For multipartite qudit systems, we can proceed analogously. A hermitian operator $W^{(k)}$ on $\mathcal{H} = \bigotimes_{m=1}^{n} \mathcal{H}_m$ is called a *k-separability witness* iff it is possible to attain $\mathrm{Tr}\left(W^{(k)}\rho\right) < 0$, but all density matrices $\rho^{(k')}$ with a higher separability $k' > k$ obey $\mathrm{Tr}(W^{(k)}\rho^{(k')}) \geq 0$. Moreover, to verify multilevel-multipartite entanglement, we may further divide the set of 1-separability witnesses into different types. For instance, we call a 1-separability witness $W_f^{(1)}$ an *f-level GME witness* iff it additionally satisfies $\mathrm{Tr}(W_f^{(1)}\sigma) \geq 0$ for all states σ which are GME in less than f-levels (and/or biseparable). Here, we again use an arbitrary f-level GME pure state $|\Psi_f\rangle$ to construct a witness. Let us denote by $\lambda(A|B)_i$ the Schmidt coefficients of the state with respect to a fixed bipartition $(A|B)$ of the system, i.e. $\mathcal{H} \cong \mathcal{K}_A \otimes \mathcal{K}_B$.

With respect to any bipartition $(A|B)$, a $(f-1)$-level state can maximally attain an (absolute square) overlap of $\sum_{i=0}^{f-2} \lambda(A|B)_i^2$. It follows that by taking the maximum of $\sum_{i=0}^{f-2} \lambda(A|B)_i^2$ over all bipartitions $\gamma = \{(A|B)\}$ we have that

$$W_f^{(1)} = \max_{\gamma} \left[\sum_{i=0}^{f-2} \lambda(A|B)_i^2 \right] \mathbb{1} - |\Psi_f\rangle \langle \Psi_f| \ , \tag{2.30}$$

constitutes a proper f-level GME witness.

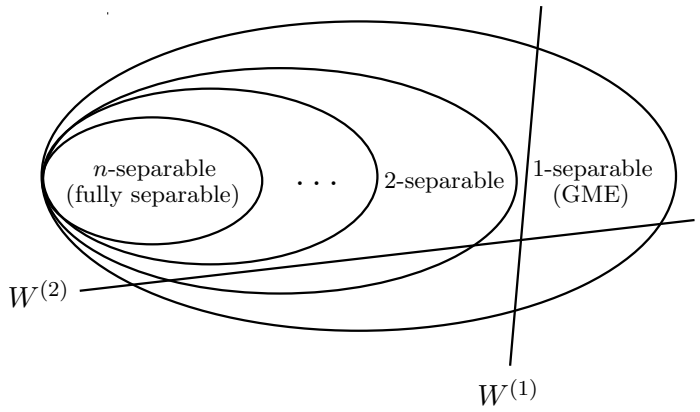

Figure 2.3: Schematic illustration of the convex structure of k-separability including two k-separability witnesses $W^{(1)}$, $W^{(2)}$.

Finally, let us come to the last method of entanglement detection that is used in this thesis. One may expect that for separable states there should be specific constraints on the matrix elements $\langle\phi| \langle\vartheta| \rho |\varphi\rangle |\psi\rangle$ of a density matrix ρ. This idea leads to the concept of *matrix element criteria* (MEC). Indeed, it was proven in Ref. [83] that the inequality

$$| \langle\phi| \langle\vartheta| \rho |\varphi\rangle |\psi\rangle | - \sqrt{\langle\phi| \langle\psi| \rho |\phi\rangle |\psi\rangle \langle\varphi| \langle\vartheta| \rho |\varphi\rangle |\vartheta\rangle} \leq 0 \ , \tag{2.31}$$

holds for all separable states ρ on $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$ and all vectors $|\phi\rangle, |\varphi\rangle \in \mathcal{H}_1$ and $|\vartheta\rangle, |\psi\rangle \in \mathcal{H}_2$. Thus, in order to detect entanglement in a given state ρ we only have to find some vectors $|\phi\rangle, |\varphi\rangle, |\vartheta\rangle, |\psi\rangle$ for which the left-hand side of (2.31) is larger than zero. In practice, one can often achieve this either by making an educated guess depending on the form of the state, or otherwise by resorting to numerical methods.

It was shown that the inequality (2.31) can be extended for the detection of multipartite entanglement [83]: This generalization can be formulated in a concise way by using a twofold copy of the density matrix $\rho^{\otimes 2}$ on $\mathcal{H} \otimes \mathcal{H} = (\bigotimes_{n=1}^{m} \mathcal{H}_n)^{\otimes 2}$. For each bipartition $(A|B)$ of $\mathcal{H} \cong \mathcal{K}_A \otimes \mathcal{K}_B$ we define a permutation operator $\mathcal{P}_A$ which permutes the subsystem A with its copy A', i.e. $\mathcal{H}^{\otimes 2} = \mathcal{K}_A \otimes \mathcal{K}_B \otimes \mathcal{K}_{A'} \otimes \mathcal{K}_{B'} \to \mathcal{K}_{A'} \otimes \mathcal{K}_B \otimes \mathcal{K}_A \otimes \mathcal{K}_{B'}$[3]. Let us again denote by $\gamma = \{(A|B)\}$ the set of all possible bipartitions. Using this notation and exploiting the convexity of the left-hand side of (2.31) in ρ, one can show that

$$| \langle\Phi| \rho |\Psi\rangle | - \sum_{\gamma} \sqrt{\langle\Phi| \otimes \langle\Psi| \mathcal{P}_A^{\dagger} \rho^{\otimes 2} \mathcal{P}_A |\Phi\rangle \otimes |\Psi\rangle} \leq 0 \tag{2.32}$$

[3]For example, for the bipartition $(1|2,\ldots,n)$ and the vector $|k\rangle^{\otimes n} \otimes |l\rangle^{\otimes n} \in \mathcal{H}^{\otimes 2}$ the corresponding operator $\mathcal{P}_1$ acts like $\mathcal{P}_1 |k\rangle^{\otimes n} \otimes |l\rangle^{\otimes n} = |l\rangle \otimes |k\rangle^{\otimes(n-1)} \otimes |k\rangle \otimes |l\rangle^{\otimes(n-1)}$

holds for all biseparable states and all n-product vectors $|\Phi\rangle = \bigotimes_{m=1}^{n} |\phi_m\rangle \in \mathcal{H}$ and $|\Psi\rangle = \bigotimes_{m=1}^{n} |\psi_m\rangle \in \mathcal{H}$. Thus, any violation of this inequality unambiguously implies that ρ is genuinely multipartite entangled.

Research contribution(s): It turns out that the matrix element criterion (2.32) is just one member of a larger family of inequalities for the detection of multipartite entanglement. Namely, there are similar expressions for arbitrary k-separability [84], particular states [85] and continuous variable systems [86]. The motivation of our paper **[P3]** was to extend this framework of inequalities for the detection of multilevel genuine multipartite entanglement. Currently, there are only a few criteria available for this kind of entanglement (see Refs. [87, 88]), and these are rather moderate in their robustness to noise. In **[P3]** we derive a set of inequalities which are optimally suited to verify the presence of f-level GME in non-pure density matrices close to the multilevel GHZ (2.16), W and Dicke state (2.17). These inequalities are shown to be stronger than the previously known projector-based witnesses. Moreover, we also discuss the usage of our criteria in experiments. Here we explain why their implementation requires only partial information about the density matrix.

2.4 Entanglement measures

For certain applications and tasks that require entanglement as a resource it is not only important to detect entanglement, but also to quantity the amount of entanglement a state contains. Maps $\rho \mapsto E(\rho) \in \mathbb{R}_0^+$ that serve this purpose are called *entanglement measures* [89, 90]. We begin with the bipartite case $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$. Any serious and meaningful entanglement measure $E(\rho)$ should have at least the following properties:

M1	$E(\rho) > 0$	only if ρ is entangled
M2	$E(\Lambda_{LOCC}(\rho)) \leq E(\rho)$	non-increasing under LOCC
M3	$E(U_1 \otimes U_2 \rho U_1^\dagger \otimes U_2^\dagger) = E(\rho)$	invariant under local unitaries

There are several candidates that fulfill these conditions: One way of formulating entanglement measures is in terms of LOCC convertibility in the asymptotic sense [91]. A well-known example is the *entanglement cost*, which is defined as the minimal number of maximally entangled states that are required per copy to produce the given state ρ (in the limit of infinitely many output states). That is, it tells us how expensive it is to create a particular state ρ. The converse of this measure is called *entanglement of distillation*. It tells us how many maximally entangled states we can extract from a state ρ in the limit $n \to \infty$ of infinitely many copies $\rho^{\otimes n}$.

Another way of quantifying entanglement is to measure the distance between the given state ρ and the closest separable state σ. Such quantifiers are referred to as *geometric entanglement measures*. Depending on the used distance function, this leads to the so-called *Bures measure of entanglement*, *relative entropy of entanglement* [92] or the *Hilbert-Schmidt entanglement*[4] [75]. In addition, there is also an information-theoretic approach to entanglement measures. Based on the quantum conditional mutual information one can formulate a measure called *squashed entanglement* with many beneficial attributes [94, 95]. Note that it is even possible to use the *(logarithmic) negativity* [96, 97] given by the PPT criterion as a measure of entanglement. This quantity is particularly easy to compute, however there are

[4]Note that up to now there is no rigorous proof that the Hilbert-Schmidt measure is monotonous under LOCC[93].

entangled states for which this measure is zero, and its physical and information-theoretic meaning is rather unclear.

In principle, any of these entanglement measures can be used to quantify entanglement. Nevertheless, it is important to note that there are subtle differences. Depending on a particular task or application, it is often demanded that the entanglement measure meets further requirements in addition to M1, M2 and M3. Frequently considered optional properties are

M4	$E(\sum_i p_i\rho_i) \leq \sum_i p_i E(\rho_i)$	convex
M5	$E(\rho) = 0 \Leftrightarrow \rho$ is separable	faithful
M6	$\|\rho_1 - \rho_2\|_{HS} \to 0 \Rightarrow \|E(\rho_1) - E(\rho_2)\| \to 0$	continuous
M7	$E(\rho_1 \otimes \rho_2) = E(\rho_1) + E(\rho_2)$	fully additive
M8	$E(\rho_1 \otimes \rho_2) \leq E(\rho_1) + E(\rho_2)$	subadditive
M9	$E(\rho^{\otimes n}) = nE(\rho)$	partially additive

A detailed comparison of the mentioned entanglement measures regarding these properties can be found in Refs. [95, 98, 99].

Let us now focus on the entanglement measures that we use in this thesis – the so-called *convex roof measures*. The idea behind them is to introduce a computable entanglement measure for pure states $E(|\Psi\rangle)$, and then to generalize it to mixed states $E(\rho)$ using a convex roof construction

$$E(\rho) = \inf_{\rho=\sum_i p_i|\Psi_i\rangle\langle\Psi_i|} \sum_i p_i E\left(|\Psi_i\rangle\right) \ , \tag{2.33}$$

where the infimum is taken over all possible pure state decomposition of $\rho = \sum_i p_i |\Psi_i\rangle \langle\Psi_i|$ with $\sum_i p_i = 1$ and $p_i \geq 0$.

For pure states $|\Psi\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_2$ it is straightforward to formulate entanglement measures via reduced density matrices $\rho_1 = \mathrm{Tr}_2 |\Psi\rangle \langle\Psi|$. Here, the mixedness of ρ_1 provides information on the amount of entanglement. It can be quantified using an entropy measure $S(\rho_1)$. The best known example of a convex roof measure constructed in this way is the *entanglement of formation* [100], which is defined as

$$E_{EOF}(\rho) = \inf_{\rho=\sum_i p_i|\Psi_i\rangle\langle\Psi_i|} \sum_i p_i S_N\left(\mathrm{Tr}_2 |\Psi_i\rangle \langle\Psi_i|\right) \ , \tag{2.34}$$

where S_N is the *von Neumann entropy*

$$S_N(\rho_1) = -\mathrm{Tr}\left(\rho_1 \log \rho_1\right) \ . \tag{2.35}$$

Entanglement of formation is a good measure of entanglement as in addition to M1, M2, M3 it also fulfills also M4, M5, M6 and M8.

However, as for most entanglement measures there is no general recipe how to compute the entanglement of formation for any mixed state of a system with arbitrary dimension. Some exact expressions were obtained for special cases [101, 102], but generally we have to resort to lower bounds [103, 104]. The only system for which we can analytically compute the entanglement of formation for all states is the bipartite qubit system. Here, the problem of determining the optimal pure state decomposition of ρ for E_{EOF} can be recast in terms of an auxiliary quantity called the *concurrence*. For a pure state $|\Psi\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_2$ the concurrence [105, 106] may be

defined as[5]

$$C(|\Psi\rangle) = \sqrt{2(1 - \mathrm{Tr}\,(\rho_1^2))}\ , \tag{2.36}$$

where ρ_1 is again the reduced density matrix $\rho_1 = \mathrm{Tr}_2\,|\Psi\rangle\,\langle\Psi|$. The concurrence can be generalized to mixed states via the convex roof construction (2.33)

$$C(\rho) = \inf_{\rho=\sum_i p_i|\Psi_i\rangle\langle\Psi_i|} \sum_i p_i C\left(|\Psi_i\rangle\right)\ . \tag{2.37}$$

At first sight this does not improve our situation, as again we would have to find the optimal pure state decomposition that yields the infimum. Nevertheless, for bipartite qubit systems $\mathcal{H} = \mathbb{C}^2 \otimes \mathbb{C}^2$ it was established in Refs. [107, 108] that

$$C(\rho) = \max\{\sqrt{\lambda^1} - \sqrt{\lambda^2} - \sqrt{\lambda^3} - \sqrt{\lambda^4}, 0\} \tag{2.38}$$

wherein λ^i are the eigenvalues of $\rho\sigma_2 \otimes \sigma_2\rho^*\sigma_2 \otimes \sigma_2$ in descending order (and $\sigma_2 = -\mathbb{i}\,|0\rangle\,\langle 1| + \mathbb{i}\,|1\rangle\,\langle 0|$). Using this result, it was found that the two-qubit entanglement of formation has the analytic solution

$$E_{EOF}(\rho) = H\left[\frac{1}{2}(1 + \sqrt{1 - C^2(\rho)})\right]\ , \tag{2.39}$$

with

$$H\,[x] = -x\log x - (1-x)\log(1-x)\ . \tag{2.40}$$

Irrespective of the remarkable connection between the concurrence and the entanglement of formation for qubits, the concurrence (for arbitrary dimension) itself constitutes a proper entanglement measure with the properties M1, M2, M3, M4, M5 and M6. To be precise, the concurrence is a convex roof measure based on the *linear entropy* $S_L\,(\rho_1) = \frac{d}{d-1}(1 - \mathrm{Tr}\,(\rho_1^2))$.

Research contribution(s): A lower bound on the qudit concurrence was derived in Refs. [109, 110]. It was found that $B(\rho) \leq C(\rho)$ where

$$B(\rho)^2 = \sum_{k_1<l_1} \sum_{k_2<l_2} X^2_{k_1,l_1,k_2,l_2}\ , \tag{2.41}$$

and

$$X_{k_1,l_1,k_2,l_2} := \max\{\sqrt{\lambda^i_{k_1,l_1,k_2,l_2}} - \sum_{i>2} \sqrt{\lambda^i_{k_1,l_1,k_2,l_2}}, 0\}\ , \tag{2.42}$$

where $\lambda^i_{k_1,l_1,k_2,l_2}$ are the eigenvalues of $\rho Y_{k_1,l_1} \otimes Y_{k_2,l_2}\rho^* Y_{k_1,l_1} \otimes Y_{k_2,l_2}$ in descending order (with $Y_{k,l} = -\mathbb{i}\,|k\rangle\,\langle l| + \mathbb{i}\,|l\rangle\,\langle k|$). Notice that this lower bound reproduces the exact solution (2.38) for $\mathcal{H} = \mathbb{C}^2 \otimes \mathbb{C}^2$.

It was noticed that $B(\rho)$ is not invariant under local unitaries. Consequently, we can improve the lower bound on $C(\rho)$ by performing suitable transformations $\rho \to U_1 \otimes U_2\rho U_1^\dagger \otimes U_2^\dagger$. In our paper **[P1]**, we give a method for efficiently optimizing $B(\rho)$ by means of the composite parameterization of $\mathcal{U}(d)$.

[5] Note that the factor 2 is only convention. Alternatively, we may define the concurrence as $C(|\Psi\rangle) = \sqrt{\frac{d}{d-1}(1 - \mathrm{Tr}\,(\rho_1^2))}$.

We also consider a possible generalization of the concurrence for systems of more than two parties. In contrast to the bipartite case, it is obviously not possible to construct one single quantity (i.e. measure) reflecting all different characteristics of multipartite entanglement. Instead, it is desirable to have several entanglement measures, each of which corresponding to a particular aspect of multipartite entanglement. In our work **[P4]**, we introduce the *GME-concurrence* – a multipartite extension of the concurrence that *strictly* quantifies the amount of genuine multipartite entanglement. For a pure state $|\Psi\rangle$ of an n-partite system $\mathcal{H} = \bigotimes_{m=1}^{n} \mathcal{H}_m$ it is defined as

$$C_{GME}(|\Psi\rangle) = \min_{\gamma} \sqrt{2(1 - \mathrm{Tr}\,(\rho_A^2))}\ , \tag{2.43}$$

where the minimum is taken over all possible bipartitions $\gamma = \{(A|B)\}$ of the system, i.e. all $\mathcal{H} \cong \mathcal{K}_A \otimes \mathcal{K}_B$. From this definition it follows that the GME-concurrence is zero for all separable and all partially entangled states. Hence, $C_{GME}(|\Psi\rangle)$ is non-zero if and only if $|\Psi\rangle$ is genuinely multipartite entangled. For mixed states we are again confronted with the incalculable convex roof

$$C_{GME}(\rho) = \inf_{\{p_i, |\psi_i\rangle\}} \sum_i p_i C_{GME}(|\psi_i\rangle)\ . \tag{2.44}$$

However, we also derive a strong lower bound on $C_{GME}(\rho)$ based on the matrix element criterion discussed in Section 2.3.

2.5 Classification of multipartite entanglement

As already mentioned, multipartite systems can be entangled in various different ways. A central problem concerns the classification of quantum states concerning their entanglement properties. A well-known approach of introducing equivalence classes among states is in terms of *invertible local operations* (ILOs) [111]. According to this scheme, two pure states $|\psi\rangle, |\phi\rangle \in \bigotimes_{m=1}^{n} \mathcal{H}_m$ belong to the same class iff there exist n invertible operators $A_m \in \mathrm{GL}(d_m, \mathbb{C})$ such that

$$|\psi\rangle = \left[\bigotimes_{m=1}^{n} A_m\right] |\phi\rangle\ . \tag{2.45}$$

For bipartite systems $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$ this is exactly the case iff two states have the same Schmidt rank r. Hence, for two qudits of dimension d we immediately see that there are d classes of states: one class for separable states and $d-1$ classes of entanglement. Unfortunately, for multipartite systems the situation is more elaborate. For instance, it was found that for three qubits there are four classes of states, two of which are genuinely tripartite entangled. Their representatives are

C1	$\|000\rangle$	fully separable
C2	$\frac{1}{\sqrt{2}}(\|000\rangle + \|011\rangle)$	biseparable (one for each bipartition)
C3	$\frac{1}{\sqrt{3}}(\|100\rangle + \|010\rangle + \|001\rangle)$	W-type genuinely tripartite entangled
C4	$\frac{1}{\sqrt{2}}(\|000\rangle + \|111\rangle)$	GHZ-type genuinely tripartite entangled

Any state $|\Psi\rangle = \sum_{i,j,k=0}^{1} c_{i,j,k} |ijk\rangle$ can be transformed into one of these four C1-C4.

For four qubits the number of classes becomes infinite. However, as shown in Ref. [112] the uncountable set of representatives can be grouped into nine continuous families. Omitting normalization, these are

F1 $\frac{a+d}{2}(|0000\rangle + |1111\rangle) + \frac{a-d}{2}(|0011\rangle + |1100\rangle)$
$+ \frac{b+c}{2}(|0101\rangle + |1010\rangle) + \frac{b-c}{2}(|0110\rangle + |1001\rangle)$

F2 $\frac{a+b}{2}(|0000\rangle + |1111\rangle) + \frac{a-b}{2}(|0011\rangle + |1100\rangle)$
$+ c(|0101\rangle + |1010\rangle) + |0110\rangle$

F3 $a(|0000\rangle + |1111\rangle) + b(|0101\rangle + |1010\rangle) + |0110\rangle + |0011\rangle$

F4 $a(|0000\rangle + |1111\rangle) + \frac{a+b}{2}(|0101\rangle + |1010\rangle) + \frac{a-b}{2}(|0110\rangle + |1001\rangle)$
$+ \frac{\mathbb{i}}{\sqrt{2}}(|0001\rangle + |0010\rangle + |0111\rangle + |1011\rangle)$

F5 $a(|0000\rangle + |0101\rangle + |1010\rangle + |1111\rangle) + (\mathbb{i}\,|0001\rangle + |0110\rangle - \mathbb{i}\,|1011\rangle)$

F6 $a(|0000\rangle + |1111\rangle) + (|0011\rangle + |0101\rangle + |0110\rangle)$

F7 $|0000\rangle + |0101\rangle + |1000\rangle + |1110\rangle$

F8 $|0000\rangle + |1011\rangle + |1101\rangle + |1110\rangle$

F9 $|0000\rangle + |0111\rangle$

with the parameters $a, b, c, d \in \mathbb{C}$. Every pure four qubit state can be converted into either of these nine families F1-F9 (up to permutations of the subsystems). An analogous classification for more than four qubits and higher dimensional systems is unknown. This is mainly because of the complexity of specifying mutually inequivalent families of states.

Research contribution(s): In our publication [**P5**], we propose a scheme that enables to introduce entanglement classes for an arbitrary number of parties. Our classification is closely related to the preparation and observation process in experiments. In detail, we define entanglement classes in terms of convex mixtures of continuous families of states including their local-unitary and permutational equivalents. One of the main advantages of our concept is that it allows for imperfect mixed states. As examples, we present three entanglement classes that can be constructed in this way. Moreover, we provide simple inequalities enabling to distinguish between these classes given an arbitrary mixed state.

Optional (not part of this thesis): The physical significance of entanglement classes is further discussed in [**P8**]. In this paper, we derive conditions for a Lorentz invariant classification of multipartite entanglement. We show that the concept given in [**P5**] is in accordance with these conditions.

2.6 Local-unitary invariant states

Symmetries play an important role in various branches of modern physics. In many cases they provide deeper insights, give rise to simple solutions and/or allow for mathematically elegant statements. One type of symmetry for quantum states is the invariance under multilateral unitary transformations. Density matrices ρ_S on $\mathcal{H} = \bigotimes_{m=1}^{n} \mathcal{H}_m$ with such a symmetry have the remarkable property that they remain unchanged under certain local-unitaries $U_1 \otimes \cdots \otimes U_n \neq \mathbb{1}$, i.e.

$$\rho_S = U_1 \otimes \cdots \otimes U_n \rho_S U_1^\dagger \otimes \cdots \otimes U_n^\dagger \ . \tag{2.46}$$

For bipartite systems $\mathcal{H} = \mathbb{C}^d \otimes \mathbb{C}^d$ there are two famous examples:
• The *Werner state* ρ_W [113]

$$\rho_W = U \otimes U \rho_W U^\dagger \otimes U^\dagger \qquad \forall\ U \in \mathcal{U}(d)\ , \tag{2.47}$$

which is invariant under all bilateral unitaries $U \otimes U$.
• The *isotropic state* ρ_I [114]

$$\rho_I = U \otimes U^* \rho_W U^\dagger \otimes U^T \qquad \forall\, U \in \mathcal{U}(d)\ , \tag{2.48}$$

which remains unaltered under any $U \otimes U^*$ transformation.

Both states contain one free parameter and may be written as [115]

$$\rho_W = \frac{\beta(\sum_{i,j=0}^{d-1} |ij\rangle\langle ji|) + \mathbb{1}}{d(d+\beta)}\ , \tag{2.49}$$

where $-1 \leq \beta \leq 1$, and

$$\rho_I = \alpha \left|\phi_d^+\right\rangle\left\langle\phi_d^+\right| + \frac{1-\alpha}{d^2}\mathbb{1}\ , \tag{2.50}$$

with $\left|\phi_d^+\right\rangle = \frac{1}{\sqrt{d}}\sum_{i=0}^{d-1} |i\rangle \otimes |i\rangle$ and $-\frac{1}{d^2-1} \leq \beta \leq 1$.

The same terminology is also used in the multipartite case, i.e. an n-partite density matrix ρ_W on $(\mathbb{C}^d)^{\otimes n}$ satisfying

$$\rho_W = U \otimes \cdots \otimes U \rho_W U^\dagger \otimes \cdots \otimes U^\dagger \qquad \forall\, U \in \mathcal{U}(d)\ , \tag{2.51}$$

is called a multipartite Werner state. For arbitrary dimension d and number of parties n, any Werner state may be expressed as [116, 117]

$$\rho_W = \sum_{i=0}^{n!-1} \gamma_i \Pi_i\ , \tag{2.52}$$

where $\gamma_i \in \mathbb{R}$ are some parameters, and Π_i are permutation operators which interchange the subsystems (including the identity $\Pi_0 = \mathbb{1}$). For example, for $n = 2$ there is only $\Pi_0 = \mathbb{1}$ and one permutation operator $\Pi_1 = |ij\rangle\langle ji|$ performing $\Pi_1 |\psi\rangle \otimes |\phi\rangle = |\phi\rangle \otimes |\psi\rangle$, which (taking into account positivity and normalization) leads to Eq. (2.49). In the general case, we have $n!$ operators Π_i as n parties can be ordered in $n!$ different ways. The main drawback of the general expression (2.52) for arbitrary n is that the parameter ranges of γ_i for which ρ_W is a density matrix are often difficult to handle. For this reason there exists no simple closed-form description of multipartite Werner states.

Apart from this issue, there are two important pure states with $U^{\otimes n}$-invariance that we would like to mention in this section:
• The *n-qubit singlet state* in $(\mathbb{C}^2)^{\otimes n}$ for an even number n of qubits [118, 119]

$$|\mathcal{S}_{n,2}\rangle = \frac{1}{(n/2)!\sqrt{n/2+1}} \sum_i z_i!(n/2-z_i)!(-1)^{n/2-z_i} \Pi_i |0\rangle^{\otimes n/2} |1\rangle^{\otimes n/2}\ , \tag{2.53}$$

where the sum runs over all distinct permutations Π_i between the first $n/2$ and the last $n/2$ subsystems. Here, each z_i corresponds to the number of subsystems that are unaffected by the particular permutation Π_i. In other words, z_i equals the number of zeros 0 occurring in the first $n/2$ subsystems of $\Pi_i |0\rangle^{\otimes n/2} |1\rangle^{\otimes n/2}$. For example, the four-qubit singlet state reads

$$|\mathcal{S}_{4,2}\rangle = \frac{1}{2\sqrt{3}}(2|0011\rangle - |0101\rangle - |0110\rangle - |1001\rangle - |1010\rangle + 2|1100\rangle)\ . \tag{2.54}$$

• The *Aharonov state* [120, 121, 122] for $(\mathbb{C}^n)^{\otimes n}$

$$|\mathcal{S}_n\rangle = \frac{1}{\sqrt{n!}} \sum_{j,\ldots,l=0}^{n-1} \varepsilon_{j,\ldots,l} \, |j,\ldots,l\rangle \ . \tag{2.55}$$

For instance, the three-qutrit Aharonov state reads

$$|\mathcal{S}_3\rangle = \frac{1}{\sqrt{6}}(|012\rangle + |120\rangle + |201\rangle - |021\rangle - |102\rangle - |210\rangle) \ . \tag{2.56}$$

Finally, let us note that any state ρ on $(\mathbb{C}^d)^{\otimes n}$ can be transformed into a Werner state via the physical map

$$\Lambda_{twirl}(\rho) = \int_{\mathcal{U}(d)} U \otimes \cdots \otimes U \rho U^\dagger \otimes \cdots \otimes U^\dagger dU \ , \tag{2.57}$$

known as *twirling*. In practical applications, this operation may be realized with a finite set of unitaries $\{U_i\}$ – called a *unitary design* [123, 124, 125, 126]

$$\Lambda_{twirl}(\rho) = \frac{1}{N} \sum_{i=1}^{N} U_i \otimes \cdots \otimes U_i \rho U_i^\dagger \otimes \cdots \otimes U_i^\dagger \ . \tag{2.58}$$

Note that the integral (2.57) can also be computed explicitly via the composite parameterization (1.16) and the formula (1.22) as stressed in **[P2]**.

2.7 Distillability problem

Highly entangled pure states constitute a valuable resource in quantum information processing. However, when generating and distributing such states we are unavoidably confronted with imperfections, disturbances and noise such that in practice we are actually dealing with mixed and non-maximally entangled states. A central problem in entanglement theory therefore concerns how to maintain and recover high-fidelity entanglement. For this purpose, *entanglement distillation protocols* have been introduced. Here, several copies of a noisy and non-maximally entangled state ρ are used and processed by LOCCs in such a way that a fewer number of states with a higher fidelity are produced. The overall amount of entanglement of course cannot increase under LOCC. Instead, distillation means that some entanglement is gathered from an ensemble of copies and concentrated into few particles.

Several entanglement distillation protocols have been introduced for this purpose. Particularly noteworthy are Bennett *et al.*'s *recurrence*, *hashing* and *breeding protocols* [127, 128] and Deutsch *et al.*'s protocol [129], as well as their adaptations and generalizations [130, 131, 132]. For some density matrices ρ, these protocols allow to successively increase the fidelity $F(\rho) = \mathrm{Tr}\,(\rho\,|\Psi_t\rangle\,\langle\Psi_t|)$ with respect to a highly entangled target state $|\Psi_t\rangle$. In this way, one asymptotically approaches $|\Psi_t\rangle$ by iteration.

It is clear that a distillation procedure will only be successful if the input state ρ fulfills some conditions. For instance, if ρ is separable then there is no chance to obtain an entangled state, no matter what distillation protocol we choose. On the other hand, we may ask if non-separability of ρ suffices for distillation. This brings us to the so-called *distillability problem*.

Let us first give a precise characterization of distillable states: For a bipartite system $\mathcal{H} = \mathbb{C}^d \otimes \mathbb{C}^d$, a state ρ is called *distillable* iff for any $\epsilon > 0$ there exist a LOCC protocol that processes a finite number of copies m

$$\rho^{\otimes m} \quad \xrightarrow{\text{LOCC}} \quad \sigma \tag{2.59}$$

in a way such that $F(\sigma) = \mathrm{Tr}\left(\sigma \left|\phi_d^+\right\rangle \left\langle\phi_d^+\right|\right) > 1 - \epsilon$ where $\left|\phi_d^+\right\rangle = \frac{1}{\sqrt{d}} \sum_{i=0}^{d-1} |i\rangle \otimes |i\rangle$. (Loosely speaking, we can come arbitrarily close to the maximally entangled state.)

Admittedly, this is not an operational condition. Now the question is, are there also practical criteria for distillability? In Ref. [133] a simple necessary condition was found. All entangled states that are not detected by the PPT criterion (Section 2.3) are undistillable. As such states indeed exist for systems beyond $\mathbb{C}^2 \otimes \mathbb{C}^3$, it already follows that there are entangled states that cannot be distilled – they are said to be *bound entangled*.

In addition, a concise necessary and sufficient requirement for distillability was also presented. Namely, a state ρ on $\mathcal{H} = \mathbb{C}^d \otimes \mathbb{C}^d$ is distillable if and only if for a finite number m of copies $\rho^{\otimes m}$ on $\mathcal{H}^{\otimes m}$ there exists an entangled $\mathbb{C}^2 \otimes \mathbb{C}^2$ subspace. Hence, there must exist rank-two projectors P_1 and P_2 on $(\mathbb{C}^d)^{\otimes m}$ such that for a particular number of copies m the state $\rho^{\otimes m}$ remains entangled under the projection $P_1 \otimes P_2 \rho^{\otimes m} P_1 \otimes P_2$. A state with this property is called m-distillable (see also Refs. [134, 135]).

The main disadvantage of this condition is once more its impracticability. In order to verify that a state is bound entangled we have to show that $P_1 \otimes P_2 \rho^{\otimes m} P_1 \otimes P_2$ is separable for all projectors P_1, P_2 and any number of copies m [136]. This difficulty arises, for example, for the Werner state (2.49). This particular state is NPPT for $-1 \leq \beta < -\frac{1}{d}$, and believed to be undistillable for $\beta \geq -\frac{1}{2}$ [115]. That is, it is conjectured that NPPT is not sufficient for distillabilty when $d \geq 3$, and it is presumed that the Werner state possesses this kind of NPPT bound entanglement [135, 137, 138]. It was proven analytically that the Werner states are not 1-distillable for $-\frac{1}{2} \leq \beta < -\frac{1}{d}$, and there is strong numerical evidence for $d = 3$ that this region remains undistillable for 2 and 3 copies of ρ_W [135, 139].

Research contribution(s): We also performed extensive numerical investigations for the Werner state of two qutrits. Here, we exploited that the composite parameterization allows to efficiently parameterize the set of all $\mathbb{C}^2 \otimes \mathbb{C}^2$ subspaces in $(\mathbb{C}^3 \otimes \mathbb{C}^3)^{\otimes m}$ by means of $2 \times 4(3^m - 2)$ parameters (as discussed in **[P1]**). Using robust numerical methods [140], we found strong numerical evidence for up to 5 copies of ρ_W that the region $-\frac{1}{2} \leq \beta < -\frac{1}{3}$ is undistillable.

While our results are in a way in favor of the conjecture of the existence of NPPT bound entanglement, it is important to note that they by no means guarantee that the considered NPPT states remain undistillable for an even larger number of copies [136]. Also note that if NPPT bound entanglement really exists, then *entanglement of distillation* (Section 2.4) is neither convex nor additive [141].

3 Foundations of quantum theory

3.1 Uncertainty and mutually unbiased bases

The *uncertainty principle* is a key feature of quantum theory. Loosely speaking, it says that there are pairs of observables that cannot be specified simultaneously. Well-known examples are the position X and the momentum P of a particle, or the spin in different directions. Mathematically, this incompatibility may be expressed in terms of an *uncertainty relation*, the most prominent of which is Heisenberg's

$$\Delta X \Delta P \geq \frac{\hbar}{2} \, , \tag{3.1}$$

where ΔX is the standard deviation $\Delta X = \sqrt{\langle \Psi | \, X^2 \, | \Psi \rangle - \langle \Psi | \, X \, | \Psi \rangle^2}$. This uncertainty relation was later generalized by Robertson [142], who showed that for an arbitrary pair of observables A and B it holds that

$$\Delta A \Delta B \geq \frac{1}{2} | \, \langle \Psi | \, [A, B] \, | \Psi \rangle \, | \, , \tag{3.2}$$

where the square brackets on the right denote the commutator $[A, B] = AB - BA$.

The main disadvantage of Robertson's relation is that the right-hand side (rhs) depends on the state $|\Psi\rangle$. In principle, we could simply replace the rhs by the minimum of $| \, \langle \Psi | \, [A, B] \, | \Psi \rangle \, |$ over all states; then, however, it can happen that this is zero even for incompatible observables. For instance, in $\mathcal{H} = \mathbb{C}^2$ and σ_1, σ_2 we have $[\sigma_1, \sigma_2] = 2i\sigma_3$, for which $\min_{|\Psi\rangle \in \mathbb{C}^2} | \, \langle \Psi | \, 2i\sigma_3 \, | \Psi \rangle \, | = 0$.

This issue does not occur in so-called *entropic uncertainty relations*: To quantify the entropy of a given state ρ with respect to an arbitrary observable A on $\mathcal{H} = \mathbb{C}^d$ with the (normalized) eigenvectors $\{|i_A\rangle\}$ we can use any Rényi entropy [143]

$$H_\alpha(A) = \frac{1}{1 - \alpha} \log \left(\sum_{i=0}^{d-1} P(A = i)^\alpha \right) \, , \tag{3.3}$$

where $P(A = i) = \mathrm{Tr} \, (\rho \, |i_A\rangle \, \langle i_A|)$ and $\alpha \geq 0$. Now, an entropic uncertainty relation [144] is an inequality of the form

$$\frac{1}{m} \sum_{k=1}^{m} H_\alpha(A_k) \geq c(A_1, \ldots, A_m) \, , \tag{3.4}$$

where the constant $c(A_1, \ldots, A_m)$ on the rhs depends only on the $m \geq 2$ involved observables $A_1, \ldots, A_m$ but not on the state ρ.

An important uncertainty relation of this type is [145, 146]

$$\frac{1}{2} \left(H(A_1) + H(A_2) \right) \geq - \log \left(\max_{i,j} \{ | \, \langle i_1 \, | j_2 \rangle \, | \} \right) \, , \tag{3.5}$$

which holds for any two non-degenerate observables $A_1 \leftrightarrow \{|i_1\rangle\}$ and $A_2 \leftrightarrow \{|i_2\rangle\}$, wherein $H(A) = \lim_{\alpha \to 1} H_\alpha(A)$ is the Shannon entropy, which explicitly reads $H(A) = - \sum_{i=0}^{d-1} P(A = i) \log P(A = i)$. Notice that now the rhs can only be zero iff A_1 and A_2 have at least one common eigenvector. On the other hand, the rhs becomes maximal for $\max_{i,j} \{ | \, \langle i_1 \, | j_2 \rangle \, | \} = \frac{1}{\sqrt{d}}$, i.e. when A_1 and A_2 are complementary.

A set of observables $\{A_k\} = \{A_1, \ldots, A_m\}$ on $\mathcal{H} = \mathbb{C}^d$ is said to be *complementary* iff the corresponding normalized eigenvectors $\mathcal{B}_k = \{|i_k\rangle\} = \{|0_k\rangle, \ldots, |d-1_k\rangle\}$ form *mutually unbiased bases* (MUBs) [147], which is when

$$|\langle i_k|j_l\rangle|^2 = \frac{1}{d} \qquad \forall\ i,j \in \{0,\ldots,d-1\}\ , \tag{3.6}$$

holds for all basis vectors $|i_k\rangle$ and $|j_l\rangle$ that belong to different bases ($\forall\ k \neq l$). These bases are mutually unbiased in the sense that if we prepare a system in a state $|i_k\rangle$ of basis k, then all measurement outcomes regarding any other basis $l \neq k$ are equally likely (i.e. evenly distributed random). Besides the fact that MUBs lead to large uncertainties, they are also of practical interest. Namely, they find application in quantum state tomography [148], cryptographic protocols [149, 150] and the mean king's problem [151, 152].

There is a vast literature on the problem of determining the maximum number of MUBs for a given Hilbert space $\mathcal{H} = \mathbb{C}^d$ of dimension d. Here, it was found that for any d there exists at least a triplet of MUBs, but there can never be more than $d+1$. A set of $d+1$ MUBs is called a *complete set*. It was shown through an explicit construction that a complete set of MUBs indeed exists if d is a prime number p, or a prime power p^n. However, for all non-prime dimensions d the maximum number of MUBs is currently unknown. It is only known that the lower bound can be improved to $x+1$, where $x = \min\{p_i^{n_i}\}$ is the smallest prime power of the factorization $d = \prod_i p_i^{n_i}$. There is strong evidence suggesting that at least in some cases (e.g. $d = 6 = 2 \times 3$) it is impossible to have a complete set of $d+1$ MUBs. However, there is no proof for that.

Fortunately, we do not have to go into technical details on the construction of complete sets, since throughout this thesis it will suffice to know how a pair of MUBs can be constructed. For this purpose it is enough to perform a discrete Fourier transform. Specifically, two bases $\mathcal{B}_1 = \{|i_1\rangle\} = \{|0_1\rangle, \ldots, |d-1_1\rangle\}$ and $\mathcal{B}_2 = \{|i_2\rangle\} = \{|0_2\rangle, \ldots, |d-1_2\rangle\}$ of $\mathcal{H} = \mathbb{C}^d$ related by

$$|i_2\rangle = \frac{1}{\sqrt{d}} \sum_{k=0}^{d-1} \omega^{ki}\, |k_1\rangle\ , \tag{3.7}$$

with $\omega = \exp(2\pi\mathbb{i}/d)$ are mutually unbiased. Regarding the construction of a complete set it is worth mentioning that the transformation of $\mathcal{B}_1$ into $\mathcal{B}_2$ can be interpreted as a special case of a complex Hadamard matrix (times the constant $\frac{1}{\sqrt{d}}$). Constructing a complete set of $d+1$ MUBs thus boils down to the characterization of d mutually unbiased complex Hadamard matrices.

Research contribution(s): In the paper [**P6**], we investigate a link between mutually unbiased bases and the separability problem. In detail, we show that for separable states there is an upper bound on correlations among complementary observables. In our scheme, correlations are quantified by means of the correlation function

$$C_{A,B} = \sum_{i=0}^{d-1} \langle i_A| \otimes \langle i_B|\, \rho\, |i_A\rangle \otimes |i_B\rangle\ , \tag{3.8}$$

where A and B represent local observables of a bipartite qudit system. For a linear combination of $C_{A,B}$ using m complementary measurement settings $\{A_1, \ldots, A_m\}$

and $\{B_1, \ldots, B_m\}$, we prove that

$$I_m = \sum_{k=1}^{m} C_{k,k} \leq 1 + \frac{m-1}{d} \,, \tag{3.9}$$

holds for all separable states. Then we show that this is a nontrivial bound, meaning that there are indeed entangled states that violate Eq. (3.9). We also extend this method of entanglement detection to multipartite systems. In addition, and more importantly from a theoretical point of view, we find that there is an intrinsic connection between the maximum number of $d+1$ MUBs and the separability of the isotropic state (2.50).

Optional (not part of this thesis): Further considerations of the uncertainty principle and complementarity can be found in **[P9]**. Therein, we introduce an effective formalism that allows to describe decaying two-state systems. This formalism is then applied to a particular physical system (meson-antimeson system). Here, we use the entropic relation (3.5) to study the uncertainty between the experimentally accessible observables under the time evolution of the system.

3.2 Quantum nonlocality and Bell inequalities

In their seminal paper [1], A. Einstein, B. Podolsky and N. Rosen (EPR) argued that quantum theory constitutes an incomplete theory. In compact form (due to D. Bohm [153]) their argument goes as follows: Consider two spin-$\frac{1}{2}$ particles in the singlet state $|\Psi^-\rangle = \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle)$. According to the laws of quantum theory, the outcome of a spin measurement of a single particle in any direction is completely random, i.e. the probability of obtaining up (0) or down (1) as an outcome is one half, regardless of which local observable we choose (the reduced density matrix is maximally mixed because the state is maximally entangled). Nevertheless, since $|\Psi^-\rangle$ is $U \otimes U$-invariant we have that the measurement outcomes of the two particles are perfectly anti-correlated whenever the same observable is chosen on both sides – in short $P(A=0, A=1) + P(A=1, A=0) = 1$ for all settings A. Hence, under these conditions, we are in the position to predict with certainty the spin of particle 2 knowing the measurement outcome of particle 1, and vice versa. In particular, this also holds for a pair of complementary observables A_1 and A_2, such as, for example, spin measurements in two mutually orthogonal directions. EPR concluded that in this situation, both complementary spin directions must have simultaneous reality: *"If, without in any way disturbing a system, we can predict with certainty (i.e., with probability equal to unity) the value of a physical quantity, then there exists an element of physical reality corresponding to this physical quantity."* In case the particles are space-like separated at the time of the measurement this is a reasonable assumption as *"...the two systems no longer interact, no real change can take place in the second system in consequence of anything that may be done to the first system."* On the other hand, according to the uncertainty principle of quantum theory, complementary aspects cannot possess definite values simultaneously. Therefore, by premise of completeness *"every element of the physical reality must have a counterpart in the physical theory"* they inferred that quantum theory is (not necessarily false because it makes predictions in agreement with experiments, but) incomplete. They concluded with the words [1] *"While we have thus shown that the wave function* (i.e. state vector) *does not provide a complete description of the physical reality, we left open the question of whether or not such a description*

exists. We believe, however, that such a theory is possible." EPR were convinced that within a more fundamental theory of nature, quantum theory will have the same status as statistical mechanics within classical mechanics.

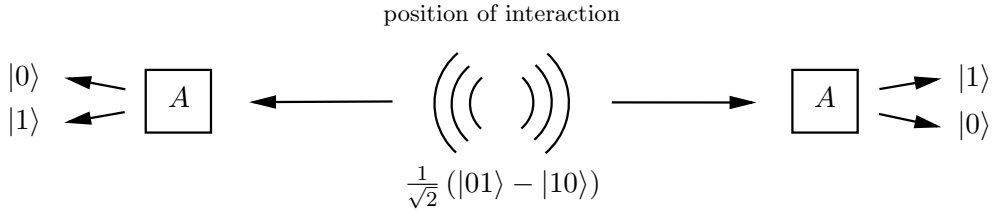

Figure 3.1: Schematic illustration of the EPR-Bohm scenario.

The fact that such a complete theory (in the sense of EPR) cannot peacefully coexist with quantum theory was first recognized by John S. Bell in 1964 [3]. The reason is the following: In order to account for the ideas of EPR in their full extent, one must assume that nature can be described by a local-realistic (LR) theory, obeying

locality	instantaneous interactions are impossible (spacelike separated objects do not influence each other)
reality	all physical observables have definite values at all times (regardless of whether they are observed or not)

These requirements lead to constraints on correlations among composite systems. For example, for a bipartite system having two local measurement outcomes $(0, 1)$ and two arbitrary observables for each party A_1, A_2 and B_1, B_2, this means (without loss of generality) that the statistics of the system can be described by 16 probabilities [154, 155]

$$P_{LR}(A_1 = j, A_2 = k; B_1 = l, B_2 = m) \geq 0 \tag{3.10}$$

normalized to

$$\sum_{j,k,l,m=0}^{1} P_{LR}(A_1 = j, A_2 = k; B_1 = l, B_2 = m) = 1 \ . \tag{3.11}$$

This yields the joint probabilities

$$P_{LR}(A_1 = j; B_1 = l) = \sum_{k,m=0}^{1} P_{LR}(A_1 = j, A_2 = k; B_1 = l, B_2 = m) \ , \tag{3.12}$$

$$P_{LR}(A_1 = j; B_2 = m) = \sum_{k,l=0}^{1} P_{LR}(A_1 = j, A_2 = k; B_1 = l, B_2 = m) \ , \tag{3.13}$$

$$P_{LR}(A_2 = k; B_1 = l) = \sum_{j,m=0}^{1} P_{LR}(A_1 = j, A_2 = k; B_1 = l, B_2 = m) \ , \tag{3.14}$$

$$P_{LR}(A_2 = k; B_2 = m) = \sum_{j,l=0}^{1} P_{LR}(A_1 = j, A_2 = k; B_1 = l, B_2 = m) \ . \tag{3.15}$$

Such a description would be compatible with quantum theory, if for all states ρ and all observables A_1, A_2, B_1 and B_2 there were a distribution (3.10) such that

$$P_{QM}(A_a = x; B_b = y) = Tr(\rho \left|x_a\right\rangle \left\langle x_a\right| \otimes \left|y_b\right\rangle \left\langle y_b\right|) = P_{LR}(A_a = x; B_b = y) \ ,$$

for all $x, y \in \{0, 1\}$ and $a, b \in \{1, 2\}$.

(Un)fortunately, this is not the case: Within the set of all possible joint probabilities that arise from quantum theory, local-realistic theories cover a closed and convex polytope which is strictly smaller [157]. Analogously to distinguishing separable from entangled through linear witnesses, we may separate local-realistic from quantum by using half-spaces. For that, we can think of the 4×4 joint probabilities $P(A_a = x; B_b = y)$ (we can insert either LR or QM) as entries of a 16-dimensional vector $\vec{P} \in \mathbb{R}^{16}$. Consequently, due to the Hahn-Banach separation theorem there exist a vector $\vec{V} \in \mathbb{R}^{16}$ and a number $v \in \mathbb{R}$ such that

$$\vec{V} \cdot \vec{P} \leq v \ , \tag{3.16}$$

for all $\vec{P}$ that lie within the local-realistic polytope (Note that $\vec{V} \cdot \vec{P}$ simply represents a linear combination of the joint probabilities $P(A_a = x; B_b = y)$). If this bound can be exceeded through quantum probabilities, i.e. if there exists observables A_1, A_2, B_1, B_2 and a state ρ such that $\vec{V} \cdot \vec{P} > v$, then (3.16) is termed a *Bell inequality* (BI). Moreover, we say that a Bell inequality is *tight* when it corresponds to a facet of the LR polytope (see Fig. 3.2).

For the current scenario (2×2 observables with two outcomes), the only relevant (tight) Bell inequality is the CHSH inequality [4], which reads

$$I_2 = E(A_1, B_1) + E(A_1, B_2) - E(A_2, B_1) + E(A_1, B_2) \leq 2 \ . \tag{3.17}$$

with $E(A, B) = P(A = 0, B = 0) + P(A = 1, B = 1) - P(A = 0, B = 1) - P(A = 1, B = 0)$. Here, quantum theory predicts values up to $I_2 = 2\sqrt{2}$.

The main advantage of Bell inequalities lies in the fact that they can be tested experimentally, in contrast to the hypothetical existence of probabilities (3.10) which we cannot directly confirm or falsify. Moreover, several experiments have demonstrated (neglecting loopholes [156]) that Bell inequalities can indeed be violated [5, 6, 158, 159]; and thus, all local-realistic models are not only incompatible with quantum theory, but also with nature.

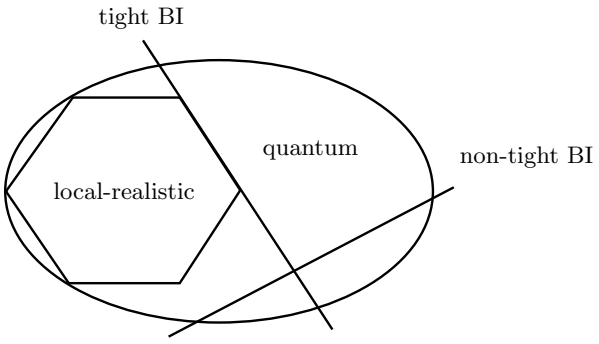

Figure 3.2: Schematic illustration of the probability space.

Let us now turn to the question why Bell inequalities are violated by quantum theory. First of all, it is straightforward to observe that a violation is a consequence

of entanglement [160]. On the other hand, it was found that not all entangled states give rise to non-local-realistic correlations [161]. If an entangled state admits a LR description, then it satisfies *all* possible Bell inequalities, i.e. proving that the CHSH inequality is not violated is not enough because it only characterizes the LR polytope of 2×2 observables; whereas it is not excluded that there exists a more restrictive polytope for an arbitrary number of $n_1 \times n_2$ observables, induced by the LR probabilities

$$P_{LR}(A_1 = j, \ldots, A_{n_1} = k; B_1 = l, \ldots, B_{n_2} = m) \geq 0 \ . \tag{3.18}$$

Note that similarly, each generalization of (3.10) which involves more than two outcomes (and/or parties) generates a convex polytope of LR correlations for a particular scenario (observables+outcomes+parties). However, the characterization of the resulting facets through Bell inequalities is generally very demanding (see e.g. Ref. [162] and references therein).

Until now, the relation between entanglement and non-local-realism is not completely clarified [163, 164, 165], and remains intriguing from a fundamental point of view [166, 167]. Besides that, Bell inequalities are also of practical use in quantum information. For instance, it was discovered that Bell inequality violations can serve to guarantee the security of cryptographic protocols [7]. In comparison to standard entanglement tests, security checks based on the violation of a Bell inequality do not rely on any assumptions about the devices carrying out the measurements, i.e. they are *device-independent* [168, 169]. Even the dimensionality of the physical system [170, 171], and multipartite aspects [172, 173] can be analyzed in a device-independent way. Moreover, Bell inequalities may also be used to certify random number generators [174, 175].

The Bell inequality that we will use in this thesis is the CGLMP inequality [176], which constitutes a generalization of the CHSH inequality to d outcomes. It reads

$$\begin{aligned} I_d = \sum_{k=0}^{\lfloor d/2 \rfloor - 1} \big(1 - \frac{2k}{d-1}\big) \big\{ + \big[& P(A_1 = B_1 + k) + P(B_1 = A_2 + k + 1) \\ & + P(A_2 = B_2 + k) + P(B_2 = A_1 + k) \big] \\ - \big[& P(A_1 = B_1 - k - 1) + P(B_1 = A_2 - k) \\ & + P(A_2 = B_2 - k - 1) + P(B_2 = A_1 - k - 1) \big] \big\} \end{aligned} \tag{3.19}$$

where $I_d \leq 2$ for LR theories. For this inequality one obtains (using suitable observables and a maximally entangled state $\left|\Phi_d^+\right\rangle = \frac{1}{\sqrt{d}} \sum_{i=0}^{d-1} |ii\rangle$)

d	2	3	4	5	6	...	$\to \infty$
I_d	2.82843	2.87293	2.89624	2.91054	2.92020	...	2.96981
violation [%]	41.4214	43.6467	44.8122	45.5272	46.0102	...	48.4906

This inequality is investigated in detail in one of our publications introduced in the next section.

3.3 Geometry of composite quantum states

In quantum physics, states are represented by density matrices on a complex Hilbert space. Thus, in comparison to classical physics where the state of the system is described by a set of real parameters, a quantum state is a less descriptive object.

However, as discussed in Section 1.4, we may also express a density matrix in terms of few real parameters using the Bloch vector representation. For a single qubit this yields an insightful geometric visualization of a quantum state as a three-dimensional real vector within a unit sphere. In this section, we consider similar geometric pictures for composite quantum states and entanglement.

Let us start with the simplest case – the bipartite qubit system [177, 178]. According to Eq. (1.29), any state ρ on $\mathcal{H} = \mathbb{C}^2 \otimes \mathbb{C}^2$ may be written as

$$\rho = \frac{1}{4}(\mathbb{1}_2 \otimes \mathbb{1}_2 + \vec{a} \cdot \vec{\sigma} \otimes \mathbb{1}_2 + \mathbb{1}_2 \otimes \vec{b} \cdot \vec{\sigma} + \sum_{m,n=1}^{3} c_{mn} \sigma_m \otimes \sigma_n) \ , \tag{3.20}$$

using two three-dimensional real vectors $\vec{a}$ and $\vec{b}$ containing local information, and a 3×3 real matrix c_{mn} related to correlations. Thus, ρ is completely characterized by 15 parameters in total. When we are not interested in the local properties of the state but only in non-local features (e.g. entanglement) we may switch to local bases for which the matrix c_{mn} is diagonal. This is always possible because of the relation

$$U\vec{n} \cdot \vec{\sigma} U^\dagger = (O\vec{n}) \cdot \vec{\sigma} \ , \tag{3.21}$$

given by the group homomorphism between $U \in \mathcal{SU}(2)$ and $O \in \mathcal{SO}(3)$. It induces that under a local basis change $U_1 \otimes U_2 \rho U_1^\dagger \otimes U_2^\dagger$, the matrix $C = (c_{mn})$ transform as $O_1 C O_2^T$. Moreover, from the singular value decomposition it follows that $O_1 C O_2^T$ becomes diagonal for an appropriate choice of O_1 and O_2. Thus, from now on we may treat the three singular values of $C = (c_{mn})$ as components of a three-dimensional real vector $\vec{c} = (c_1, c_2, c_3)$, for which (3.20) reduces to

$$\rho = \frac{1}{4}(\mathbb{1}_2 \otimes \mathbb{1}_2 + \vec{a}' \cdot \vec{\sigma} \otimes \mathbb{1}_2 + \mathbb{1}_2 \otimes \vec{b}' \cdot \vec{\sigma} + \sum_{m=1}^{3} c_m \sigma_m \otimes \sigma_m) \ . \tag{3.22}$$

Using the four projectors $P_1 = |\Psi^+\rangle\langle\Psi^+|, P_2 = |\Psi^-\rangle\langle\Psi^-|, P_3 = |\Phi^+\rangle\langle\Phi^+|$ and $P_4 = |\Phi^-\rangle\langle\Phi^-|$ defined by the Bell states $|\Psi^\pm\rangle = \frac{1}{\sqrt{2}}(|01\rangle \pm |10\rangle)$ and $|\Phi^\pm\rangle = \frac{1}{\sqrt{2}}(|00\rangle \pm |11\rangle)$, we find via $\mathrm{Tr}\,(P_n\rho) \geq 0$ four necessary conditions for non-negativity

$$1 + c_1 + c_2 - c_3 \geq 0 \ , \tag{3.23}$$
$$1 - c_1 - c_2 - c_3 \geq 0 \ , \tag{3.24}$$
$$1 + c_1 - c_2 + c_3 \geq 0 \ , \tag{3.25}$$
$$1 - c_1 + c_2 + c_3 \geq 0 \ . \tag{3.26}$$

These inequalities describe a *regular tetrahedron* spanned by the four Bell states P_n which correspond to the vectors $\vec{a}_n = 0$, $\vec{b}_n = 0$ and

$$P_1 = \left|\Psi^+\right\rangle\left\langle\Psi^+\right| \quad \Leftrightarrow \quad \vec{c}_1 = (+1, +1, -1) \ , \tag{3.27}$$
$$P_2 = \left|\Psi^-\right\rangle\left\langle\Psi^-\right| \quad \Leftrightarrow \quad \vec{c}_2 = (-1, -1, -1) \ , \tag{3.28}$$
$$P_3 = \left|\Phi^+\right\rangle\left\langle\Phi^+\right| \quad \Leftrightarrow \quad \vec{c}_3 = (+1, -1, +1) \ , \tag{3.29}$$
$$P_4 = \left|\Phi^-\right\rangle\left\langle\Phi^-\right| \quad \Leftrightarrow \quad \vec{c}_4 = (-1, +1, +1) \ . \tag{3.30}$$

Moreover, we observe that the conditions (3.23) – (3.26) are also sufficient for all *locally maximally mixed* (LMM) states ($\vec{a} = \vec{b} = 0$), as they become Bell-diagonal through the diagonalization of $C = (c_{mn})$.

In order to determine which states within the tetrahedron are entangled, we can use the PPT criterion as it is necessary and sufficient for two qubits. In the Bloch vector representation (3.20), the partial transpose ρ^{T_1} leads to the reflection $(c_1, c_2, c_3) \rightarrow (c_1, -c_2, c_3)$, because $\sigma_1^T = \sigma_1$ and $\sigma_3^T = \sigma_3$, whereas $\sigma_2^T = -\sigma_2$. Consequently, separable states lie within the cross section of the original tetrahedron and its reflected counterpart. This cross section is an *octahedron* with the extremal points $(\pm 1, 0, 0)$, $(0, \pm 1, 0)$ and $(0, 0, \pm 1)$. All states that lie outside this octahedron are entangled (see Fig. 3.3). Again, this is a necessary and sufficient statement for all LMM states.

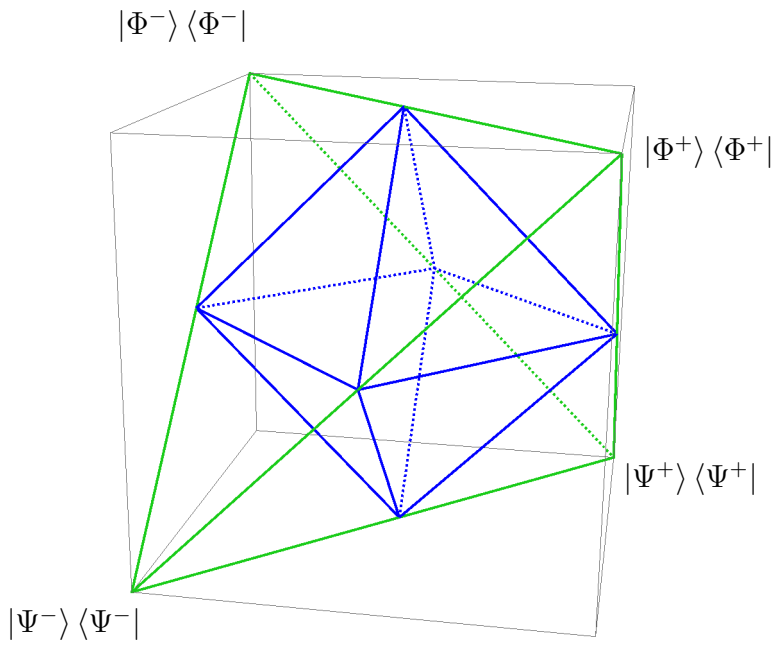

Figure 3.3: Illustration of the tetrahedron spanned by the four Bell states (green), and the octahedron of separable states (blue).

The obtained tetrahedron provides an illustrative visualization for two qubits. Is it possible to find such a simple picture also for bipartite systems of arbitrary dimension $\mathcal{H} = \mathbb{C}^d \otimes \mathbb{C}^d$? First of all, a direct generalization in terms of the Bloch vector representation is not an option, as there is no simple characterization of the state space because of the fact that non-negativity of ρ is hard to handle. Furthermore, there is no relation analogous to (3.21) for higher dimensions, which would be needed to diagonalize the $d^2-1 \times d^2-1$ dimensional generalization of the correlation matrix C (for a more detailed discussion on this issue see Ref. [160]).

However, as shown in Refs. [179, 180], we may interpret the tetrahedron as a special case of a regular (d^2-1)-dimensional simplex for $\mathcal{H} = \mathbb{C}^d \otimes \mathbb{C}^d$ spanned by mutually orthogonal Bell states. By means of the Weyl operators

$$W_{k,l} = \sum_{s=0}^{d-1} \omega^{sk} |s\rangle \langle (s+l) \bmod d| \qquad k, l \in \{0, ..., d-1\} \ , \tag{3.31}$$

with $\omega = \exp(2\pi \mathbb{i}/d)$, it is possible to construct an orthonormal basis for $\mathcal{H} = \mathbb{C}^d \otimes \mathbb{C}^d$

via the d^2 states

$$|\Omega_{k,l}\rangle = (W_{k,l} \otimes \mathbb{1}_d)\,|\Omega_{0,0}\rangle \qquad\qquad k,l \in \{0,...,d-1\}\ , \tag{3.32}$$

starting from the Schmidt form of a maximally entangled state $|\Omega_{0,0}\rangle = \frac{1}{\sqrt{d}}\sum_{i=0}^{d-1}|ii\rangle$. These states can be used to construct a (d^2-1)-dimensional regular simplex $\mathcal{W}$ of Bell-diagonal states

$$\mathcal{W} = \{\sum_{k,l=0}^{d-1} c_{k,l}P_{k,l} \ \ | \ \ c_{k,l} \geq 0, \sum_{k,l=0}^{d-1} c_{k,l} = 1\}\ , \tag{3.33}$$

where $P_{k,l} = |\Omega_{k,l}\rangle\langle\Omega_{k,l}|$. Notice that $\mathcal{W}$ constitutes an appropriate extension to higher dimensions as for $d = 2$ it coincides with the tetrahedron of LMM states.

Elements of $\mathcal{W}$ possess a discrete local-unitary symmetry [130]. Namely, all $\rho \in \mathcal{W}$ are invariant under the transformation

$$W_{k,l} \otimes W_{-k,l}\rho W_{k,l}^\dagger \otimes W_{-k,l}^\dagger = \rho\ , \tag{3.34}$$

for all $k,l \in \{0,\ldots,d-1\}$. Thus, even though an arbitrary state $\rho \in \mathbb{C}^d \otimes \mathbb{C}^d$ might not have a direct representative within the simplex $\mathcal{W}$ for $d > 2$, we may use the map

$$\Pi(\rho) = \frac{1}{d^2}\sum_{k,l=0}^{d-1} W_{k,l} \otimes W_{-k,l}\rho W_{k,l}^\dagger \otimes W_{-k,l}^\dagger\ , \tag{3.35}$$

to symmetrize ρ over the associated symmetry group $\mathcal{G} = \{W_{k,l} \otimes W_{-k,l}\}$.

In order to detect entanglement within $\mathcal{W}$, we can resort to a combination of established methods. A vast region of entangled states can readily be obtained via the PPT criterion. Here, we can exploit the structure of $\mathcal{W}$ to simplify the problem of testing whether or not ρ^{T_1} has a negative eigenvalue. In explicit form, the elements of $\mathcal{W}$ read

$$\rho = \frac{1}{d}\sum_{s,t,k,l=0}^{d-1} c_{k,l}\omega^{k(s-t)}\,|s-l,s\rangle\langle t-l,t|\ , \tag{3.36}$$

where the labels of the vectors are treated modulo d. Partial transpose on the first subsystem yields

$$\rho^{T_1} = \frac{1}{d}\sum_{s,t,k,l=0}^{d-1} c_{k,l}\omega^{k(s-t)}\,|t-l,s\rangle\langle s-l,t|\ . \tag{3.37}$$

By substituting the running index l by $l = s+t-m$ we obtain

$$\rho^{T_1} = \frac{1}{d}\sum_{s,t,k,m=0}^{d-1} c_{k,s+t-m}\omega^{k(s-t)}\,|m-s,s\rangle\langle m-t,t|\ , \tag{3.38}$$

$$= \sum_{m=0}^{d-1}\left[\frac{1}{d}\sum_{s,t,k=0}^{d-1} c_{k,s+t-m}\omega^{k(s-t)}\,|m-s,s\rangle\langle m-t,t|\right]\ , \tag{3.39}$$

$$= \sum_{m=0}^{d-1} B_m\ . \tag{3.40}$$

Here, each operator B_m acts on a d-dimensional subspace spanned by the vectors $\{|m-s\rangle\otimes|s\rangle\}_{s=0,..,d-1}$, meaning that (3.40) may be written as a direct sum $\bigoplus_m B_m$. Consequently, computing the eigenvalues of ρ^{T_1} can be reduced to determining the eigenvalues of the matrices B_m, which is less expensive.

The symmetries of $\mathcal{W}$ also lead to simplifications concerning entanglement witnesses. Since any $\rho \in \mathcal{W}$ is invariant under the symmetry group $\mathcal{G} = \{W_{k,l} \otimes W_{-k,l}\}$, we can restrict to witnesses W sharing this particular symmetry. The most general form of such an operator is

$$W = \sum_{k,l} \kappa_{k,l} P_{k,l} \ , \tag{3.41}$$

with $\kappa_{k,l} \in \mathbb{R}$. Such an operator W is an entanglement witness only if it has non-negative expectation values for all product states. By considering

$$\langle\psi| \otimes \langle\eta| W |\psi\rangle \otimes |\eta\rangle \ , \tag{3.42}$$

$$= \frac{1}{d} \sum_{k,l,s,t=0}^{d-1} \kappa_{k,l} \langle\psi| \otimes \langle\eta| W_{k,l} \otimes \mathbb{1}_d |s\rangle \otimes |s\rangle \langle t| \otimes \langle t| W_{k,l}^\dagger \otimes \mathbb{1}_d |\psi\rangle \otimes |\eta\rangle \ , \tag{3.43}$$

$$= \frac{1}{d} \sum_{k,l,s,t=0}^{d-1} \kappa_{k,l} \langle\psi| W_{k,l} |s\rangle \langle\eta|s\rangle \langle t|\eta\rangle \langle t| W_{k,l}^\dagger |\psi\rangle \ , \tag{3.44}$$

$$= \frac{1}{d} \langle\psi| \left[\sum_{k,l=0}^{d-1} \kappa_{k,l} W_{k,l} |\phi\rangle \langle\phi| W_{k,l}^\dagger \right] |\psi\rangle \ , \tag{3.45}$$

we observe that this is the case iff the matrix $M_\phi = \sum_{k,l=0}^{d-1} \kappa_{k,l} W_{k,l} |\phi\rangle \langle\phi| W_{k,l}^\dagger$ of dimension $d \times d$ is non-negative for all $|\phi\rangle \in \mathbb{C}^d$. Thus, we have again reduced the complexity of the problem from a $d^2 \times d^2$ matrix problem to a $d \times d$ matrix problem.

Research contribution(s): The aim of our paper [**P7**] was to compare entanglement with Bell inequality violations within this geometric framework. For that, we analytically determine the region within the tetrahedron that leads to a violation of the CHSH inequality. Beyond two qubits, we show how to numerically optimize the measurement setting to achieve a maximum outcome of a Bell test given an arbitrary state. Using this method, we study the violation of the CGLMP inequality (3.19) within low-dimensional subsections of the simplex $\mathcal{W}$ for bipartite qutrits. In addition, we also investigate the difference between Bell inequality violations and entanglement measures.

Optional (not part of this thesis): In an earlier paper [**P10**], we generalized the concept of the tetrahedron to multipartite qubits. We constructed a set of states with a similar geometric structure as bipartite qubits. We investigated the properties of these states concerning separability, distillability and Bell inequality violations.

Summary

The aim of this doctoral thesis was to investigate entanglement and non-local-realistic correlations in composite finite-dimensional quantum systems. This summary gives an overview of the main results obtained in this cumulative dissertation:

- We presented a new parameterization of the unitary $\mathcal{U}(d)$ and the special unitary group $\mathcal{SU}(d)$ of arbitrary dimension d. This parameterization has an insightful matrix notation and is beneficial in a variety of (numerical) problems arising in quantum information. In particular, it is computationally advantageous due to its factorized form, and moreover can be used to describe orthonormal vectors, density matrices and subspaces with a minimal number of parameters. The usefulness of the parameterization was demonstrated in the context of distillability conditions, lower bounds on the concurrence and Bell inequalities.

- We considered the Haar measure in terms of the introduced parameterization. This measure has applications in unbiased randomizations and the computation of group integrals (not necessarily polynomials). We showed that the well-defined structure of the parameterization leads to a concise formula for the normalized Haar measure on $\mathcal{U}(d)$ and $\mathcal{SU}(d)$. In addition, we gave examples of integrals that can be solved analytically in this way.

- We discussed the categorization of multilevel entanglement in multipartite systems. Here, we introduced a precise characterization of f-level genuine multipartite entanglement. Multilevel generalizations of the well-known GHZ, W and Dicke states were considered. In order to verify genuine multipartite entanglement and the number of involved levels, we constructed a set of noise-robust detection criteria for mixed states. These criteria are simple functions of a few density matrix elements and thus are easily computable. Moreover, they are also advantageous in experiments as they can be implemented with a reduced number of local measurements. That is, a full state tomography is not required.

- We introduced the GME-concurrence – a functional measure of multipartite entanglement based on the well-known concurrence. The GME-concurrence is defined in such a way that it is zero for all partially entangled states and non-zero for all genuinely multipartite entangled states. This property holds for pure, as well as for mixed states. Since the computation of the GME-concurrence involves a nontrivial optimization for mixed states, we derived a computable lower bound and showed that it is exact for GHZ-like states. Furthermore, it was discussed how to reliably estimate the GME-concurrence in an experimental situation.

- We proposed a simple scheme for the classification of genuine multipartite entanglement. It enables to define equivalence classes of states with similar physical properties. These substructures are formulated in terms of convex mixtures of continuous families of states and their equivalents with respect to local unitaries and permutations of the subsystems. The advantages of this concept are that it is not restricted to pure states and that it also works for rather complicated multipartite systems. We introduced three exemplary classes of genuinely multipartite entangled states for n qubits: the double states (which

correspond to a class of GHZ-like states), the n-tuple states (W-like states), and the $(n-1)$-tuple states (Dicke-like states). We also presented three inequalities which are each satisfied for all elements of one particular class, thus enabling to examine arbitrary mixed states according to their membership.

- We investigated correlations with regard to complementary observables. In this way, we saw that mutually unbiased bases can serve for the detection of entanglement in various systems and states. This was demonstrated for bipartite systems by the example of the isotropic state, and for multipartite systems by the aid of a noisy Aharonov state. A main advantage of entanglement criteria based on mutually unbiased bases is that the detection strength is comparatively high in relation to the number of used measurement settings. Moreover, the number of settings is variable, allowing for a compromise between the noise robustness and the experimental effort. By varying the number of settings for the isotropic state, we noticed that the criterion becomes necessary and sufficient for $d+1$ mutually unbiased bases (where d is the dimension of the subsystem). We showed that any further hypothetical complementary observable would lead to a substantial inconsistency, with the consequence that there cannot exist more than $d+1$. Hence, we established a link between the separability problem and the maximum number of mutually unbiased bases.

- We studied geometric aspects of quantum entanglement and Bell inequality violations. A simplex structure given by mutually orthogonal generalized Bell states was used to visualize subsections of the Hilbert space for bipartite qudits. Violations of the CGLMP-Bell inequality were compared with entanglement within this particular set of states. We found that the dissimilarities of entanglement and quantum non-local-realism are reflected in their geometries. That is, there is no simple relation between the shape of the separability boundary and the shape of the boundary resulting from the Bell inequality. Moreover, one also finds a difference between the contour of the concurrence in comparison to the strength of the Bell inequality violation. Here, we showed that Bell inequality violations and entanglement measures are generally non-monotonically related.

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Appendix

```
%
%   COMPOSITE PARAMETERIZATION of SU(d) /// version 1.5 /// 12.04.2011
%
%   (c) Christoph Spengler 2011, Faculty of Physics, University of Vienna
%       Contact: christoph.spengler@univie.ac.at
%
%       available @ Matlab Central:
%       http://www.mathworks.com/matlabcentral/
%
%   Usage : UCS(lambda)
%
%   lambda - dxd real matrix (lambda(d,d) is ignored)
%   lambda(a,b) diagonal components a=b - absolute phases for a in [0,2*pi]
%   lambda(a,b) upper right components a<b - rotations in a-b plane in [0,pi/2]
%   lambda(a,b) lower left components a>b - relative phases between a-b in [0,pi]
%

function unitary=UCS(lambda)

d=length(lambda);

unitary=1;
ex2=1;

for m=(d-1):-1:1
    ex1(1,d-m)=0;
    ex2(d-m+1,1)=0;
    unitary=[ex1;unitary];
    unitary=[ex2 unitary];
    for n=(d-m+1):-1:2
        A=eye(d-m+1);
        A(1,1)=exp(1i*lambda(n+m-1,m))*cos(lambda(m,n+m-1));
        A(n,n)=exp(-1i*lambda(n+m-1,m))*cos(lambda(m,n+m-1));
        A(n,1)=-exp(-1i*lambda(n+m-1,m))*sin(lambda(m,n+m-1));
        A(1,n)=exp(1i*lambda(n+m-1,m))*sin(lambda(m,n+m-1));
        unitary=A*unitary;
    end
end

for k=1:d-1
    unitary(:,k)=unitary(:,k)*exp(1i*lambda(k,k));
    unitary(:,d)=unitary(:,d)*exp(-1i*lambda(k,k));
end


end
```

Appendix

```
%
%   COMPOSITE PARAMETERIZATION of U(d) /// version 1.5 /// 12.04.2011
%
%   (c) Christoph Spengler 2011, Faculty of Physics, University of Vienna
%       Contact: christoph.spengler@univie.ac.at
%
%       available @ Matlab Central:
%       http://www.mathworks.com/matlabcentral/
%
%   Usage : UC(lambda)
%
%   lambda - dxd real matrix
%   lambda(a,b) diagonal components a=b - absolute phases for a in [0,2*pi]
%   lambda(a,b) upper right components a<b - rotations in a-b plane in [0,pi/2]
%   lambda(a,b) lower left components a>b - relative phases between a-b in [0,2*pi]
%

function unitary=UC(lambda)

d=length(lambda);

unitary=1;
ex2=1;

for m=(d-1):-1:1
    ex1(1,d-m)=0;
    ex2(d-m+1,1)=0;
    unitary=[ex1;unitary];
    unitary=[ex2 unitary];
    for n=(d-m+1):-1:2
        A=eye(d-m+1);
        A(1,1)=cos(lambda(m,n+m-1));
        A(n,n)=exp(1i*lambda(n+m-1,m))*cos(lambda(m,n+m-1));
        A(n,1)=-exp(1i*lambda(n+m-1,m))*sin(lambda(m,n+m-1));
        A(1,n)=sin(lambda(m,n+m-1));
        unitary=A*unitary;
    end
end

for k=1:d
    unitary(:,k)=unitary(:,k)*exp(1i*lambda(k,k));
end

end
```

Appendix

Composite parameterization of SU(d) // v1.0 for mathematica // 23.08.2011

(c) Christoph Spengler 2011, Faculty of Physics, University of Vienna
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[1] Ch.Spengler, M.Huber, B.C.Hiesmayr
'A composite parameterization of unitary groups, density matrices and subspaces'
J.Phys.A : Math.Theor.43, 385306 (2010)

[2] Ch.Spengler, M.Huber, B.C.Hiesmayr
'Composite parameterization and Haar measure for all unitary and special unitary groups'
J. Math. Phys. 53, 013501 (2012)

Code:

```
basis[dimension_] :=
 Do[Do[basevector[n] = Transpose[{UnitVector[dimension, n]}], {n, 1, dimension}];
  u = Array[basevector, dimension]]

Y[j_, k_] := -I * u[[j]].ConjugateTranspose[u[[k]]] + I * u[[k]].ConjugateTranspose[u[[j]]]

Z[j_, k_] := 1 * u[[j]].ConjugateTranspose[u[[j]]] - 1 * u[[k]].ConjugateTranspose[u[[k]]]

UC[d_] := {basis[d], J = 1, U1 = IdentityMatrix[d],
  U2 = IdentityMatrix[d], Do[U2 = U2.MatrixExp[I * λ[l, l] * Z[l, d]], {l, 1, d - 1}],
  Do[Do[U1 = U1.MatrixExp[I * λ[k, j] * Z[j, k]].MatrixExp[I * λ[j, k] * Y[j, k]], {k, j + 1, d}],
   {j, 1, d - 1}], U = U1.U2,
  Do[Do[J = J * (2 * (k - j)) * Sin[λ[j, k]] * Cos[λ[j, k]]^(2 (k - j) - 1), {k, j + 1, d}],
   {j, 1, d - 1}], J = Pi^(-d (d + 1) / 2 + 1) * 2^(1 - d) * J,
  Do[Do[If[m > n, range[m, n] = {λ[m, n], 0, Pi}, If[m == n, range[m, n] = {λ[m, n], 0, 2 * Pi},
      range[m, n] = {λ[m, n], 0, Pi / 2}]], {m, 1, d}], {n, 1, d}];
  domain = Delete[Flatten[Array[range, {d, d}], 1], d^2]}
```

Usage:

1) Run the code.
2) Initialization with UC[d]; where d is the required dimension.
3) U yields a parameterized special unitary matrix of dimension dxd expressed in terms of d^2-1 real parameters λ(m,n). For details on the meaning of the parameters λ(m,n) see the references [1],[2].
4) J yields the absolute value of the normalized Jacobian determinant |det(dU/dλ)|, such that dU= Jdλ(1,1)...dλ(d,d-1) is a normalized Haar measure $\int$J dλ(1,1)...dλ(d,d-1) = 1.
5) domain//InputForm yields the ranges of the parameters λ(m,n) in InputForm. Copy&paste this to compute group integrals, i.e. $\int$f(U) dU= $\int$f(U(λ(1,1),...,λ(d,d-1))) Jdλ(1,1)...dλ(d,d-1).

Appendix

Composite parameterization of U(d) // v1.0 for mathematica // 23.08.2011

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'Composite parameterization and Haar measure for all unitary and special unitary groups'
J. Math. Phys. 53, 013501 (2012)

Code:

```
basis[dimension_] :=
 Do[Do[basevector[n] = Transpose[{UnitVector[dimension, n]}], {n, 1, dimension}];
  u = Array[basevector, dimension]]

Y[j_, k_] := -I * u[[j]].ConjugateTranspose[u[[k]]] + I * u[[k]].ConjugateTranspose[u[[j]]]

P[n_] := u[[n]].ConjugateTranspose[u[[n]]]

UC[d_] := {basis[d], J = 1, U1 = IdentityMatrix[d],
  U2 = IdentityMatrix[d], Do[U2 = U2.MatrixExp[I * λ[l, l] * P[l]], {l, 1, d}],
  Do[Do[U1 = U1.MatrixExp[I * λ[k, j] * P[k]].MatrixExp[I * λ[j, k] * Y[j, k]], {k, j + 1, d}],
   {j, 1, d - 1}], U = U1.U2,
  Do[Do[J = J * (2 * (k - j)) * Sin[λ[j, k]] * Cos[λ[j, k]]^(2 (k - j) - 1), {k, j + 1, d}],
   {j, 1, d - 1}], J = (2 * Pi)^(-d (d + 1) / 2) * J,
  Do[Do[If[m >= n, range[m, n] = {λ[m, n], 0, 2 * Pi}, range[m, n] = {λ[m, n], 0, Pi / 2}],
    {m, 1, d}], {n, 1, d}]; domain = Flatten[Array[range, {d, d}], 1]}
```

Usage:

1) Run the code.
2) Initialization with UC[d]; where d is the required dimension.
3) U yields a parameterized unitary matrix of dimension dxd expressed in terms of d^2 real parameters $\lambda(1,1),...,\lambda(d,d)$. For details on the meaning of the parameters $\lambda(m,n)$ see the references [1],[2].
4) J yields the absolute value of the normalized Jacobian determinant $|\det(dU/d\lambda)|$, such that $dU = J d\lambda(1,1)...d\lambda(d,d)$ is a normalized Haar measure $\int J\, d\lambda(1,1)...d\lambda(d,d) = 1$.
5) domain//InputForm yields the ranges of the parameters $\lambda(m,n)$ in InputForm. Copy&paste this to compute group integrals, i.e. $\int f(U)\, dU = \int f(U(\lambda(1,1),...,\lambda(d,d)))\, J d\lambda(1,1)...d\lambda(d,d)$.

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A composite parameterization of unitary groups, density matrices and subspaces

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Abstract
Unitary transformations and density matrices are central objects in quantum physics and various tasks require to introduce them in a parameterized form. In this paper we present a parameterization of the unitary group $\mathcal{U}(d)$ of arbitrary dimension d which is constructed in a composite way. We show explicitly how any element of $\mathcal{U}(d)$ can be composed of matrix exponential functions of generalized anti-symmetric σ-matrices and one-dimensional projectors. The specific form makes it considerably easy to identify and discard redundant parameters in several cases. In this way, redundancy-free density matrices of arbitrary rank k can be formulated. Our construction can also be used to derive an orthonormal basis of any k-dimensional subspaces of $\mathbb{C}^d$ with the minimal number of parameters. As an example it is shown that this feature leads to a significant reduction of parameters in the case of investigating distillability of quantum states via lower bounds of an entanglement measure (the m-concurrence).

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1. Introduction

In quantum information many quantities or properties of quantum systems are related to optimization problems that necessitate to vary over the set of all unitary transformations, density matrices or subspaces. Such problems arise, for instance, in the detection and quantification of entanglement (see [1–3] and references therein), the properties of quantum states with respect to Bell inequalities [4, 5] or the question of distillability [6, 7]. In general, such a variation can only be done efficiently by parameterizing the object of interest. In this work the focus is on the parameterization of the unitary group $\mathcal{U}(d)$. Density matrices and orthonormal subspaces can then easily be formulated in terms of this representation. It should

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be emphasized that parameterizations are in general equivalent to each other and one should not be misled to conclude that one parameterization is better than the other. However, depending on the problem a certain parameterization can be advantageous by providing more insightful results or by leading to a reduction of the number of involved parameters. The simplest parameterization of $\mathcal{U}(d)$ is the canonical parameterization which is given by $U = \exp(\mathrm{i}H)$, wherein the Hermitian matrix H can be composed of a real-valued linear combination of the $d^2 - 1$ generalized Gell–Mann matrices and the unity $\mathbb{1}_d$. Despite its simple form, this parameterization has the disadvantage that there is no way how redundant parameters, which appear for some tasks, can be removed beforehand (except for one parameter for the special unitary group $\mathcal{SU}(d)$). Thus, the number of parameters is always d^2 or $d^2 - 1$, respectively, independent of the given problem. A different parameterization of $\mathcal{U}(d)$ and $\mathcal{SU}(d)$ in terms of the generalized Euler angle was introduced by Tilma and Sudershan [8, 9]. It has the advantage that it allows us to eliminate redundant 'unphysical' global phases in several cases. A further parameterization of $\mathcal{U}(d)$ was recently found by Jarlskog [10, 11]. Here, the unitary matrices are formulated in a recursive way, meaning that the elements of $\mathcal{U}(d)$ are expressed in terms of the elements of $\mathcal{U}(d-1)$ and a further unitary matrix containing the parameters which enables the extension to d. This parameterization also enables one to remove invariant phases; however, this is a nontrivial task as shown in [12].

In this work we introduce a parameterization (see section 2) which is ideal for the formulation of density matrices (see section 3) and orthonormal subspaces (see section 4), since all redundancies can be easily identified and removed beforehand without having to consider fixed dimensions or special cases explicitly. Due to its concise notation and formulation in terms of the matrix exponential functions of dyadic vector products, the parameterization can be easily implemented in computational programs. Moreover, the parameters have simple ranges; when gathered in a $d \times d$ matrix in a particular order, they permit an insightful interpretation of numerical computations. Concrete numerical examples, in which our parameterization reduces the number of involved variables, are given in section 5. Here we state which parameters can be discarded with respect to optimizing lower bounds of an entanglement measure (the m-concurrence), as well as for clarifying the distillability of quantum states.

2. Composite parameterization of the unitary group $\mathcal{U}(d)$

Consider the unitary operators U acting on a Hilbert space $\mathcal{H} = \mathbb{C}^d$ with $d \geqslant 2$ spanned by the orthonormal basis $\{|1\rangle, \ldots, |d\rangle\}$. For any $U \in \mathcal{U}(d)$ there exist d^2 real values $\lambda_{m,n}$ with $m, n \in \{1, \ldots, d\}$ and $\lambda_{m,n} \in [0, 2\pi]$ for $m \geqslant n$ and $\lambda_{m,n} \in \left[0, \frac{\pi}{2}\right]$ for $m < n$ such that U equals[3]

$$U_C = \left[\prod_{m=1}^{d-1}\left(\prod_{n=m+1}^{d}\exp(\mathrm{i}P_n\lambda_{n,m})\exp(\mathrm{i}\sigma_{m,n}\lambda_{m,n})\right)\right]\cdot\left[\prod_{l=1}^{d}\exp(\mathrm{i}P_l\lambda_{l,l})\right]. \quad (1)$$

Here, the P_l are one-dimensional projectors,

$$P_l = |l\rangle\langle l|, \quad (2)$$

and $\sigma_{m,n}$ are the generalized anti-symmetric σ-matrices

$$\sigma_{m,n} = -\mathrm{i}|m\rangle\langle n| + \mathrm{i}|n\rangle\langle m|, \quad (3)$$

with $1 \leqslant m < n \leqslant d$.

Before we prove that any unitary operator of $\mathcal{U}(d)$ can be written in the form (1) let us comment on the concept behind it: unitary transformations have the characteristic trait

[3] The sequence of the product is $\prod_{i=1}^{N} A_i = A_1 \cdot A_2 \cdots A_N$.

that they map orthonormal bases onto orthonormal bases, i.e. for a given set of vectors $\{|1\rangle, \ldots, |d\rangle\}$ forming an orthonormal basis of a Hilbert space $\mathbb{C}^d$, the unitarily transformed set $\{|1'\rangle, \ldots, |d'\rangle\} = \{U|1\rangle, \ldots, U|d\rangle\}$ is also orthonormal. We are interested in the most general unitary operations transforming $\{|1\rangle, \ldots, |d\rangle\}$ into any arbitrary orthonormal basis $\{|1'\rangle, \ldots, |d'\rangle\}$; hence, our object is the unitary group of dimension d. We know that for the dimension d the unitary group $\mathcal{U}(d)$ is a d^2-parameter group. This means that in order to cover all unitary transformations we must find a transformation that contains at least d^2 parameters (if a parameterization involves more than d^2 parameters it also contains redundancies, which is undesirable).

Regarding the basis $\{|1\rangle, \ldots, |d\rangle\}$, we first find that d parameters can be embedded in global phases for each vector, i.e. $\{e^{i\alpha_1}|1\rangle, \ldots, e^{i\alpha_d}|d\rangle\}$. This corresponds to the product $\prod_{l=1}^{d} \exp(iP_l\lambda_{l,l})$ of our parameterization (1). The notion behind the left part of (1) is to pairwise embed two parameters in the distinctive transformations

$$\Lambda_{m,n} = \exp(iP_n\lambda_{n,m})\exp(i\sigma_{m,n}\lambda_{m,n}) \tag{4}$$

containing two parameters $\lambda_{n,m}$ and $\lambda_{m,n}$. These transformations perform the following operations: the term $\exp(i\sigma_{m,n}\lambda_{m,n})$ generates a rotation in the two-dimensional subspace spanned by the vectors $|m\rangle$ and $|n\rangle$, while $\exp(iP_n\lambda_{n,m})$ adds a relative phase between the vector components of the rotated vectors. Note that $\mathcal{U}(2)$ is actually a 4-parameter group; however, as will be proven later, the neglected two parameters would only lead to redundancies. In order to parameterize $\mathcal{U}(d)$, all terms $\Lambda_{m,n}$ have to be taken into account. There are $\binom{d}{2} = d(d-1)/2$ ways to combine two vectors of $\{|1\rangle, \ldots, |d\rangle\}$, which corresponds to the $d(d-1)/2$ generalized anti-symmetric σ-matrices. One opportunity to involve all terms $\Lambda_{m,n}$ is given by building the product $\prod_{m=1}^{d-1}\left(\prod_{n=m+1}^{d}\Lambda_{m,n}\right)$, which is clearly not unique. We now have embedded further $2 \times d(d-1)/2 = d^2 - d$ parameters, which in sum with the d global phases gives d^2 parameters $\lambda_{m,n}$ in total. For convenience, these parameters $\lambda_{m,n}$ are gathered in a $d \times d$ 'parameterization' matrix

$$\begin{pmatrix} \lambda_{1,1} & \cdots & \lambda_{1,d} \\ \vdots & \ddots & \vdots \\ \lambda_{d,1} & \cdots & \lambda_{d,d} \end{pmatrix}. \tag{5}$$

In this convention, the diagonal entries represent global phase transformations: the upper right are related to rotations, while the lower left are relative phases (with respect to the basis $\{|1\rangle, \ldots, |d\rangle\}$).

We have thus constructed a d^2 parameter set of unitary operators. It remains to prove that this construction covers the entire unitary group $\mathcal{U}(d)$, which is equivalent to showing that for any U there exists a U_C such that $U_C^\dagger U = \mathbb{1}$.

Proof. Let $U = \sum_{r,s=1}^{d} a_{r,s}|r\rangle\langle s|$ be an arbitrary unitary operator, i.e. $\sum_{i=1}^{d} a_{m,i}^* a_{n,i} = \sum_{i=1}^{d} a_{i,m}^* a_{i,n} = \delta_{mn}$. The conjugate transpose of U_C is

$$U_C^\dagger = \left[\prod_{l=1}^{d} \exp(-iP_{d+1-l}\lambda_{d+1-l,d+1-l})\right] \cdot \left[\prod_{m=1}^{d-1}\left(\prod_{n=1}^{m}\Lambda_{d-m,d+1-n}^\dagger\right)\right], \tag{6}$$

implying that $\Lambda_{1,2}^\dagger$ acts first on U. For $U' = \Lambda_{1,2}^\dagger U = \sum_{r,s=1}^{d} a'_{r,s}|r\rangle\langle s|$, this leads to

$$a'_{1,s} = \cos(\lambda_{1,2})a_{1,s} - e^{-i\lambda_{2,1}}\sin(\lambda_{1,2})a_{2,s}, \tag{7}$$

$$a'_{2,s} = \sin(\lambda_{1,2})a_{1,s} + e^{-i\lambda_{2,1}}\cos(\lambda_{1,2})a_{2,s}. \tag{8}$$

For $d > 2$, all other components are unchanged, i.e. $a'_{r,s} = a_{r,s}$ for $r > 2$. As can easily be confirmed, $a'_{2,1}$ can always be made zero via certain parameters $\lambda_{1,2}$ and $\lambda_{2,1}$. If $a_{1,1}$ and $a_{2,1}$ both are zero, both parameters $\lambda_{1,2}$ and $\lambda_{2,1}$ can be chosen freely; if only $a_{1,1} = 0$ we choose $\lambda_{1,2} = \frac{\pi}{2}$ and for $a_{2,1} = 0$ we take $\lambda_{1,2} = 0$. If none of them is zero, then $a'_{2,1}$ vanishes for $\lambda_{2,1}$ and $\lambda_{1,2}$ obeying

$$\arg(\mathrm{e}^{-\mathrm{i}\lambda_{2,1}} a_{2,1}) = \arg(-a_{1,1}), \tag{9}$$

$$\tan(\lambda_{1,2}) = \frac{|a_{2,1}|}{|a_{1,1}|}, \tag{10}$$

which is achievable in any case with $\lambda_{2,1} \in [0, 2\pi]$ and $\lambda_{1,2} \in \left[0, \frac{\pi}{2}\right]$. In the same way, the component $a''_{3,1}$ of $U'' = \Lambda^{\dagger}_{1,3} U'$ can be made zero for $d > 2$. By proceeding in this way for $d > 2$, we can attain $a_{r,s} = 0$ for all components with $r > s$ via $\prod_{m=1}^{d-1} \left(\prod_{n=1}^{m} \Lambda^{\dagger}_{d-m,d+1-n} \right)$. Then, if $a_{r,1} = 0$ for all $r > 1$, it follows $|a_{1,1}| = 1$ due to the unitarity $\left(\sum_{i=1}^{d} a^*_{i,1} a_{i,1} = 1 \right)$ of $U_P = \left[\prod_{m=1}^{d-1} \left(\prod_{n=1}^{m} \Lambda^{\dagger}_{d-m,d+1-n} \right) \right] U$. Moreover, since U_P also satisfies $\sum_{i=1}^{d} a^*_{1,i} a_{1,i} = 1$, we can infer that $a_{1,r} = 0$ for all $r > 1$. When taking into account the unitarity constraints $\sum_{i=1}^{d} a^*_{m,i} a_{n,i} = \sum_{i=1}^{d} a^*_{i,m} a_{i,n} = \delta_{mn}$ for all rows and columns, we conclude that U_P has the diagonal form

$$U_P = \sum_{r=1}^{d} a_{r,r} |r\rangle\langle r|, \tag{11}$$

with $a_{r,r}$ obeying $|a_{r,r}| = 1$, which is a complex number of magnitude 1, i.e. $a_{r,r} = \mathrm{e}^{\mathrm{i}\alpha_r}$. The choice $\lambda_{r,r} = \alpha_r$ then yields $U_C^{\dagger} U = \left[\prod_{l=1}^{d} \exp(-\mathrm{i} P_{d+1-l} \lambda_{d+1-l,d+1-l}) \right] U_P = \mathbb{1}$, which was to be proven. □

3. Parameterization of density matrices with rank *k*

Now we use our parameterization of $\mathcal{U}(d)$ to formulate density matrices. Any density matrix ρ acting on $\mathcal{H} = \mathbb{C}^d$ can be written in the form

$$\rho = \sum_{n=1}^{k} p_n |\Psi_n\rangle\langle\Psi_n|, \tag{12}$$

with $p_n \geqslant 0$ and $\sum_{n=1}^{k} p_n = 1$, where $k \leqslant d$ is the rank of ρ and $\{|\Psi_1\rangle, \ldots, |\Psi_k\rangle\}$ are the orthonormal vectors. For $k = 1$, i.e. pure states, we only have one $p_1 = 1$. Without loss of generality, the coefficients $\{p_n\}$ of an arbitrary state of rank $k > 1$ or smaller can be expressed by means of $k - 1$ real parameters $\theta_i \in \left[0, \frac{\pi}{2}\right]$ as

$$p_1 = \cos^2 \theta_1 \tag{13}$$

$$p_n = \cos^2 \theta_n \prod_{i=1}^{n-1} \sin^2 \theta_i \qquad \forall\, n : 1 < n < k \tag{14}$$

$$p_k = \prod_{i=1}^{k-1} \sin^2 \theta_i. \tag{15}$$

Any desired set of k orthonormal vectors $\{|\Psi_1\rangle, \ldots, |\Psi_k\rangle\}$ can be constructed out of $\{|1\rangle, \ldots, |k\rangle\}$ by applying U_C. Thus, any ρ with rank k can be parameterized via

$$\rho = \sum_{n=1}^{k} p_n U_C |n\rangle\langle n| U_C^{\dagger}. \tag{16}$$

A parameterization of density matrices via diagonal elements and unitary transformations can in principle be achieved with any parameterization of the unitary group $\mathcal{U}(d)$ (see for instance [13–15]). However, the composite form of U_C makes it easy to identify and eliminate all redundant parameters. The first observation is that the diagonal entries $\lambda_{n,n}$ are redundant, since they cancel out in the outer product, i.e.

$$\left[\prod_{l=1}^{d}\exp(\mathrm{i}P_l\lambda_{l,l})\right]|n\rangle\langle n|\left[\prod_{l=1}^{d}\exp(-\mathrm{i}P_{d+1-l}\lambda_{d+1-l,d+1-l})\right]=|n\rangle\langle n| \qquad \forall\, n\in\{1,\ldots,d\}. \tag{17}$$

The second observation is that for density matrices of rank $k < d$ we can eliminate further parameters when the composite parameterization is used. As can easily be seen, ρ is independent of all parameters $\lambda_{m,n}$ where both $m > k$ and $n > k$. Thus, it suffices to utilize

$$\rho=\sum_{n=1}^{k}p_nU_{CD}|n\rangle\langle n|U_{CD}^{\dagger}, \tag{18}$$

with

$$U_{CD}=\prod_{m=1}^{k}\left(\prod_{n=m+1}^{d}\exp(\mathrm{i}P_n\lambda_{n,m})\exp(\mathrm{i}\sigma_{m,n}\lambda_{m,n})\right), \tag{19}$$

where the index m is only running from 1 to k instead of 1 to $d-1$. Using the introduced representation in terms of the parameterization matrix, this is U_C with

$$\underbrace{\left.\begin{pmatrix} 0 & \lambda_{1,2} & \cdots \\ \lambda_{2,1} & \ddots & \ddots \\ \vdots & \ddots & 0 \\ \lambda_{k+1,1} & \cdots & \lambda_{k+1,k} \\ \vdots & \ddots & \vdots \\ \lambda_{d,1} & \cdots & \lambda_{d,k} \end{pmatrix}\right\}k}_{k}\quad\underbrace{\left.\begin{pmatrix} \lambda_{1,k+1} & \cdots & \lambda_{1,d} \\ \vdots & \ddots & \vdots \\ \lambda_{k,k+1} & \cdots & \lambda_{k,d} \\ 0 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & 0 \end{pmatrix}\right\}d-k}_{d-k}. \tag{20}$$

Consequently, any density matrix of rank k or smaller acting on $\mathbb{C}^d$ can be expressed with a maximum of $2dk-k^2-1$ parameters ($k-1$ parameters θ_i and $k(2d-k-1)$ parameters $\lambda_{m,n}$). The extremal scenarios are pure states with $2(d-1)$ parameters and full rank density matrices with d^2-1 parameters.

4. Parameterization of k-dimensional subspaces

In the previous section, we have shown that any set of k orthonormal vectors can be constructed (up to global phases) with $k(2d-k-1)$ parameters. Now, we prove that even less, namely $2k(d-k)$, parameters are necessary to construct an orthonormal basis of an arbitrary k-dimensional subspace of $\mathbb{C}^d$. Consider a general subspace spanned by k orthonormal vectors $\{|\Psi_1\rangle,\ldots,|\Psi_k\rangle\}$ in a d-dimensional complex Hilbert space $\mathcal{H}=\mathbb{C}^d$. Let $a_{m,n}$ be the coefficients of $|\Psi_n\rangle$ in the complete basis $\{|1\rangle,\ldots,|d\rangle\}$ of $\mathcal{H}=\mathbb{C}^d$, i.e. $|\Psi_n\rangle=\sum_{m=1}^{d}a_{m,n}|m\rangle$. A different basis of the same subspace then is of course given by the orthonormal set of vectors

$$\{|\Psi_1\rangle,\ldots,|\Psi_{k-2}\rangle,\cos(\lambda_{k-1,k})|\Psi_{k-1}\rangle-\mathrm{e}^{(\mathrm{i}\lambda_{k,k-1})}\sin(\lambda_{k-1,k})|\Psi_k\rangle, \tag{21}$$

$$\sin(\lambda_{k-1,k})|\Psi_{k-1}\rangle + \mathrm{e}^{(\mathrm{i}\lambda_{k,k-1})}\cos(\lambda_{k-1,k})|\Psi_k\rangle\}, \tag{22}$$

which is $\{\Lambda'_{k-1,k}|\Psi_1\rangle, \ldots, \Lambda'_{k-1,k}|\Psi_k\rangle\}$ where $\Lambda'_{k-1,k}$ is given as in (4) but with $P_l = |\Psi_l\rangle\langle\Psi_l|$ and $\sigma_{m,n} = -\mathrm{i}|\Psi_m\rangle\langle\Psi_n| + \mathrm{i}|\Psi_n\rangle\langle\Psi_m|$. The $(k-1)$st vector of this set is

$$\cos(\lambda_{k-1,k})|\Psi_{k-1}\rangle - \mathrm{e}^{(\mathrm{i}\lambda_{k,k-1})}\sin(\lambda_{k-1,k})|\Psi_k\rangle \tag{23}$$

$$= \sum_{m=1}^{d}(\cos(\lambda_{k-1,k})a_{m,k-1} - \mathrm{e}^{(\mathrm{i}\lambda_{k,k-1})}\sin(\lambda_{k-1,k})a_{m,k})|m\rangle, \tag{24}$$

whose kth coefficient $\cos(\lambda_{k-1,k})a_{k,k-1} - \mathrm{e}^{(\mathrm{i}\lambda_{k,k-1})}\sin(\lambda_{k-1,k})a_{k,k}$ can be made zero analogously to (7)–(10). In this way, with $\{\prod_{n=1}^{k-1}\Lambda'_{n,k}|\Psi_1\rangle, \ldots, \prod_{n=1}^{k-1}\Lambda'_{n,k}|\Psi_k\rangle\}$, a basis of the subspace can be obtained where all kth coefficients of all vectors except the last one are zero. This can then be repeated for all rows $< k$, such that with $\{\prod_{m=2}^{k}\prod_{n=1}^{m-1}\Lambda'_{n,m}|\Psi_1\rangle, \ldots, \prod_{m=2}^{k}\prod_{n=1}^{m-1}\Lambda'_{n,m}|\Psi_k\rangle\}$ we arrive at an orthonormal basis, let us say $\{|\Psi'_1\rangle, \ldots, |\Psi'_k\rangle\}$, of the same subspace where all coefficients $a_{m,n} = 0$ for all m with $n < m \leqslant k$. Such a set of vectors, however, can be constructed (up to global phases) from $\{|1\rangle, \ldots, |k\rangle\}$ via $\{U_{CS}|1\rangle, \ldots, U_{CS}|k\rangle\}$ where

$$U_{CS} = \prod_{m=1}^{k}\left(\prod_{n=k+1}^{d}\exp(\mathrm{i}P_n\lambda_{n,m})\exp(\mathrm{i}\sigma_{m,n}\lambda_{m,n})\right). \tag{25}$$

Here, only $2k(d-k)$ parameters $\lambda_{m,n}$ are involved since the index n of the second product $\prod$ lies within $k < n \leqslant d$. In terms of the parameterization matrix, this is U_C with

$$\underbrace{\begin{pmatrix} 0 & \cdots & 0 & \lambda_{1,k+1} & \cdots & \lambda_{1,d} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & 0 & \lambda_{k,k+1} & \cdots & \lambda_{k,d} \\ \lambda_{k+1,1} & \cdots & \lambda_{k+1,k} & 0 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ \lambda_{d,1} & \cdots & \lambda_{d,k} & 0 & \cdots & 0 \end{pmatrix}}_{\begin{matrix} k & & & d-k & & \end{matrix}} \begin{matrix} \left.\begin{matrix} \\ \\ \\ \end{matrix}\right\} k \\ \left.\begin{matrix} \\ \\ \\ \end{matrix}\right\} d-k \end{matrix} \tag{26}$$

.

Proof. The proof is completely analogous to the one in section 2 and therefore is not given in detail. One only has to take an arbitrary set of vectors $\{|\Psi'_1\rangle, \ldots, |\Psi'_k\rangle\}$ with the mentioned properties, for which via $\{U_{CS}^{\dagger}|\Psi'_1\rangle, \ldots, U_{CS}^{\dagger}|\Psi'_k\rangle\} = \{\sum_{m=1}^{d}a_{m,1}|m\rangle, \ldots, \sum_{m=1}^{d}a_{m,k}|m\rangle\}$ it is possible to attain $|a_{m,n}| = \delta_{m,n}$ for all $m \in [1, \ldots, d]$ and $n \in [1, \ldots, k]$. □

5. Application: optimization of lower bounds of entanglement measures

The m-concurrence introduced in [16] constitutes a building block of entanglement measures for multipartite systems of arbitrary dimension (see also [17]) with simple computable lower bounds. These bounds are not invariant under local unitary transformations. Optimization procedures can be realized efficiently via the previously introduced parameterization of the unitary group.

5.1. Optimal lower bounds

First we introduce the m-concurrence for bipartite quantum systems in $\mathbb{C}^d \otimes \mathbb{C}^d$. The linear entropy $S_L(\rho) := \frac{d}{d-1}(1 - \mathrm{Tr}(\rho^2))$ of the reduced density matrices $\rho_{A/B} := \mathrm{Tr}_{B/A}(\rho)$ of a bipartite pure state $|\psi\rangle \in \mathbb{C}^d \otimes \mathbb{C}^d$ can be expressed as

$$\frac{2(d-1)}{d} S_L(\rho_A) = \sum_{k_A<l_A} \sum_{k_B<l_B} \mathrm{Tr}(|\psi\rangle\langle\psi|\sigma_{k_A,l_A} \otimes \sigma_{k_B,l_B}(|\psi\rangle\langle\psi|)^* \sigma_{k_A,l_A} \otimes \sigma_{k_B,l_B}) \tag{27}$$

$$=: C_m^2(|\psi\rangle\langle\psi|). \tag{28}$$

Via a convex roof extension one can generalize the m-concurrence $C_m^2(|\psi\rangle\langle\psi|)$ to mixed states:

$$C_m^2(\rho) := \inf_{\{p_i,|\psi_i\rangle\}} \sum_i p_i C_m^2(|\psi_i\rangle\langle\psi_i|)$$

$$= \inf_{\{p_i,|\psi_i\rangle\}} \sum_i p_i \sum_{k_A<l_A} \sum_{k_B<l_B} \mathrm{Tr}(|\psi_i\rangle\langle\psi_i|\sigma_{k_A,l_A} \otimes \sigma_{k_B,l_B}(|\psi_i\rangle\langle\psi_i|)^* \sigma_{k_A,l_A} \otimes \sigma_{k_B,l_B}).$$

As the infimum of this expression cannot straightforwardly be computed, it is of great importance to find strong lower bounds. Those can be obtained with

$$C_m^2(\rho) \geqslant \sum_{k_A<l_A} \sum_{k_B<l_B} \inf_{\{p_i,|\psi_i\rangle\}} \sum_i p_i \mathrm{Tr}(|\psi_i\rangle\langle\psi_i|\sigma_{k_A,l_A} \otimes \sigma_{k_B,l_B}(|\psi_i\rangle\langle\psi_i|)^* \sigma_{k_A,l_A} \otimes \sigma_{k_B,l_B})$$

by exploiting that the individual infima are known (see [18, 19]):

$$\inf_{\{p_i,|\psi_i\rangle\}} \sum_i p_i \mathrm{Tr}(|\psi_i\rangle\langle\psi_i|\sigma_{k_A,l_A} \otimes \sigma_{k_B,l_B}(|\psi_i\rangle\langle\psi_i|)^* \sigma_{k_A,l_A} \otimes \sigma_{k_B,l_B}) = X^2_{k_A,l_A,k_B,l_B}, \tag{30}$$

with

$$X_{k_A,l_A,k_B,l_B} := \max\left[2\max\left[\left\{x^i_{k_A,l_A,k_B,l_B}\right\}\right] - \sum_i x^i_{k_A,l_A,k_B,l_B}, 0\right], \tag{31}$$

where $\left\{x^i_{k_A,l_A,k_B,l_B}\right\}$ are the square roots of the eigenvalues of

$$\rho\sigma_{k_A,l_A} \otimes \sigma_{k_B,l_B}\rho^*\sigma_{k_A,l_A} \otimes \sigma_{k_B,l_B}. \tag{32}$$

In summary, we have obtained the following bound:

$$C_m^2(\rho) \geqslant \sum_{k_A<l_A} \sum_{k_B<l_B} X^2_{k_A,l_A,k_B,l_B} =: B^2(\rho). \tag{33}$$

This bound is not invariant under local unitaries and thus can be optimized with an appropriate choice $U_A \otimes U_B$. Consequently, the optimal lower bound for the m-concurrence for bipartite systems is given by

$$B^2_{\mathrm{opt}}(\rho) := \max\left[\sum_{k_A<l_A} \sum_{k_B<l_B} X^2_{k_A,l_A,k_B,l_B}\right], \tag{34}$$

where the eigenvalues of $\rho\sigma_{k_A,l_A} \otimes \sigma_{k_B,l_B}\rho^*\sigma_{k_A,l_A} \otimes \sigma_{k_B,l_B}$ are replaced by the eigenvalues of

$$U_A \otimes U_B \rho U_A^\dagger \otimes U_B^\dagger \sigma_{k_A,l_A} \otimes \sigma_{k_B,l_B} U_A^* \otimes U_B^* \rho^* U_A^T \otimes U_B^T \sigma_{k_A,l_A} \otimes \sigma_{k_B,l_B} \tag{35}$$

and the maximum is taken over all $U_A, U_B \in \mathcal{U}(d)$. In many cases, this problem can be solved numerically by parameterizing U_A, U_B and utilizing numerical methods such as 'Nelder–Mead' [20], 'simulated annealing' [21] or 'differential evolution' [22]. In order to remove redundant parameters we exploit that

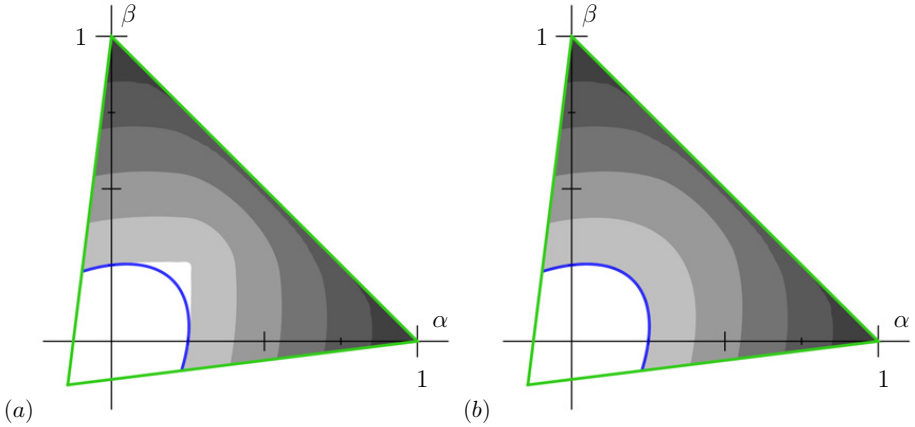

Figure 1. Contour plots of the lower bounds $B(\rho)$ and $B_{\text{opt}}(\rho)$ of the normalized m-concurrence $\frac{C_m(\rho)}{C_m(|\Psi_1\rangle\langle\Psi_1|)}$ for the set of states $\rho = \alpha|\Psi_1\rangle\langle\Psi_1| + \beta|\Psi_2\rangle\langle\Psi_2| + \frac{1-\alpha-\beta}{9}\mathbb{1}$ constructed with two mutually orthogonal maximally entangled states $|\Psi_1\rangle = \frac{1}{\sqrt{3}}(|11\rangle + |22\rangle + |33\rangle)$ and $|\Psi_2\rangle = \frac{1}{\sqrt{3}}(|12\rangle + |23\rangle + |31\rangle)$ of $\mathbb{C}^3 \otimes \mathbb{C}^3$ (bipartite qutrit system) combined with uncolored noise $\frac{1}{9}\mathbb{1}$. All values of the parameters α and β within the green triangle correspond to density matrices (positive semidefinite). Density matrices within the blue ellipse are positive under partial transposition (PPT criterion). In the gray shaded areas the bounds of the m-concurrence are nonzero. The gray scale corresponds to the value of the bounds lying in the range of 0–1. The shades of gray are related to an increment of 0.2 starting from 0. The left picture (a) illustrates the contour plot of the bounds computed according to equation (33) without optimization. The right picture (b) illustrates the contour plot of the numerically optimized bounds (34) using our parameterization for $\mathcal{U}(3)$ and the Nelder–Mead method. Without optimization (a), the lower bounds are zero for some states with negative partial transposition. After the numerical optimization (b), the lower bounds of all states that are negative under partial transposition are greater than zero. As can also be seen, the shapes of the contours of (b) differ considerably from (a), and indicate an improvement of the lower bounds.

(This figure is in colour only in the electronic version)

$$\text{EV}\big(U_A \otimes U_B \rho U_A^\dagger \otimes U_B^\dagger \sigma_{k_A,l_A} \otimes \sigma_{k_B,l_B} U_A^* \otimes U_B^* \rho^* U_A^T \otimes U_B^T \sigma_{k_A,l_A} \otimes \sigma_{k_B,l_B}\big) \tag{36}$$

$$= \text{EV}\big(\rho\big(U_A^\dagger \sigma_{k_A,l_A} U_A^*\big) \otimes \big(U_B^\dagger \sigma_{k_B,l_B} U_B^*\big) \rho^* \big(U_A^T \sigma_{k_A,l_A} U_A\big) \otimes \big(U_B^T \sigma_{k_B,l_B} U_B\big)\big), \tag{37}$$

where EV stands for the set of eigenvalues. If we now insert $U_A^\dagger$ and $U_B^\dagger$ into the parameterized form (1), i.e. $U_A^\dagger = U_{C,A}$ and $U_B^\dagger = U_{C,B}$, and let them act on the σ-matrices, it is easy to see that all diagonal entries $\lambda_{m,m}$ of both unitaries cancel out. Consequently, we can reduce (34) to a $2(d^2 - d)$-dimensional global optimization problem. (If we would insert $U_A = U_{C,A}$ and $U_B = U_{C,B}$, only one diagonal entry $\lambda_{m,m}$ of each U_C could generally be set zero.) An illustrative example, where the bounds of the m-concurrence are optimized in this way using the Nelder–Mead method [20] for convex combinations of two mutually orthogonal maximally entangled states and uncolored noise, is given in figure 1. With optimization, the bounds are greater than zero for all states detected by the partial transposition criterion (PPT).

For multipartite systems we can use the same principle (for a detailed introduction see [16, 17]). First we introduce the set of all bipartitions $\mathcal{B} = \{(\alpha|\beta)\}$ of a given n-partite system. Here, α denotes a union of subsystems in the first part of the bipartition and β is its complement. The dimensions of the corresponding complex Hilbert spaces $\mathcal{H}_\alpha$ and $\mathcal{H}_\beta$ are

d_α and d_β, respectively. In this way, the general definition of the m-concurrence also valid for multipartite systems is

$$C_m^2(\rho) = \inf_{\{p_i,|\psi_i\rangle\}} \sum_i p_i \sum_{\mathcal{B}} \sum_{k_A<l_A} \sum_{k_B<l_B} \mathrm{Tr}\big(|\psi_i\rangle\langle\psi_i|\sigma^{\alpha\beta}_{k_A,l_A} \otimes \sigma^{\alpha\beta}_{k_B,l_B}(|\psi_i\rangle\langle\psi_i|)^* \sigma^{\alpha\beta}_{k_A,l_A} \otimes \sigma^{\alpha\beta}_{k_B,l_B}\big),$$

where $\{\sigma^{\alpha\beta}_{k_A,l_A}\}$ and $\{\sigma^{\alpha\beta}_{k_B,l_B}\}$ are the generalized anti-symmetric σ-matrices defined with respect to the bipartition $(\alpha|\beta)$, i.e. acting on $\mathcal{H}_\alpha$ and $\mathcal{H}_\beta$, respectively. Consequently, according to (29)–(33),

$$C_m^2(\rho) \geqslant \sum_{\mathcal{B}} \sum_{k_A<l_A} \sum_{k_B<l_B} \big(X^{\alpha\beta}_{k_A,l_A,k_B,l_B}\big)^2, \tag{38}$$

where $X^{\alpha\beta}_{k_A,l_A,k_B,l_B}$ is defined as in (31) but with the eigenvalues of

$$\rho\sigma^{\alpha\beta}_{k_A,l_A} \otimes \sigma^{\alpha\beta}_{k_B,l_B}\rho^*\sigma^{\alpha\beta}_{k_A,l_A} \otimes \sigma^{\alpha\beta}_{k_B,l_B}. \tag{39}$$

By proceeding analogously to (34)–(37), this lower bound can be optimized by replacing ρ by $U_A^{\alpha\beta} \otimes U_B^{\alpha\beta}\rho U_A^{\dagger\alpha\beta} \otimes U_B^{\dagger\alpha\beta}$ for each bipartition. In this sense, the optimal lower bound is given by

$$B^2_{\mathrm{opt}}(\rho) := \max\left[\sum_{\mathcal{B}} \sum_{k_A<l_A} \sum_{k_B<l_B} \big(X^{\alpha\beta}_{k_A,l_A,k_B,l_B}\big)^2\right]; \tag{40}$$

over all $U_A^{\alpha\beta} \in \mathcal{U}(d_\alpha)$ and $U_B^{\alpha\beta} \in \mathcal{U}(d_\beta)$.

5.2. Distillation

If entanglement is used as a resource it is often required that the system is in a pure maximally entangled state. States that can be transformed into such maximally entangled states via LOCC (local operations and classical communication) are called distillable. It was proven by Horodecki *et al* in [6] that all distillable states have an entangled $\mathbb{C}^2 \otimes \mathbb{C}^2$ subsystem (see also [23]). As the bounds for the m-concurrence are exact in those systems it suffices to optimize one of the terms in the sum of (34) to investigate distillability since all terms are local-unitarily related. Thus, a state ρ is distillable only if

$$\max X^2_{1,2,1,2} > 0, \tag{41}$$

where the maximum is taken over all $U_A \in \mathcal{U}(d)$ and $U_B \in \mathcal{U}(d)$. According to (37), the value of $X_{1,2,1,2}$ is a function of the eigenvalues of

$$\rho\big(U_A^\dagger\sigma_{1,2}U_A^*\big) \otimes \big(U_B^\dagger\sigma_{1,2}U_B^*\big)\rho^*\big(U_A^T\sigma_{1,2}U_A\big) \otimes \big(U_B^T\sigma_{1,2}U_B\big). \tag{42}$$

These eigenvalues, however, are completely determined by the 2×2-dimensional subspace spanned by the tensorproducts of the vectors $U_A^\dagger|1\rangle$ and $U_A^\dagger|2\rangle$ with $U_B^\dagger|1\rangle$ and $U_B^\dagger|2\rangle$. Consequently, for $U_A^\dagger$ and $U_B^\dagger$ we can take $U_A^\dagger = U_{CS,A}$ and $U_B^\dagger = U_{CS,B}$ defined as in (25) with $k = 2$, where each transformation only depends on $4d - 8$ parameters $\lambda_{m,n}$. In this way, the question of whether a state ρ is distillable or not can efficiently be clarified via a (numerical) optimization algorithm with a reduced number of parameters. (Note that in contrast to a naive parameterization of $\mathcal{U}(d)$, the number of parameters is linear in d instead of quadratic. As distillability is generally studied for high-dimensional n-copy states, i.e. $\rho^{\otimes n}$, this reduction is of great importance for numerical tractability.)

Multipartite systems can be treated equivalently for each bipartition. Hence, for a fixed bipartition $4(d_\alpha + d_\beta) - 16$ variables have to be optimized. However, in this case, if the unitary operators related to a fixed bipartition are not locally implementable with respect to

the subsystems, also unlockable bound entanglement can appear (see also [24, 25]). The set of locally distillable states can be determined by restricting all transformations to unitaries which are local with respect to all subsystems.

6. Summary

In this paper we introduced a parameterization of the unitary group $\mathcal{U}(d)$ which besides its simple form has the advantage that redundancies can easily be identified and removed in several cases. The efficiency for the representation of density matrices of rank k and k-dimensional subspaces in $\mathbb{C}^d$ was shown. We found that only $2dk - k^2 - 1$ real parameters are necessary to parameterize density matrices of rank k, since we were able to discard all irrelevant parameters related to transformations in uninvolved subspaces and invariant phases beforehand. For the construction of an orthonormal basis of any k-dimensional subspace of $\mathbb{C}^d$ even less parameters are needed, namely $2k(d-k)$, due to the unitary equivalence of basis vectors within the subspace.

Furthermore, examples of the usefulness of the parameterization with respect to a multipartite entanglement measure (referred to as the m-concurrence) and distillability were given. We described how lower bounds can be derived for this entanglement measure. The bounds were obtained by the observation that the linear entropy of reduced density matrices can be rewritten by an operator sum, where each operator acts in a two-dimensional subspace. We showed how these bounds can be optimized and how invariant parameters can be removed when our parameterization is utilized. Finally, we revealed that further parameters can be discarded if only the distillability of quantum states is of interest. We found that only a number of variables linear in the dimensions of the subsystems have to be optimized to solve this problem.

We believe that the parameterization presented in this paper is advantageous with respect to the tractability of a variety of high-dimensional optimization procedures in quantum information as well as for other problems in quantum theory.

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Composite parameterization and Haar measure for all unitary and special unitary groups

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We adopt the concept of the composite parameterization of the unitary group $\mathcal{U}(d)$ to the special unitary group $\mathcal{SU}(d)$. Furthermore, we also consider the Haar measure in terms of the introduced parameters. We show that the well-defined structure of the parameterization leads to a concise formula for the normalized Haar measure on $\mathcal{U}(d)$ and $\mathcal{SU}(d)$. With regard to possible applications of our results, we consider the computation of high-order integrals over unitary groups. © *2012 American Institute of Physics*. [doi:10.1063/1.3672064]

I. INTRODUCTION

Unitary and special unitary groups play an important role in various fields of physics. Several problems that arise in the context of these groups require to express them in terms of a set of real parameters. In general, such parameterizations are not unique in the sense that the considered groups can be parameterized in many different ways. With regard to the diversity of problems it is reasonable to have a repertoire of different parameterizations available, in order to be able to choose the most convenient one for a given problem. In Ref. 8, we recently introduced the composite parameterization of the unitary group $\mathcal{U}(d)$ as an alternative to the canonical parameterization $U = \exp(iH)$ via Hermitian matrices H and those presented in Refs. 9–11. It was shown that our parameterization enables a simple identification of redundant parameters when it is applied to describing orthonormal bases, density matrices of arbitrary rank and subspaces. For all these objects, we found representations containing the minimal number of parameters needed. Due to its concise notation, simple implementation and computational benefits it has already found widespread applications in research on lattice correlation functions,[12] quantum nonlocality,[13] genuine multipartite entanglement,[14–16] and quantum secret sharing.[17]

The aim of the present paper is twofold. First, we adopt our concept that was used in Ref. 8 to obtain a novel parameterization of the special unitary group $\mathcal{SU}(d)$. The need of additional representations of this group is not only apparent because of its vital relevance in all kinds of fields involving quantum physics (see Ref. 18 for an overview), but moreover is given because the number of available parameterizations is relatively low compared to $\mathcal{U}(d)$. Here, our parameterization is proposed as an alternative to the canonical parameterization $U = \exp(iH)$ via *traceless* Hermitian matrices H and the generalized Euler angle parameterization[19] introduced by Tilma and Sudarshan.

Second, we rigorously derive the normalized Haar measure in terms of the introduced parameters for both the unitary $\mathcal{U}(d)$ and the special unitary group $\mathcal{SU}(d)$ of arbitrary dimension. In form of an infinitesimal volume element of a group, the Haar measure contains all information about the distribution density in its parameter representation. This in return is essential for the capability of generating uniformly distributed random unitaries, density matrices, and subspaces, as they are important in, for instance, Monte Carlo simulations[20] or quantum data hiding.[21,22] Explicit

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expressions of the normalized Haar measure can, furthermore, be useful to tackle group integrals as they appear in lattice QCD,[23] quantum optics,[24] stochastic processes,[25] and mesoscopic systems.[26] In quantum information, they can be found in the context of symmetric states (*Werner* and isotropic states[27–29]) and the *a priori entanglement* of quantum systems.[30–32]

Within recent years much attention has been paid to integrals over unitary groups, i.e., $\int_{\mathcal{U}(d)} f(U, U^*)dU$ whose integrand is a polynomial in U and U^*. It was shown that such integrals can be replaced by a sum of function values $f(U_i, U_i^*)$ using a finite set of unitaries $\{U_i\}_N$. Such sets are termed *unitary t-designs*,[32–34] wherein t denotes that the degree of the polynomial in U and U^* is at most t. Whereas the existence of a unitary t-design was proven for all dimensions d and all polynomial degrees t (see Ref. 35), it is generally unknown how to construct them for arbitrary d and t. In addition, there currently exists no *simple* analytic method for solving any integral over any polynomial. Due to this, there have been several attempts to find schemes to approximate unitary t-designs. Here, the usefulness of our results in the context of unitary t-designs and their approximations is obvious: Since we do not only provide the Haar measure but also the exact parameter ranges for group covering, the integration of polynomials can be performed explicitly and solved analytically in many cases. This in return allows to verify (or falsify) suggested unitary designs and to test the accuracy of approximations. Apart from that, our tools for computing integrals are not limited to polynomials, but are applicable to arbitrary functions.

The paper is organized as follows. In Sec. II, we review the composite parameterization of the unitary group $\mathcal{U}(d)$. In Sec. III, we introduce the composite parameterization of the special unitary group $\mathcal{SU}(d)$. In Sec. IV, the general formula for the Haar measure on $\mathcal{U}(d)$ is stated and proven. An analogous formula for the Haar measure on the special unitary group $\mathcal{SU}(d)$ can be found in Sec. V. Finally, in Sec. VI we make useful remarks on computing integrals over $\mathcal{U}(d)$ and $\mathcal{SU}(d)$ using the composite parameterization and the associated Haar measure.

II. COMPOSITE PARAMETERIZATION OF THE UNITARY GROUP $\mathcal{U}(d)$

Consider a d-dimensional ($d \geq 2$) complex Hilbert space $\mathcal{H} = \mathbb{C}^d$ spanned by the orthonormal basis $\{|1\rangle, \ldots, |d\rangle\}$. On this space define d one-dimensional projectors

$$P_l = |l\rangle \langle l|, \qquad 1 \leq l \leq d, \tag{1}$$

and $d(d-1)/2$ anti-symmetric matrices[1]

$$Y_{m,n} = -i\,|m\rangle \langle n| + i\,|n\rangle \langle m|, \qquad 1 \leq m < n \leq d \tag{2}$$

each acting on a two-dimensional subspace spanned by $|m\rangle$ and $|n\rangle$. In our previous paper,[8] using these operators we have proven the following theorem.

Theorem 1: *Any operator of the unitary group $\mathcal{U}(d)$ can be written as*[2]

$$U_C = \left[\prod_{m=1}^{d-1}\left(\prod_{n=m+1}^{d} \exp\left(i\,P_n\lambda_{n,m}\right)\exp\left(i\,Y_{m,n}\lambda_{m,n}\right)\right)\right]\cdot\left[\prod_{l=1}^{d}\exp(i\,P_l\lambda_{l,l})\right], \tag{3}$$

using d^2 real parameters $\{\lambda_{m,n}\}_{m,n=1,\ldots,d}$ in the ranges $\lambda_{m,n} \in [0, 2\pi]$ for $m \geq n$ and $\lambda_{m,n} \in \left[0, \frac{\pi}{2}\right]$ for $m < n$.

The idea behind this construction was to compose the unitary group out of "elementary operations" such as rotations and phase shifts. Here, these operations are realized through the matrix exponential functions $\exp(iY_{m,n}\alpha)$ (generates a rotation) and $\exp(iP_l\alpha)$ (shifts a phase). To make an ansatz for an arbitrary unitary operator it is useful to think of unitaries as orthonormal basis transformations. In this way, the form (3) can be interpreted as one option of incorporating d global phase operations

$$\exp(i\,P_l\lambda_{l,l}) \tag{4}$$

as well as $d(d-1)/2$ rotations followed by relative phase shifts

$$\Lambda_{m,n} = \exp\left(i P_n \lambda_{n,m}\right) \exp\left(i Y_{m,n} \lambda_{m,n}\right) \tag{5}$$

that result from partitioning the Hilbert space into two-dimensional subspaces according to (2). That this d^2 parameter set of unitary operators indeed covers the whole unitary group $\mathcal{U}(d)$ was proven in Ref. 8. This was done by showing that for any $U \in \mathcal{U}(d)$ there exists a U_C such that $U_C^\dagger U = \mathbb{1}$.

III. COMPOSITE PARAMETERIZATION OF THE SPECIAL UNITARY GROUP $\mathcal{SU}(d)$

Unitary operators obeying $\det U = 1$ constitute a subgroup of $\mathcal{U}(d)$ called the special unitary group $\mathcal{SU}(d)$. The first new result of this paper is that this group can be parameterized similarly as $\mathcal{U}(d)$ using the concept of the composite parameterization. First, let us note that as special unitary operators satisfy an additional constraint the special unitary group $\mathcal{SU}(d)$ can be described by $d^2 - 1$ real parameters. As redundant parameters are undesirable we have to find a parameterization that contains exactly this number of parameters. Second, it is known that $U = \exp(iH\alpha)$ is special unitary for all $\alpha \in \mathbb{R}$ only if H is Hermitian and *traceless*. In the composite parameterizaton of the unitary group $\mathcal{U}(d)$, we have used matrix exponentials of P_l and $Y_{m,n}$ as defined in Eqs. (1) and (2). The latter is already traceless but any one-dimensional projector P_l has $\mathrm{Tr}(P_l) = 1$. As the projectors P_l were used to create phase shifts it is clear that they have to be replaced by a set of diagonal *traceless* operators. For that we introduce the following operators:

$$Z_{m,n} = |m\rangle\langle m| - |n\rangle\langle n|, \qquad 1 \le m < n \le d\,. \tag{6}$$

These are possible generalizations of the diagonal Pauli matrix σ_z acting on the subspace spanned by $|m\rangle$ and $|n\rangle$. In (5) the operation $\exp(iP_n\lambda_{n,m})$ was used to generate a relative phase shift between the vector components $|m\rangle$ and $|n\rangle$. However, the same effect can also be achieved with $\exp(iZ_{m,n}\lambda_{n,m})$ meaning that (5) can be replaced by

$$\Lambda_{m,n} = \exp\left(i Z_{m,n} \lambda_{n,m}\right) \exp\left(i Y_{m,n} \lambda_{m,n}\right)\,. \tag{7}$$

It now remains to turn our attention to the last part of (3), i.e., $\left[\prod_{l=1}^{d} \exp(i P_l \lambda_{l,l})\right]$. Here, each $\exp(iP_l\lambda_{l,l})$ is regarded as a global phase operation on $|l\rangle$. Special unitarity implies that there are only $d-1$ independent global phase operations instead of d for $\mathcal{U}(d)$. There is no unique way how these operations can be realized using matrix exponentials of (6). However, a possible and convenient choice is

$$\exp(i Z_{l,d} \lambda_{l,l}), \qquad 1 \le l \le d-1\,. \tag{8}$$

In this version, the first $d-1$ vectors $|1\rangle, \ldots, |d-1\rangle$ experience the phase shifts $e^{i\lambda_{1,1}}|1\rangle, \ldots, e^{i\lambda_{d-1,d-1}}|d-1\rangle$, while the last vector $|d\rangle$ gets phase shifted in the overall inverse direction, i.e. $e^{-i\sum_{l=1}^{d-1}\lambda_{l,l}}|d\rangle$. Note that according to our labeling there is no parameter $\lambda_{d,d}$. Thus, in total we have the desired number of $d^2 - 1$ parameters $\lambda_{m,n}$. In summary, this leads to the next theorem.

Theorem 2: *Any operator of the special unitary group $\mathcal{SU}(d)$ can be written as*

$$U_C = \left[\prod_{m=1}^{d-1}\left(\prod_{n=m+1}^{d} \exp\left(i Z_{m,n}\lambda_{n,m}\right)\exp\left(i Y_{m,n}\lambda_{m,n}\right)\right)\right]\cdot\left[\prod_{l=1}^{d-1}\exp(i Z_{l,d}\lambda_{l,l})\right]\,, \tag{9}$$

using $d^2 - 1$ real parameters $\{\lambda_{m,n}\}$[3] in the ranges $\lambda_{m,n} \in [0, \pi]$ for $m > n$, $\lambda_{m,n} \in \left[0, \frac{\pi}{2}\right]$ for $m < n$ and $\lambda_{m,n} \in [0, 2\pi]$ for $m = n$.

Proof: Proving that any $U \in \mathcal{SU}(d)$ may be written as (9) is equivalent to showing that $U_C^\dagger U = \mathbb{1}$ can be achieved for all group elements. Let $U = \sum_{r,s=1}^{d} a_{r,s}|r\rangle\langle s|$ be an arbitrary special unitary operator, i.e., U fulfils $\sum_{i=1}^{d} a_{m,i}^* a_{n,i} = \sum_{i=1}^{d} a_{i,m}^* a_{i,n} = \delta_{mn}$ and $\det U = 1$. The conjugate transpose

of U_C as given in (9) using the abbreviation (7) is

$$U_C^\dagger = \left[\prod_{l=1}^{d-1} \exp(-i\, Z_{d-l,d}\lambda_{d-l,d-l})\right] \cdot \left[\prod_{m=1}^{d-1}\left(\prod_{n=1}^{m} \Lambda_{d-m,d+1-n}^\dagger\right)\right] . \tag{10}$$

The order of the factors in $U_C^\dagger$ implies that $\Lambda_{1,2}^\dagger$ acts first on U. For $U' = \Lambda_{1,2}^\dagger U = \sum_{r,s=1}^d a'_{r,s} |r\rangle \langle s|$, one obtains

$$a'_{1,s} = e^{-i\lambda_{2,1}} \cos(\lambda_{1,2}) a_{1,s} - e^{i\lambda_{2,1}} \sin(\lambda_{1,2}) a_{2,s} , \tag{11}$$

$$a'_{2,s} = e^{-i\lambda_{2,1}} \sin(\lambda_{1,2}) a_{1,s} + e^{i\lambda_{2,1}} \cos(\lambda_{1,2}) a_{2,s} . \tag{12}$$

All other components remain unchanged, i.e., $a'_{r,s} = a_{r,s}$ for $r > 2$ if $d > 2$. We observe that $a'_{2,1}$ can always be made zero using particular values for $\lambda_{1,2}$ and $\lambda_{2,1}$: In case $a_{1,1}$ and $a_{2,1}$ both are zero, both parameters $\lambda_{1,2}$ and $\lambda_{2,1}$ can be chosen freely. If only $a_{1,1} = 0$, one chooses $\lambda_{1,2} = \frac{\pi}{2}$. If both are unequal zero, then $a'_{2,1}$ vanishes for

$$\arg(e^{i2\lambda_{2,1}} a_{2,1}) = \arg(-a_{1,1}) , \tag{13}$$

$$\tan(\lambda_{1,2}) = \frac{|a_{2,1}|}{|a_{1,1}|} . \tag{14}$$

This can always be achieved with $\lambda_{2,1} \in [0, \pi]$ and $\lambda_{1,2} \in [0, \frac{\pi}{2}]$. Analogously, one can make the component $a''_{3,1}$ of $U'' = \Lambda_{1,3}^\dagger U'$ zero for the case $d > 2$. In this way, all components $\overline{a}_{r,s}$ with $r > s$ of $\overline{U} = \prod_{m=1}^{d-1}\left(\prod_{n=1}^{m} \Lambda_{d-m,d+1-n}^\dagger\right) U = \sum_{r,s=1}^d \overline{a}_{r,s} |r\rangle \langle s|$ can be made zero. The unitarity constraints $\sum_{i=1}^d \overline{a}_{m,i}^* \overline{a}_{n,i} = \sum_{i=1}^d \overline{a}_{i,m}^* \overline{a}_{i,n} = \delta_{mn}$ imply that also all $\overline{a}_{r,s}$ with $r < s$ have become zero during this procedure. Hence, $\overline{U}$ is diagonal $\overline{U} = \sum_{r=1}^d \overline{a}_{r,r} |r\rangle \langle r|$, where $\overline{a}_{r,r}$ are complex numbers of magnitude one, i.e., $\overline{a}_{r,r} = e^{i\alpha_r}$. The first $d - 1$ phases $\alpha_1, \ldots, \alpha_{d-1}$ can be compensated via $\left[\prod_{l=1}^{d-1} \exp(-i\, Z_{d-l,d}\lambda_{d-l,d-l})\right] \overline{U}$ by choosing $\lambda_{r,r} = \alpha_r$. This is guaranteed to be achievable with $\lambda_{r,r} \in [0, 2\pi]$. Recall that so far we have only multiplied special unitary operators implying that $U_C^\dagger U = \left[\prod_{l=1}^{d-1} \exp(-i\, Z_{d-l,d}\lambda_{d-l,d-l})\right] \overline{U}$ is still a member of $\mathcal{SU}(d)$. We have achieved that $U_C^\dagger U$ is diagonal and that the first $d - 1$ diagonal entries are all equal 1. Now, the fact that $\det(U_C^\dagger U) = 1$ still holds implies that also the last diagonal entry equals 1. Hence, $U_C^\dagger U = \mathbb{1}$, which proves the theorem. □

A. Remarks on the composite parameterization

It is worth mentioning some properties of the composite parameterization. In our previous paper[8] on the parameterization of $\mathcal{U}(d)$, we have shown that it can be rather insightful to gather the parameters $\lambda_{m,n}$ in a matrix

$$\text{relative phases} \rightarrow \begin{bmatrix} \lambda_{1,1} & \cdots & \lambda_{1,d} \\ \vdots & \ddots & \vdots \\ \lambda_{d,1} & \cdots & \lambda_{d,d} \end{bmatrix} \leftarrow \text{rotations} \quad . \tag{15}$$

In this notation, the lower left entries represent relative phase shifts, the diagonal global phase shifts and the upper right rotations (with respect to the computational basis $\{|1\rangle, \ldots, |d\rangle\}$). Using this representation is particularly useful for illustrating which parameters are irrelevant for certain tasks. For instance, we have shown that for parameterizing an orthonormal set of k vectors $\{|\Psi_1\rangle, \ldots,$

$|\Psi_k\rangle\}$ only the $k(2d - k - 1)$ non-zero parameters of the following matrix are relevant:

$$\left[\begin{array}{cccccc} 0 & \lambda_{1,2} & \cdots & \lambda_{1,k+1} & \cdots & \lambda_{1,d} \\ \lambda_{2,1} & \ddots & \ddots & \vdots & \ddots & \vdots \\ \vdots & \ddots & 0 & \lambda_{k,k+1} & \cdots & \lambda_{k,d} \\ \lambda_{k+1,1} & \cdots & \lambda_{k+1,k} & 0 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ \lambda_{d,1} & \cdots & \lambda_{d,k} & 0 & \cdots & 0 \end{array}\right] \begin{array}{l} \left.\begin{array}{l} \\ \\ \\ \end{array}\right\} k \\ \left.\begin{array}{l} \\ \\ \\ \end{array}\right\} d-k \end{array} \tag{16}$$

$$\underbrace{\qquad\qquad}_{k} \quad \underbrace{\qquad\qquad\qquad}_{d-k} \qquad .$$

A similar example was given for parameterizing the set of k-dimensional subspaces in $\mathbb{C}^d$ where the corresponding $2k(d - k)$ relevant parameters $\lambda_{m,n}$ were illustrated. For the composite parameterization of the special unitary group $\mathcal{SU}(d)$ all this remains valid as the operations (5) and (7) are equivalent up to a global phase and are applied in the same order in both cases. Using this matrix representation for the special unitary group, one should only keep in mind that there is no diagonal element $\lambda_{d,d}$.

Let us illustrate another important feature of the composite parameterization. The $(d - k)^2$ or $(d - k)^2 - 1$, respectively, non-zero parameters

$$\left[\begin{array}{cccccc} 0 & 0 & \cdots & 0 & \cdots & 0 \\ 0 & \ddots & \ddots & \vdots & \ddots & \vdots \\ \vdots & \ddots & 0 & 0 & \cdots & 0 \\ 0 & \cdots & 0 & \lambda_{k+1,k+1} & \cdots & \lambda_{k+1,d} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & 0 & \lambda_{d,k+1} & \cdots & \lambda_{d,d} \end{array}\right] \begin{array}{l} \left.\begin{array}{l} \\ \\ \\ \end{array}\right\} k \\ \left.\begin{array}{l} \\ \\ \\ \end{array}\right\} d-k \end{array} \tag{17}$$

$$\underbrace{\qquad\qquad}_{k} \quad \underbrace{\qquad\qquad\qquad}_{d-k}$$

correspond to the (special) unitary group for the $(d - k)$-dimensional subspace defined by $\text{span}(|k+1\rangle, \ldots, |d\rangle)$. This directly follows from the correct number of required parameters in combination with the fact that the subspace $\text{span}(U_C|1\rangle, \ldots, U_C|k\rangle)$ is independent of the illustrated parameters. Note that this feature will be helpful in an upcoming proof.

IV. HAAR MEASURE ON THE UNITARY GROUP $\mathcal{U}(d)$

Let us now assign an infinitesimal volume element dU_d to the unitary group $\mathcal{U}(d)$ in terms of the composite parameterization $U_C = U_C(\lambda_{1,1}, \ldots, \lambda_{d,d})$. This can be achieved by determining the associated Haar measure. This means that, as for any compact Lie group, we must find a measure of volume which is left and right invariant.[36,37] Explicitly, we require that dU_d satisfies

$$dU_d = d(U_C) = d(U_1 U_C) = d(U_C U_2)\,, \tag{18}$$

for all $U_1, U_2 \in \mathcal{U}(d)$. Generally, an invariant measure is (up to an irrelevant constant) determined by the absolute value of the Jacobian determinant

$$J_d = \left|\det(j_{k,l})\right| = \left|\det \frac{\partial(u_1, \ldots, u_{d^2})}{\partial(\alpha_1, \ldots, \alpha_{d^2})}\right|\,, \tag{19}$$

wherein $\{u_k\}$ are coefficients of the unitary $U = U(\alpha_1, \ldots, \alpha_{d^2})$ expanded in an orthogonal operator basis $\{b_k\}$ of $\mathbb{C}^d \times \mathbb{C}^d$, i.e.,

$$u_k = \frac{\mathrm{Tr}(b_k^\dagger U)}{\mathrm{Tr}(b_k^\dagger b_k)} \qquad \left(\Rightarrow U = \sum_{k=1}^{d^2} u_k b_k \right) , \tag{20}$$

and where $\{\alpha_l\}$ are any d^2 parameters that cover $\mathcal{U}(d)$. Here, a left or right translation $U_1, U_2 \in \mathcal{U}(d)$ merely induces a unitary basis transformation of $\{b_k\}$ which is length and angle preserving. Hence, J_d is invariant under these transformations and

$$dU_d = J_d \prod_{l=1}^{d^2} d\alpha_l \tag{21}$$

is a Haar measure.[4] Our aim is to derive a general expression of dU_d for arbitrary d in terms of the parameterization introduced in Sec. II, i.e.,

$$dU_d = \frac{J_d}{N_d} \prod_{k,l=1}^{d} d\lambda_{k,l} , \tag{22}$$

where N_d is a normalization constant such that $\int_{\mathcal{U}(d)} dU_d = 1$. We obtain the following.

Theorem 3: *In terms of the d^2 parameters $\lambda_{m,n}$ introduced in Theorem 1, the (normalized) Haar measure on the unitary group $\mathcal{U}(d)$ reads*

$$dU_d = \frac{1}{N_d} \prod_{m=1}^{d-1} \prod_{n=m+1}^{d} \sin(\lambda_{m,n}) \cos^{2(n-m)-1}(\lambda_{m,n}) \prod_{k,l=1}^{d} d\lambda_{k,l} , \tag{23}$$

with

$$N_d = \frac{(2\pi)^{d(d+1)/2}}{\prod_{m=1}^{d-1} \prod_{n=m+1}^{d} 2(n-m)} \tag{24}$$

such that $\int_{\mathcal{U}(d)} dU_d = 1$.

Proof: For simplicity, let us start with the case $d = 2$. Using the canonical operator basis $\{b_k\}$ $= \{|1\rangle\langle 1|, |1\rangle\langle 2|, |2\rangle\langle 1|, |2\rangle\langle 2|\}$ and the order of the parameters $\{\alpha_l\} = \{\lambda_{1,1}, \lambda_{1,2}, \lambda_{2,1}, \lambda_{2,2}\}$, we obtain the Jacobian matrix

$$\frac{\partial(u_1, u_2, u_3, u_4)}{\partial(\lambda_{1,1}, \lambda_{1,2}, \lambda_{2,1}, \lambda_{2,2})} = \tag{25}$$

$$\begin{pmatrix} ie^{i\lambda_{1,1}} \cos\lambda_{1,2} & -e^{i\lambda_{1,1}} \sin\lambda_{1,2} & 0 & 0 \\ 0 & e^{i\lambda_{2,2}} \cos\lambda_{1,2} & 0 & ie^{i\lambda_{2,2}} \sin\lambda_{1,2} \\ -ie^{i\lambda_{1,1}+i\lambda_{2,1}} \sin\lambda_{1,2} & -e^{i\lambda_{1,1}+i\lambda_{2,1}} \cos\lambda_{1,2} & -ie^{i\lambda_{1,1}+i\lambda_{2,1}} \sin\lambda_{1,2} & 0 \\ 0 & -e^{i\lambda_{2,1}+i\lambda_{2,2}} \sin\lambda_{1,2} & ie^{i\lambda_{2,1}+i\lambda_{2,2}} \cos\lambda_{1,2} & ie^{i\lambda_{2,1}+i\lambda_{2,2}} \cos\lambda_{1,2} \end{pmatrix} .$$

Using the Laplace expansion and elementary simplifications, one finds

$$J_2 = 2\sin(\lambda_{1,2})\cos(\lambda_{1,2}) = \sin(2\lambda_{1,2}) . \tag{26}$$

The relation (22) combined with normalization

$$\int_{\lambda_{2,2}=0}^{2\pi} \int_{\lambda_{2,1}=0}^{2\pi} \int_{\lambda_{1,2}=0}^{\pi/2} \int_{\lambda_{1,1}=0}^{2\pi} \frac{J_2}{N_2} d\lambda_{1,1} d\lambda_{1,2} d\lambda_{2,1} d\lambda_{2,2} = 1 , \tag{27}$$

yields the normalized Haar measure

$$dU_2 = \frac{1}{4\pi^3} \sin(\lambda_{1,2}) \cos(\lambda_{1,2}) d\lambda_{1,1} d\lambda_{1,2} d\lambda_{2,1} d\lambda_{2,2} , \tag{28}$$

which is in accordance with Theorem 3.

One could in principle compute dU_d analogously for arbitrary d, i.e., using the canonical operator basis $\{b_k\} = \{|1\rangle\langle 1|, |1\rangle\langle 2|, |1\rangle\langle 3|, \ldots, |d\rangle\langle d-1|, |d\rangle\langle d|\}$ and the naive order $\{\alpha_l\} = \{\lambda_{1,1}, \lambda_{1,2}, \lambda_{1,3}, \ldots, \lambda_{d,d-1}, \lambda_{d,d}\}$. For instance, a long and cumbersome computation reveals that

$$dU_3 = \frac{1}{4\pi^6} \sin(\lambda_{1,2}) \cos(\lambda_{1,2}) \sin(\lambda_{1,3}) \cos^3(\lambda_{1,3}) \sin(\lambda_{2,3}) \cos(\lambda_{2,3}) \prod_{k,l=1}^{3} d\lambda_{k,l} \tag{29}$$

demonstrating the validity of Theorem 3 for $d = 3$. Unfortunately, in this way, computing the determinant of the $d^2 \times d^2$ Jacobian matrix becomes increasingly unfeasible the larger d gets. More importantly, this approach is not suitable to prove a general expression such as (23) for all d. However, the Jacobian matrix can be considerably simplified by taking into account the invariance of the Haar measure, the structure of the composite parameterization as well as the freedom in the choice of the operator basis and the order of the derivatives $\partial/\partial\lambda_{x,y}$. In this way, the correctness of Theorem 3 can be verified for all d.

First, due to the left invariance of the Jacobian determinant $J_d = \left|\det(j_{k,l})\right|$, we are allowed to perform any transformation

$$j_{k,l} = \frac{\partial u_k}{\partial \alpha_l} = \frac{\mathrm{Tr}(b_k^\dagger \frac{\partial U}{\partial \alpha_l})}{\mathrm{Tr}(b_k^\dagger b_k)} \quad \longrightarrow \quad j'_{k,l} = \frac{\mathrm{Tr}(b_k^\dagger U_1 \frac{\partial U}{\partial \alpha_l})}{\mathrm{Tr}(b_k^\dagger b_k)} \tag{30}$$

with $U_1 \in \mathcal{U}(d)$. Here, it is beneficial to choose $U_1 = -iU_C^\dagger$ since the matrix $-iU_C^\dagger \frac{\partial U_C}{\partial \lambda_{x,y}}$ has a simpler form due to the fact that $U_C^\dagger$ and $\frac{\partial U_C}{\partial \lambda_{x,y}}$ cancel each other out partially. For instance, since all projectors $P_l = |l\rangle\langle l|$ commute, for any derivative with respect to a global phase transformation $\partial/\partial\lambda_{l,l}$ one obtains

$$-iU_C^\dagger \frac{\partial U_C}{\partial \lambda_{l,l}} = -iU_C^\dagger U_C i P_l = P_l = |l\rangle\langle l| \ . \tag{31}$$

As can directly be inferred from the structure of U_C (3), the derivatives $\partial U_C/\partial\lambda_{x,y}$ are

$$\left[\prod_{m=1}^{x-1}\prod_{n=m+1}^{d} \Lambda_{m,n}\right]\left[\prod_{n=x+1}^{y} \Lambda_{x,n}\right] i Y_{x,y} \left[\prod_{n=y+1}^{d} \Lambda_{x,n}\right]\left[\prod_{m=x+1}^{d-1}\prod_{n=m+1}^{d} \Lambda_{m,n}\right]\prod_{l=1}^{d} \exp(i P_l \lambda_{l,l})$$

for $x < y$, and

$$\left[\prod_{m=1}^{y-1}\prod_{n=m+1}^{d} \Lambda_{m,n}\right]\left[\prod_{n=y+1}^{x-1} \Lambda_{y,n}\right] i P_x \left[\prod_{n=x}^{d} \Lambda_{y,n}\right]\left[\prod_{m=y+1}^{d-1}\prod_{n=m+1}^{d} \Lambda_{m,n}\right]\prod_{l=1}^{d} \exp(i P_l \lambda_{l,l})$$

for $x > y$. Consequently, if we apply $-iU_C^\dagger$ from the left, the products to the left of $iY_{x,y}$ (respectively, iP_x) cancel out and we get

$$-iU_C^\dagger \frac{\partial U_C}{\partial \lambda_{x,y}} = \begin{cases} U_{x,y}^\dagger Y_{x,y} U_{x,y} & \text{for } x < y \ , \\ U_{x,y}^\dagger P_x U_{x,y} & \text{for } x > y \ , \end{cases} \tag{32}$$

where

$$U_{x,y} = \begin{cases} \left[\prod_{n=y+1}^{d} \Lambda_{x,n}\right]\left[\prod_{m=x+1}^{d-1}\prod_{n=m+1}^{d} \Lambda_{m,n}\right]\prod_{l=x}^{d} \exp(i P_l \lambda_{l,l}) & \text{for } x < y \ , \\ \left[\prod_{n=x}^{d} \Lambda_{y,n}\right]\left[\prod_{m=y+1}^{d-1}\prod_{n=m+1}^{d} \Lambda_{m,n}\right]\prod_{l=y}^{d} \exp(i P_l \lambda_{l,l}) & \text{for } x > y \ . \end{cases} \tag{33}$$

Here, it is important to realize that $U_{x,y}^\dagger Y_{x,y} U_{x,y}$ and $U_{x,y}^\dagger P_x U_{x,y}$ do no longer contain operations $\Lambda_{m,n}$ with $m < \min\{x, y\}$, meaning that there are no off-diagonal elements $|m\rangle\langle n|$ and $|n\rangle\langle m|$ with $m < \min\{x, y\}$. This and the observation (31) imply that when we choose the following orthogonal

operator basis and order:

$$
\begin{aligned}
b_1 &= |1\rangle\langle 2| + |2\rangle\langle 1| \ , & \alpha_1 &= \lambda_{2,1} \ , \\
b_2 &= -i\,|1\rangle\langle 2| + i\,|2\rangle\langle 1| \ , & \alpha_2 &= \lambda_{1,2} \ , \\
b_3 &= |1\rangle\langle 3| + |3\rangle\langle 1| \ , & \alpha_3 &= \lambda_{3,1} \ , \\
b_4 &= -i\,|1\rangle\langle 3| + i\,|3\rangle\langle 1| \ , & \alpha_4 &= \lambda_{1,3} \ , \\
&\vdots & &\vdots \\
b_{2(d-1)-1} &= |1\rangle\langle d| + |d\rangle\langle 1| \ , & \alpha_{2(d-1)-1} &= \lambda_{d,1} \ , \\
b_{2(d-1)} &= -i\,|1\rangle\langle d| + i\,|d\rangle\langle 1| \ , & \alpha_{2(d-1)} &= \lambda_{1,d} \ , \\
b_{2(d-1)+1} &= |2\rangle\langle 3| + |3\rangle\langle 2| \ , & \alpha_{2(d-1)+1} &= \lambda_{3,2} \ , \\
b_{2(d-1)+2} &= -i\,|2\rangle\langle 3| + i\,|3\rangle\langle 2| \ , & \alpha_{2(d-1)+2} &= \lambda_{2,3} \ , \\
b_{2(d-1)+3} &= |2\rangle\langle 4| + |4\rangle\langle 2| \ , & \alpha_{2(d-1)+3} &= \lambda_{4,2} \ , \\
b_{2(d-1)+4} &= -i\,|2\rangle\langle 4| + i\,|4\rangle\langle 2| \ , & \alpha_{2(d-1)+4} &= \lambda_{2,4} \ , \\
&\vdots & &\vdots \\
b_{d^2-d-1} &= |d-1\rangle\langle d| + |d\rangle\langle d-1| \ , & \alpha_{d^2-d-1} &= \lambda_{d,d-1} \ , \\
b_{d^2-d} &= -i\,|d-1\rangle\langle d| + i\,|d\rangle\langle d-1| \ , & \alpha_{d^2-d} &= \lambda_{d-1,d} \ , \\
b_{d^2-d+1} &= |1\rangle\langle 1| \ , & \alpha_{d^2-d+1} &= \lambda_{1,1} \ , \\
b_{d^2-d+2} &= |2\rangle\langle 2| \ , & \alpha_{d^2-d+2} &= \lambda_{2,2} \ , \\
&\vdots & &\vdots \\
b_{d^2} &= |d\rangle\langle d| \ , & \alpha_{d^2} &= \lambda_{d,d} \ ,
\end{aligned}
\tag{34}
$$

the Jacobian matrix becomes a lower block-triangular matrix as graphically illustrated in Figure 1.

Thus, the Jacobian determinant simplifies to a product of the determinants of the blocks M_i and D, i.e.,

$$
J_d = \left|\det(j'_{k,l})\right| = \left(\prod_{i=1}^{d-1} |\det M_i|\right) |\det D| \ . \tag{35}
$$

Furthermore, we have that $|\det D| = 1$ since D is a $d \times d$ identity matrix due to (31) and the choice (34). It now remains to investigate the blocks M_i. Let us first consider $-iU_C^\dagger \frac{\partial U_C}{\partial \lambda_{x,y}}$ for the Hilbert

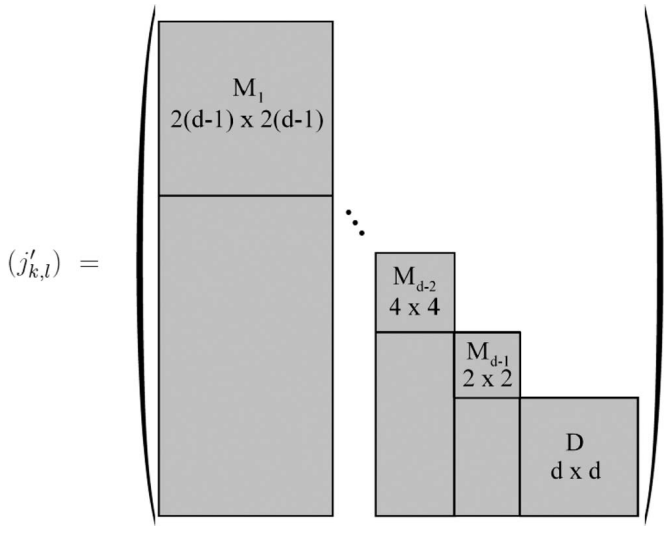

FIG. 1. Schematic illustration of the Jacobian matrix $(j'_{k,l})$ for the operator basis (34). All entries outside the gray-shaded blocks are zero.

space $\mathcal{H}' = \mathbb{C}^{d-1}$ whose dimension is lower by one. In this case, we have

$$-iU_C^\dagger \frac{\partial U_C}{\partial \lambda_{x,y}} = \begin{cases} U_{x,y}^\dagger Y_{x,y} U_{x,y} & \text{for } x < y, \\ U_{x,y}^\dagger P_x U_{x,y} & \text{for } x > y\,, \end{cases} \tag{36}$$

where

$$U_{x,y} = \begin{cases} \left[\prod_{n=y+1}^{d-1} \Lambda_{x,n}\right]\left[\prod_{m=x+1}^{d-2}\prod_{n=m+1}^{d-1} \Lambda_{m,n}\right]\prod_{l=x}^{d-1} \exp(i\,P_l \lambda_{l,l}) & \text{for } x < y, \\ \left[\prod_{n=x}^{d-1} \Lambda_{y,n}\right]\left[\prod_{m=y+1}^{d-2}\prod_{n=m+1}^{d-1} \Lambda_{m,n}\right]\prod_{l=y}^{d-1} \exp(i\,P_l \lambda_{l,l}) & \text{for } x > y\,. \end{cases} \tag{37}$$

By substituting $\lambda_{m,n} \to \lambda_{m+1,n+1}$, $|m\rangle \to |m+1\rangle$ and $\langle m| \to \langle m+1|$, one can directly see that these matrices are equal to $-iU_C^\dagger \frac{\partial U_C}{\partial \lambda_{x,y}}$ with $x, y \geq 2$ and U_C for the Hilbert space $\mathcal{H} = \mathbb{C}^d$ of full dimension d. Hence, since $J_d = |\det M_1| \prod_{i=2}^{d-1} |\det M_i|$ we have established the recursion formula

$$J_d = |\det M_1|\, J_{d-1}\,, \tag{38}$$

where the parameters in J_{d-1} are to be substituted according to $\lambda_{m,n} \to \lambda_{m+1,n+1}$. This relation is a direct consequence of the fact that each $-iU_C^\dagger \frac{\partial U_C}{\partial \lambda_{x,y}}$ with $x, y \geq 2$ only contains parameters $\lambda_{m,n}$ with $m, n \geq 2$. As discussed in Sec. III A the set of $(d-1)^2$ parameters $\lambda_{m,n}$ satisfying $m, n \geq 2$ correspond to the unitary group $\mathcal{U}(d-1)$ for the $(d-1)$-dimensional subspace span$(|2\rangle, \ldots, |d\rangle)$. Consequently, (38) simply reflects the well-known fact[9,19] that the infinitesimal volume element dU_d on $\mathcal{U}(d)$ is the product of the infinitesimal volume element dU_{d-1} on $\mathcal{U}(d-1)$ times a to-be-determined function $g(d)$, i.e.,

$$dU_d = g(d) dU_{d-1}\,. \tag{39}$$

Now, due to the above mentioned reasons, for the composite parameterization dU_{d-1} is a function of the parameters $\lambda_{m,n}$ with $m, n \geq 2$. In addition to that, g(d) is a function of the $2d-1$ parameters $\{\lambda_{1,1}, \lambda_{1,2}, \ldots, \lambda_{1,d}\}$ and $\{\lambda_{2,1}, \ldots, \lambda_{d,1}\}$ since they extend the unitary group $\mathcal{U}(d-1)$ acting on span$(|2\rangle, \ldots, |d\rangle)$ to the entire $\mathcal{U}(d)$ on $\mathcal{H} = \mathbb{C}^d$, hence, $g(d) = g(d; \lambda_{1,1}, \lambda_{1,2}, \ldots, \lambda_{1,d}; \lambda_{2,1}, \ldots, \lambda_{d,1})$. For the sake of clarity, let us illustrate this by the example $dU_2 \to dU_3$ by comparing (28) and (29): dU_2 is (up to a constant) given by $\sin\lambda_{1,2}\cos\lambda_{1,2} d\lambda_{1,1} d\lambda_{1,2} d\lambda_{2,1} d\lambda_{2,2}$. According to our considerations, dU_3 must contain the same expression in terms of $\lambda_{2,2}$, $\lambda_{2,3}$, $\lambda_{3,2}$, $\lambda_{3,3}$ and it must look like

$$dU_3 \sim g(3; \lambda_{1,1}, \lambda_{1,2}, \lambda_{1,3}; \lambda_{2,1}, \lambda_{3,1}) \sin\lambda_{2,3}\cos\lambda_{2,3} d\lambda_{2,2} d\lambda_{2,3} d\lambda_{3,2} d\lambda_{3,3}\,. \tag{40}$$

Equation (29) shows that this is indeed the case since it can easily be observed that

$$g(3; \lambda_{1,1}, \lambda_{1,2}, \lambda_{1,3}; \lambda_{2,1}, \lambda_{3,1}) \sim \sin\lambda_{1,2}\cos\lambda_{1,2}\sin\lambda_{1,3}\cos^3\lambda_{1,3} d\lambda_{1,1} d\lambda_{1,2} d\lambda_{1,3} d\lambda_{2,1} d\lambda_{3,1}\,.$$

It now remains to find a general expression for $|\det M_1|$ for arbitrary d, since the formula of J_d can then be derived via (38) and induction. In general, the matrix M_1 does not have a simple form which makes it difficult to compute its determinant. Here, it is useful to exploit that, first, there is no explicit dependence of J_d on parameters corresponding to phase operations, i.e., all $\lambda_{m,n}$ with $m \geq n$. This can directly be followed from the construction of the composite parameterization in combination with the Haar measure on $\mathcal{U}(2)$ and the Jacobian matrix (25). Since in the Jacobian matrix (25) and in its determinant the phase operations $\lambda_{1,1}$, $\lambda_{2,1}$, $\lambda_{2,2}$ only appear as $e^{i\lambda_{1,1}}, e^{i\lambda_{2,1}}, e^{i\lambda_{2,2}}$, i.e., complex numbers of magnitude 1, and since in the end we are only interested in the absolute value of this determinant, it is clear that dU_2 (28) is independent of these parameters. As the composite parameterization only combines $\mathcal{U}(2)$-operations by incorporating all possible 2-dimensional subspaces in $\mathbb{C}^d$ the same statement holds of course true for all d (see, for instance, (29) for the case $d = 3$). Second, the circumstance that $g(d)$ is independent of all parameters $\lambda_{m,n}$ with $\min\{m, n\} \geq 2$ implies that these parameters do not affect $|\det M_1|$.[5] For these reasons, one can set the parameters $\lambda_{m,n}$ with $\min\{m, n\} \geq 2$ and $m \geq n$ to zero in (33) without altering $|\det M_1|$, i.e.,

$$|\det M_1| = \left|\det\left(M_1|_{\{\lambda_{m,n}=0 | (m,n) \notin \{(1,2),\ldots,(1,d)\}\}}\right)\right| \equiv |\det \overline{M}_1|\,. \tag{41}$$

Here, (32) reduces to

$$U_{1,y}^{\dagger} Y_{1,y} U_{1,y}\Big|_{\{\lambda_{m,n}=0|(m,n)\notin\{(1,2),\ldots,(1,d)\}\}} = \left[\prod_{n=y+1}^{d} \exp(iY_{1,n}\lambda_{1,n})\right]^{\dagger} Y_{1,y} \left[\prod_{n=y+1}^{d} \exp(iY_{1,n}\lambda_{1,n})\right] ,$$
$$\equiv O_{1,y}^{T} Y_{1,y} O_{1,y},$$
$$U_{x,1}^{\dagger} P_x U_{x,1}\Big|_{\{\lambda_{m,n}=0|(m,n)\notin\{(1,2),\ldots,(1,d)\}\}} = \left[\prod_{n=x}^{d} \exp(iY_{1,n}\lambda_{1,n})\right]^{\dagger} P_x \left[\prod_{n=x}^{d} \exp(iY_{1,n}\lambda_{1,n})\right] ,$$
$$\equiv O_{x,1}^{T} P_x O_{x,1} ,$$

where $O_{x,1}$ and $O_{1,y}$ are orthogonal (real) matrices since they are a product of the operations $\exp(iY_{1,n}\lambda_{1,n})$ which explicitly read

$$\cos(\lambda_{1,n})\,|1\rangle\langle 1| + \sin(\lambda_{1,n})\,|1\rangle\langle n| - \sin(\lambda_{1,n})\,|n\rangle\langle 1| + \cos(\lambda_{m,n})\,|n\rangle\langle n| + \sum_{k\neq 1,n} |k\rangle\langle k| \ . \tag{42}$$

According to (34), the $2(d-1)\times 2(d-1)$ elements of $\overline{M}_1$ are now determined by

$$\mathrm{Tr}\left(b_k^{\dagger} O_{1,y}^{T} Y_{1,y} O_{1,y}\right) = \mathrm{Tr}\left(O_{1,y} b_k^{\dagger} O_{1,y}^{T} Y_{1,y}\right) \tag{43}$$

and

$$\mathrm{Tr}\left(b_k^{\dagger} O_{x,1}^{T} P_x O_{x,1}\right) = \mathrm{Tr}\left(O_{x,1} b_k^{\dagger} O_{x,1}^{T} P_x\right) \tag{44}$$

with $x, y \in \{2,\ldots,d\}$, and

$$b_k = b_k^{\dagger} = \begin{cases} |1\rangle\langle(k+3)/2| + |(k+3)/2\rangle\langle 1| & = X_{1,(k+3)/2} \quad k\text{ - odd}, \\ -i\,|1\rangle\langle(k+2)/2| + i\,|(k+2)/2\rangle\langle 1| & = Y_{1,(k+2)/2} \quad k\text{ - even}, \end{cases} \tag{45}$$

with $k \in \{1,\ldots,2(d-1)\}$. Now consider the coefficients (43) and (44) depending on different $X_{1,m}$ and $Y_{1,m}$ $(2 \le m \le d)$ of (45).

• $\mathrm{Tr}\left(O_{1,y} X_{1,m} O_{1,y}^{T} Y_{1,y}\right)$ for arbitrary m:

$$\mathrm{Tr}\left(O_{1,y} X_{1,m} O_{1,y}^{T} Y_{1,y}\right) = 0 . \tag{46}$$

Note: $O_{1,y} X_{1,m} O_{1,y}^{T}$ is symmetric, while $Y_{1,y}$ is antisymmetric.

• $\mathrm{Tr}\left(O_{1,y} Y_{1,m} O_{1,y}^{T} Y_{1,y}\right)$ for $m < y$:

$$\mathrm{Tr}\left(O_{1,y} Y_{1,m} O_{1,y}^{T} Y_{1,y}\right) = 0 . \tag{47}$$

Note: $O_{1,y} Y_{1,m} O_{1,y}^{T}$ is orthogonal to $Y_{1,y}$ for $m < y$ since the product in $O_{1,y} = \prod_{n=y+1}^{d} \exp(iY_{1,n}\lambda_{1,n})$ starts with $n = y+1$.

• $\mathrm{Tr}\left(O_{x,1} Y_{1,m} O_{x,1}^{T} P_x\right)$ for arbitrary m:

$$\mathrm{Tr}\left(O_{x,1} Y_{1,m} O_{x,1}^{T} P_x\right) = \langle x|\, O_{x,1} Y_{1,m} O_{x,1}^{T}\, |x\rangle , \tag{48}$$

$$= -i\,\langle x|\, O_{x,1}\, |1\rangle\langle m|\, O_{x,1}^{T}\, |x\rangle + i\,\langle x|\, O_{x,1}\, |m\rangle\langle 1|\, O_{x,1}^{T}\, |x\rangle , \tag{49}$$

$$= 0 . \tag{50}$$

Note: $O_{x,1}$ is an orthogonal (real) matrix.

• $\mathrm{Tr}\left(O_{x,1}X_{1,m}O_{x,1}^T P_x\right)$ for $m < x$:

$$\mathrm{Tr}\left(O_{x,1}X_{1,m}O_{x,1}^T P_x\right) = \langle x|\, O_{x,1}X_{1,m}O_{x,1}^T\, |x\rangle \ , \tag{51}$$

$$= \langle x|\, O_{x,1}\, |1\rangle\, \langle m|\, O_{x,1}^T\, |x\rangle + \langle x|\, O_{x,1}\, |m\rangle\, \langle 1|\, O_{x,1}^T\, |x\rangle \ , \tag{52}$$

$$= 0\ . \tag{53}$$

Note: $O_{x,1} = \prod_{n=x}^{d} \exp(iY_{1,n}\lambda_{1,n})$ has no off-diagonal elements $\langle x|O_{x,1}|m\rangle$ for $m < x$.

These four observations imply for the operator basis and parameter order

$$\begin{aligned}
b_1 &= |1\rangle\langle 2| + |2\rangle\langle 1| \ , & \alpha_1 &= \lambda_{2,1}\ ,\\
b_2 &= -i\,|1\rangle\langle 2| + i\,|2\rangle\langle 1| \ , & \alpha_2 &= \lambda_{1,2}\ ,\\
b_3 &= |1\rangle\langle 3| + |3\rangle\langle 1| \ , & \alpha_3 &= \lambda_{3,1}\ ,\\
b_4 &= -i\,|1\rangle\langle 3| + i\,|3\rangle\langle 1| \ , & \alpha_4 &= \lambda_{1,3}\ ,\\
&\vdots & &\vdots\\
b_{2(d-1)-1} &= |1\rangle\langle d| + |d\rangle\langle 1| \ , & \alpha_{2(d-1)-1} &= \lambda_{d,1}\ ,\\
b_{2(d-1)} &= -i\,|1\rangle\langle d| + i\,|d\rangle\langle 1| \ , & \alpha_{2(d-1)} &= \lambda_{1,d}\ ,
\end{aligned} \tag{54}$$

that $\overline{M}_1$ is a lower triangular matrix (see Figure 2). For the determinant we can now restrict on determining the diagonal entries of $\overline{M}_1$ which are given by

• $\mathrm{Tr}\big(O_{1,y}Y_{1,m}O_{1,y}^T Y_{1,y}\big)/\mathrm{Tr}(Y_{1,m}^2)$ for $m = y$:

$$\mathrm{Tr}\left(O_{1,m}Y_{1,m}O_{1,m}^T Y_{1,m}\right) = \langle 1|\, O_{1,m}Y_{1,m}O_{1,m}^T Y_{1,m}\, |1\rangle + \langle m|\, O_{1,m}Y_{1,m}O_{1,m}^T Y_{1,m}\, |m\rangle \ , \tag{55}$$

$$= i\,\langle 1|\, O_{1,m}Y_{1,m}O_{1,m}^T\, |m\rangle - i\,\langle m|\, O_{1,m}Y_{1,m}O_{1,m}^T\, |1\rangle \ , \tag{56}$$

$$\begin{aligned}
&= \langle 1|\, O_{1,m}\, |1\rangle\, \langle m|\, O_{1,m}^T\, |m\rangle - \langle 1|\, O_{1,m}\, |m\rangle\, \langle 1|\, O_{1,m}^T\, |m\rangle\\
&\quad - \langle m|\, O_{1,m}\, |1\rangle\, \langle m|\, O_{1,m}^T\, |1\rangle + \langle m|\, O_{1,m}\, |m\rangle\, \langle 1|\, O_{1,m}^T\, |1\rangle \ ,
\end{aligned} \tag{57}$$

$$= 2\,\langle 1|\, O_{1,m}\, |1\rangle\, \langle m|\, O_{1,m}\, |m\rangle\ . \tag{58}$$

Note: $O_{1,m} = \prod_{n=m+1}^{d} \exp(iY_{1,n}\lambda_{1,n})$ does not have off-diagonal element $\langle 1|O_{1,m}|m\rangle$ since the product starts with $n = m + 1$.

• $\mathrm{Tr}\left(O_{x,1}X_{1,m}O_{x,1}^T P_x\right)/\mathrm{Tr}(X_{1,m}^2)$ for $m = x$:

$$\mathrm{Tr}\left(O_{m,1}X_{1,m}O_{m,1}^T P_m\right) = \langle m|\, O_{m,1}X_{1,m}O_{m,1}^T\, |m\rangle \ , \tag{59}$$

$$\overline{M}_1 = \left(j'_{k,l}\right)_{k,l\,=\,1,\ldots,2(d\,-\,1)} =$$

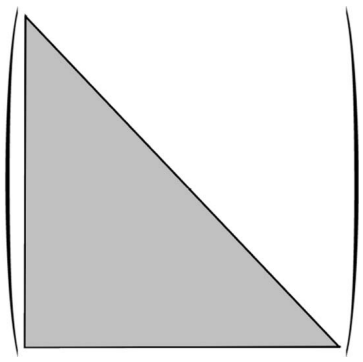

FIG. 2. Schematic illustration of the matrix block $\overline{M}_1$. Only the gray-shaded entries are non-zero.

$$= \langle m|\, O_{m,1}\, |1\rangle \, \langle m|\, O_{m,1}^T\, |m\rangle + \langle m|\, O_{m,1}\, |m\rangle \, \langle 1|\, O_{m,1}^T\, |m\rangle \ , \tag{60}$$

$$= 2\, \langle m|\, O_{m,1}\, |1\rangle \, \langle m|\, O_{m,1}\, |m\rangle \ . \tag{61}$$

We have thus found simple relations between the diagonal entries of $\overline{M}_1$ and the matrix elements ($2 \leq m \leq d$),

$$\langle 1|\, O_{1,m}\, |1\rangle = \prod_{n=m+1}^{d} \cos\lambda_{1,n} \ , \tag{62}$$

$$\langle m|\, O_{1,m}\, |m\rangle = 1 \ , \tag{63}$$

$$\langle m|\, O_{m,1}\, |1\rangle = -\sin\lambda_{1,m} \prod_{n=m+1}^{d} \cos\lambda_{1,n} \ , \tag{64}$$

$$\langle m|\, O_{m,1}\, |m\rangle = \cos\lambda_{1,m} \ , \tag{65}$$

which can easily be obtained via the definitions of $O_{m,1}$ and $O_{1,m}$ together with (42). Hence, since $\mathrm{Tr}(X_{1,m}^2) = \mathrm{Tr}(Y_{1,m}^2) = 2$, we find that the diagonal entries of $\overline{M}_1$ are

$$\mathrm{Tr}\left(O_{1,m} Y_{1,m} O_{1,m}^T Y_{1,m}\right) / \mathrm{Tr}(Y_{1,m}^2) = \prod_{n=m+1}^{d} \cos\lambda_{1,n} \ , \tag{66}$$

$$\mathrm{Tr}\left(O_{m,1} X_{1,m} O_{m,1}^T P_m\right) / \mathrm{Tr}(X_{1,m}^2) = -\sin\lambda_{1,m} \prod_{n=m}^{d} \cos\lambda_{1,n} \ . \tag{67}$$

If we multiply all these entries ($m = 2, \ldots, d$), we finally obtain

$$\left|\det \overline{M}_1\right| = \left[\prod_{k=2}^{d} \left(\prod_{n=k+1}^{d} \cos\lambda_{1,n} \right)\right] \cdot \left[\prod_{l=2}^{d} \left(\sin\lambda_{1,l} \prod_{n=l}^{d} \cos\lambda_{1,n} \right)\right] \ , \tag{68}$$

$$= \prod_{n=2}^{d} \sin(\lambda_{1,n}) \cos^{2(n-1)-1}(\lambda_{1,n}) \ . \tag{69}$$

Using the recursion formula (38) and induction, one finds the final result

$$J_d = \prod_{m=1}^{d-1} \prod_{n=m+1}^{d} \sin(\lambda_{m,n}) \cos^{2(n-m)-1}(\lambda_{m,n}) \ . \tag{70}$$

The corresponding normalizing constant N_d is given by the integral

$$N_d = \int_{\mathcal{U}(d)} J_d \prod_{k,l=1}^{d} d\lambda_{k,l} \ , \tag{71}$$

$$= \int_{\lambda_{k,l}=0}^{2\pi \ (k\geq l)} \int_{\lambda_{k,l}=0}^{\pi/2 \ (k<l)} \left[\prod_{m=1}^{d-1} \prod_{n=m+1}^{d} \sin(\lambda_{m,n}) \cos^{2(n-m)-1}(\lambda_{m,n})\right] \prod_{k,l=1}^{d} d\lambda_{k,l} \ , \tag{72}$$

which can straightforwardly be computed

$$N_d = (2\pi)^{d(d+1)/2} \prod_{m=1}^{d-1} \prod_{n=m+1}^{d} \frac{-1}{2(n-m)} \cos^{2(n-m)}(\lambda_{m,n}) \Big|_{\lambda_{m,n}=0}^{\pi/2} , \tag{73}$$

$$= \frac{(2\pi)^{d(d+1)/2}}{\prod_{m=1}^{d-1} \prod_{n=m+1}^{d} 2(n-m)} . \tag{74}$$

□

V. HAAR MEASURE ON THE SPECIAL UNITARY GROUP $\mathcal{SU}(d)$

Theorem 4: *In terms of the $d^2 - 1$ parameters $\lambda_{m,n}$ introduced in Theorem 2, the (normalized) Haar measure on the special unitary group $\mathcal{SU}(d)$ reads*

$$dU_d = \frac{1}{N_d} \prod_{m=1}^{d-1} \prod_{n=m+1}^{d} \sin(\lambda_{m,n}) \cos^{2(n-m)-1}(\lambda_{m,n}) \prod_{k,l} d\lambda_{k,l} , \tag{75}$$

with

$$N_d = \frac{2^{d-1} \pi^{d(d+1)/2-1}}{\prod_{m=1}^{d-1} \prod_{n=m+1}^{d} 2(n-m)} \tag{76}$$

such that $\int_{\mathcal{SU}(d)} dU_d = 1$.

Proof: The proof is similar to the previous one – only minor modifications have to be made. Given the special unitary group $\mathcal{SU}(d)$ in parameterized form $U(\alpha_1, \ldots, \alpha_{d^2-1})$, to construct the Haar measure one must determine the absolute value $J_d = |\det(j_{k,l})|$ of the determinant of the Jacobian matrix

$$(j_{k,l}) = \frac{\partial(u_1, \ldots, u_{d^2-1})}{\partial(\alpha_1, \ldots, \alpha_{d^2-1})} , \tag{77}$$

wherein $\{u_k\}$ are coefficients of the special unitary operator $U(\alpha_1, \ldots, \alpha_{d^2-1})$ expanded in an orthogonal basis $\{b_k\}$ of traceless operators[6] of $\mathbb{C}^d \times \mathbb{C}^d$, i.e.,

$$u_k = \frac{\mathrm{Tr}(b_k^\dagger U)}{\mathrm{Tr}(b_k^\dagger b_k)} \qquad \left(\Rightarrow \frac{\partial U}{\partial \alpha_l} = \sum_{k=1}^{d^2-1} \frac{\partial u_k}{\partial \alpha_l} b_k \right) . \tag{78}$$

In this terminology, the (normalized) Haar measure reads

$$dU_d = \frac{J_d}{N_d} \prod_{l=1}^{d^2-1} d\alpha_l . \tag{79}$$

Our aim is to derive a general expression of dU_d for arbitrary d in terms of the parameterization introduced in Sec. III, i.e.,

$$dU_d = \frac{J_d}{N_d} \prod_{k,l} d\lambda_{k,l} . \tag{80}$$

As in the previous proof, we make use of the left invariance of the Haar measure on $\mathcal{SU}(d)$, i.e., $J_d = |\det(j_{k,l})| = |\det(j'_{k,l})|$, where

$$j_{k,l} = \frac{\mathrm{Tr}(b_k^\dagger \frac{\partial U}{\partial \alpha_l})}{\mathrm{Tr}(b_k^\dagger b_k)} \qquad \longrightarrow \qquad j'_{k,l} = \frac{\mathrm{Tr}(b_k^\dagger U_1 \frac{\partial U}{\partial \alpha_l})}{\mathrm{Tr}(b_k^\dagger b_k)} . \tag{81}$$

If for the composite parameterization (Theorem 2), U_1 is chosen to be $-iU_C^\dagger$ one obtains analogously to (31)–(33) that

$$-iU_C^\dagger \frac{\partial U_C}{\partial \lambda_{x,y}} = \begin{cases} U_{x,y}^\dagger Y_{x,y} U_{x,y} & \text{for } x < y, \\ Z_{x,d} & \text{for } x = y, \\ U_{x,y}^\dagger Z_{y,x} U_{x,y} & \text{for } x > y\ , \end{cases} \tag{82}$$

where

$$U_{x,y} = \begin{cases} \left[\prod_{n=y+1}^{d} \Lambda_{x,n}\right] \left[\prod_{m=x+1}^{d-1} \prod_{n=m+1}^{d} \Lambda_{m,n}\right] \prod_{l=x}^{d-1} \exp(i Z_{l,d} \lambda_{l,l}) & \text{for } x < y, \\ \left[\prod_{n=x}^{d} \Lambda_{y,n}\right] \left[\prod_{m=y+1}^{d-1} \prod_{n=m+1}^{d} \Lambda_{m,n}\right] \prod_{l=y}^{d-1} \exp(i Z_{l,d} \lambda_{l,l}) & \text{for } x > y\ . \end{cases} \tag{83}$$

These operators are now to be expressed in an orthogonal basis $\{b_k\}$ of traceless operators. Since the first $d^2 - d$ operators that were used in (34) already are mutually orthogonal and traceless, only the d diagonal operators $|k\rangle\langle k|$ with $1 \le k \le d$ have to be replaced by $d - 1$ diagonal operators with vanishing trace. A convenient choice is the $d - 1$ mutually orthogonal operators[7,38]

$$L_k = \sqrt{\frac{2}{(d-k)(d-k+1)}} \left(-(d-k)\,|k\rangle\langle k| + \sum_{n=k+1}^{d} |n\rangle\langle n| \right), \tag{84}$$

with $1 \le k \le d - 1$ obeying $\mathrm{Tr}(L_k^\dagger L_k) = \mathrm{Tr}(L_k^2) = 2$. For the order

$$\begin{aligned}
b_1 &= |1\rangle\langle 2| + |2\rangle\langle 1|\ , & \alpha_1 &= \lambda_{2,1}\ , \\
b_2 &= -i\,|1\rangle\langle 2| + i\,|2\rangle\langle 1|\ , & \alpha_2 &= \lambda_{1,2}\ , \\
b_3 &= |1\rangle\langle 3| + |3\rangle\langle 1|\ , & \alpha_3 &= \lambda_{3,1}\ , \\
b_4 &= -i\,|1\rangle\langle 3| + i\,|3\rangle\langle 1|\ , & \alpha_4 &= \lambda_{1,3}\ , \\
&\vdots & &\vdots \\
b_{2(d-1)-1} &= |1\rangle\langle d| + |d\rangle\langle 1|\ , & \alpha_{2(d-1)-1} &= \lambda_{d,1}\ , \\
b_{2(d-1)} &= -i\,|1\rangle\langle d| + i\,|d\rangle\langle 1|\ , & \alpha_{2(d-1)} &= \lambda_{1,d}\ , \\
b_{2(d-1)+1} &= |2\rangle\langle 3| + |3\rangle\langle 2|\ , & \alpha_{2(d-1)+1} &= \lambda_{3,2}\ , \\
b_{2(d-1)+2} &= -i\,|2\rangle\langle 3| + i\,|3\rangle\langle 2|\ , & \alpha_{2(d-1)+2} &= \lambda_{2,3}\ , \\
b_{2(d-1)+3} &= |2\rangle\langle 4| + |4\rangle\langle 2|\ , & \alpha_{2(d-1)+3} &= \lambda_{4,2}\ , \\
b_{2(d-1)+4} &= -i\,|2\rangle\langle 4| + i\,|4\rangle\langle 2|\ , & \alpha_{2(d-1)+4} &= \lambda_{2,4}\ , \\
&\vdots & &\vdots \\
b_{d^2-d-1} &= |d-1\rangle\langle d| + |d\rangle\langle d-1|\ , & \alpha_{d^2-d-1} &= \lambda_{d,d-1}\ , \\
b_{d^2-d} &= -i\,|d-1\rangle\langle d| + i\,|d\rangle\langle d-1|\ , & \alpha_{d^2-d} &= \lambda_{d-1,d}\ , \\
b_{d^2-d+1} &= L_1\ , & \alpha_{d^2-d+1} &= \lambda_{1,1}\ , \\
b_{d^2-d+2} &= L_2\ , & \alpha_{d^2-d+2} &= \lambda_{2,2}\ , \\
&\vdots & &\vdots \\
b_{d^2-1} &= L_{d-1}\ , & \alpha_{d^2-1} &= \lambda_{d-1,d-1}\ ,
\end{aligned} \tag{85}$$

the $(d^2 - 1) \times (d^2 - 1)$ Jacobian matrix is again lower block-triangular as depicted in Figure 3.

Here, the block D is not diagonal but lower triangular since

$$\mathrm{Tr}(L_k^\dagger Z_{m,d}) = \begin{cases} 0 & \text{for } k < m, \\ \sqrt{\frac{2}{(d-k)(d-k+1)}}(k-d-1) & \text{for } k = m, \\ -\sqrt{\frac{2}{(d-k)(d-k+1)}} & \text{for } k > m\ . \end{cases} \tag{86}$$

Since the diagonal entries of D are merely real numbers, we find again that

$$J_d = \left|\det(j'_{k,l})\right| = c_d \prod_{i=1}^{d-1} |\det M_i|\ , \tag{87}$$

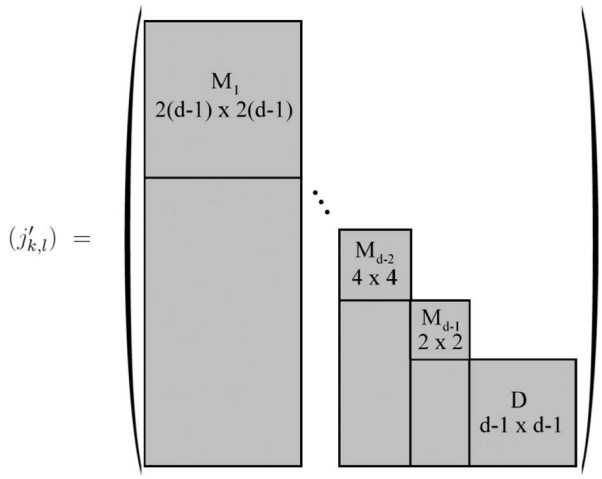

FIG. 3. Schematic illustration of the Jacobian matrix $(j'_{k,l})$ for the operator basis (85).

where c_d is a constant that can be dropped since the Haar measure will be normalized at the end anyhow. As the composite parameterization of the unitary group and the special unitary group share the same structure the discussion between (38)–(41) essentially remains the same, meaning that (ignoring irrelevant constants) one finds again the recursion formula

$$J_d = \left|\det \overline{M}_1\right| J_{d-1} \,, \tag{88}$$

where $\overline{M}_1 = M_1|_{\{\lambda_{m,n}=0|(m,n)\notin\{(1,2),\ldots,(1,d)\}\}}$ and $\lambda_{m,n} \to \lambda_{m+1,n+1}$ in J_{d-1}. Here, the relevant operators of (82) have the form

$$\begin{aligned} U_{1,y}^\dagger Y_{1,y} U_{1,y}\Big|_{\{\lambda_{m,n}=0|(m,n)\notin\{(1,2),\ldots,(1,d)\}\}} &= \left[\prod_{n=y+1}^{d} \exp(iY_{1,n}\lambda_{1,n})\right]^\dagger Y_{1,y} \left[\prod_{n=y+1}^{d} \exp(iY_{1,n}\lambda_{1,n})\right] \,, \\ &\equiv O_{1,y}^T Y_{1,y} O_{1,y} \,, \\ U_{x,1}^\dagger Z_{1,x} U_{x,1}\Big|_{\{\lambda_{m,n}=0|(m,n)\notin\{(1,2),\ldots,(1,d)\}\}} &= \left[\prod_{n=x}^{d} \exp(iY_{1,n}\lambda_{1,n})\right]^\dagger Z_{1,x} \left[\prod_{n=x}^{d} \exp(iY_{1,n}\lambda_{1,n})\right] \,, \\ &\equiv O_{x,1}^T Z_{1,x} O_{x,1} \,, \end{aligned}$$

containing the orthogonal matrices $O_{x,1}$ and $O_{1,y}$ that also appeared in the previous proof. The $2(d-1)\times 2(d-1)$ elements of $\overline{M}_1$ are determined by (compare with the order (85))

$$\mathrm{Tr}\left(b_k^\dagger O_{1,y}^T Y_{1,y} O_{1,y}\right) = \mathrm{Tr}\left(O_{1,y} b_k^\dagger O_{1,y}^T Y_{1,y}\right) \tag{89}$$

and

$$\mathrm{Tr}\left(b_k^\dagger O_{x,1}^T Z_{1,x} O_{x,1}\right) = \mathrm{Tr}\left(O_{x,1} b_k^\dagger O_{x,1}^T Z_{1,x}\right) \tag{90}$$

with $x, y \in \{2,\ldots,d\}$, and

$$b_k = b_k^\dagger = \begin{cases} |1\rangle\langle(k+3)/2| + |(k+3)/2\rangle\langle 1| &= X_{1,(k+3)/2} \quad k \text{ - odd}, \\ -i\,|1\rangle\langle(k+2)/2| + i\,|(k+2)/2\rangle\langle 1| &= Y_{1,(k+2)/2} \quad k \text{ - even}\,, \end{cases} \tag{91}$$

with $k \in \{1,\ldots,2(d-1)\}$. Now consider the coefficients of (89) and (90) for the different operator basis elements occurring in (91): First, notice that $\overline{M}_1$ is again lower triangular as in the previous proof since (89) and (43) are identical and

- $\mathrm{Tr}\left(O_{x,1} Y_{1,m} O_{x,1}^T Z_{1,x}\right) = 0$ for arbitrary m:
  Note: $O_{1,y} Y_{1,m} O_{1,y}^T$ is antisymmetric, while $Z_{1,x}$ is symmetric.

• $\mathrm{Tr}\left(O_{x,1}X_{1,m}O_{x,1}^T Z_{1,x}\right) = 0$ for $m < x$:

$$\mathrm{Tr}\left(O_{x,1}X_{1,m}O_{x,1}^T Z_{1,x}\right) = \langle 1|\, O_{x,1}X_{1,m}O_{x,1}^T\,|1\rangle - \langle x|\, O_{x,1}X_{1,m}O_{x,1}^T\,|x\rangle\ , \tag{92}$$

$$= \langle 1|\, O_{x,1}\,|1\rangle\,\langle m|\, O_{x,1}^T\,|1\rangle - \langle 1|\, O_{x,1}\,|m\rangle\,\langle 1|\, O_{x,1}^T\,|1\rangle$$

$$- \langle x|\, O_{x,1}\,|1\rangle\,\langle m|\, O_{x,1}^T\,|x\rangle - \langle x|\, O_{x,1}\,|m\rangle\,\langle 1|\, O_{x,1}^T\,|x\rangle\ , \tag{93}$$

$$= 0\ . \tag{94}$$

Note: $O_{x,1} = \prod_{n=x}^{d} \exp(iY_{1,n}\lambda_{1,n})$ does not have off-diagonal elements $\langle 1|O_{x,1}|m\rangle$ and $\langle x|O_{x,1}|m\rangle$ for $m < x$.

Thus, it again suffices to compute the diagonal entries of $\overline{M}_1$, half of which are already known from (66)

$$\mathrm{Tr}\left(O_{1,m}Y_{1,m}O_{1,m}^T Y_{1,m}\right)/\mathrm{Tr}(Y_{1,m}^2) = \prod_{n=m+1}^{d}\cos\lambda_{1,n}\ . \tag{95}$$

The remaining ones are found to be

$$\mathrm{Tr}\left(O_{1,m}X_{1,m}O_{1,m}^T Z_{1,m}\right)/\mathrm{Tr}(X_{1,m}^2) = 2\sin\lambda_{1,m}\prod_{n=m}^{d}\cos\lambda_{1,n}\ , \tag{96}$$

which directly follow from

$$\mathrm{Tr}\left(O_{1,m}X_{1,m}O_{1,m}^T Z_{1,m}\right) = \langle 1|\, O_{m,1}X_{1,m}O_{m,1}^T\,|1\rangle - \langle m|\, O_{m,1}X_{1,m}O_{m,1}^T\,|m\rangle\ , \tag{97}$$

$$= \langle 1|\, O_{m,1}\,|1\rangle\,\langle m|\, O_{m,1}^T\,|1\rangle + \langle 1|\, O_{m,1}\,|m\rangle\,\langle 1|\, O_{m,1}^T\,|1\rangle$$

$$- \langle m|\, O_{m,1}\,|1\rangle\,\langle m|\, O_{m,1}^T\,|m\rangle - \langle m|\, O_{m,1}\,|m\rangle\,\langle 1|\, O_{m,1}^T\,|m\rangle\ ,$$

$$= 2\,\langle 1|\, O_{m,1}\,|m\rangle\,\langle 1|\, O_{m,1}\,|1\rangle - 2\,\langle m|\, O_{m,1}\,|1\rangle\,\langle m|\, O_{m,1}\,|m\rangle \tag{98}$$

and the definition of $O_{m,1}$ together with (42)

$$\langle 1|\, O_{m,1}\,|m\rangle = \sin\lambda_{1,m}\ , \tag{99}$$

$$\langle 1|\, O_{m,1}\,|1\rangle = \prod_{n=m}^{d}\cos\lambda_{1,n}\ , \tag{100}$$

$$\langle m|\, O_{m,1}\,|1\rangle = -\sin\lambda_{1,m}\prod_{n=m+1}^{d}\cos\lambda_{1,n}\ , \tag{101}$$

$$\langle m|\, O_{m,1}\,|m\rangle = \cos\lambda_{1,m}\ . \tag{102}$$

Since (96) differs only by the factor two from (66), we again obtain for J_d the result (70)

$$J_d = c_d'\prod_{m=1}^{d-1}\prod_{n=m+1}^{d}\sin(\lambda_{m,n})\cos^{2(n-m)-1}(\lambda_{m,n})\ , \tag{103}$$

up to an irrelevant multiplicative constant c_d'. Hence, the Haar measure on $\mathcal{SU}(d)$ reads

$$dU_d = \frac{1}{N_d}\prod_{m=1}^{d-1}\prod_{n=m+1}^{d}\sin(\lambda_{m,n})\cos^{2(n-m)-1}(\lambda_{m,n})\prod_{k,l}d\lambda_{k,l}\ . \tag{104}$$

The normalizing constant N_d is given by the integral

$$N_d = \int_{\lambda_{k,l}=0}^{2\pi\ (k=l)}\int_{\lambda_{k,l}=0}^{\pi\ (k>l)}\int_{\lambda_{k,l}=0}^{\pi/2\ (k<l)}\left[\prod_{m=1}^{d-1}\prod_{n=m+1}^{d}\sin(\lambda_{m,n})\cos^{2(n-m)-1}(\lambda_{m,n})\right]\prod_{k,l}d\lambda_{k,l}\ .$$

Since there are $d-1$ parameters $\lambda_{k,l}$ with $k=l$ and $d(d-1)/2$ parameters $\lambda_{k,l}$ with $k>l$, one finally obtains

$$N_d = 2^{d-1}\pi^{d(d+1)/2-1}\prod_{m=1}^{d-1}\prod_{n=m+1}^{d}\frac{-1}{2(n-m)}\cos^{2(n-m)}(\lambda_{m,n})\Big|_{\lambda_{m,n}=0}^{\pi/2}, \tag{105}$$

$$= \frac{2^{d-1}\pi^{d(d+1)/2-1}}{\prod_{m=1}^{d-1}\prod_{n=m+1}^{d}2(n-m)}. \tag{106}$$

□

VI. REMARKS ON INTEGRALS OVER UNITARY GROUPS

As previously mentioned, our results can be used to compute group integrals, i.e., integrals of the form $\int f(U,U^*)dU$ where one integrates over the entire group $\mathcal{U}(d)$ or $\mathcal{SU}(d)$, respectively. At least three things are needed when one intends to *explicitly* compute such integrals: A parameterization of the corresponding group, exact knowledge of the parameter ranges and the normalized Haar measure. All this is provided in the present paper. Theorems 1–4 can straightforwardly be applied without knowledge of further technicalities (e.g., details appearing in the proofs). Whether or not a given integral can be solved analytically in this way of course depends on the integrand. However, for many physical problems the function $f(U,U^*)$ is a polynomial in the components of U and U^*. In this case, when U and dU are inserted in parameterized form according to Theorems 1–4, we have that the integrand is a polynomial in $\cos\lambda_{m,n}$, $\sin\lambda_{m,n}$, and $e^{\pm i\lambda_{m,n}}$. Neglecting the computational effort, such integrals can always be solved analytically (see Ref. 39 and references therein). Besides that, our results constitute a good starting point for the integration of non-polynomial functions using numerical methods.

A detailed analysis on integrals that can be solved in this way shall be presented in a subsequent paper. We are convinced that due to the simplicity of the parameterization and the associated Haar measure, it is possible to find several general results and to gain a better understanding of integrals over $\mathcal{U}(d)/\mathcal{SU}(d)$. In order not to go beyond the scope of this paper, we conclude with simple examples that can be compared with existing results as a consistency check.

A. Example 1

In Ref. 40, it was shown that

$$\int_{\mathcal{U}(d)} |\langle 1|U|1\rangle|^4 dU = \frac{2}{d(d+1)}. \tag{107}$$

By means of our results, it is straightforward to analytically confirm this relation and to find the general solution for $\int|\langle 1|U|1\rangle|^p dU$ for arbitrary $p\in\mathbb{N}$. In parameterized form, we have $\langle 1|U_C|1\rangle = e^{i\lambda_{1,1}}\prod_{n=2}^{d}\cos(\lambda_{1,n})$, and accordingly $|\langle 1|U_C|1\rangle|^p = \prod_{n=2}^{d}\cos^p(\lambda_{1,n})$ only depends on $\lambda_{1,2},\ldots,\lambda_{1,d}$. Due to this, the integral simplifies as follows (see also Appendix C):

$$\int_{\mathcal{U}(d)} |\langle 1|U|1\rangle|^p dU, \tag{108}$$

$$= \int_{\lambda_{k,l}=0}^{2\pi\ (k\geq l)}\int_{\lambda_{k,l}=0}^{\pi/2\ (k<l)}\prod_{n=2}^{d}\cos^p(\lambda_{1,n})\,dU_d, \tag{109}$$

$$= \int_{\lambda_{1,2}=0}^{\pi/2}\cdots\int_{\lambda_{1,d}=0}^{\pi/2}\prod_{n=2}^{d}\cos^p(\lambda_{1,n})2(n-1)\sin(\lambda_{1,n})\cos^{2(n-1)-1}(\lambda_{1,n})d\lambda_{1,2}\cdots d\lambda_{1,d},$$

$$= \int_{\lambda_{1,2}=0}^{\pi/2}\cdots\int_{\lambda_{1,d}=0}^{\pi/2}\prod_{n=2}^{d}2(n-1)\sin(\lambda_{1,n})\cos^{2(n-1)-1+p}(\lambda_{1,n})d\lambda_{1,2}\cdots d\lambda_{1,d}. \tag{110}$$

This integral can easily be solved, i.e.,

$$= \left[\prod_{n=2}^{d} 2(n-1) \frac{-\cos^{2(n-1)+p}(\lambda_{1,n})}{2(n-1)+p} \right] \Bigg|_{\lambda_{1,n}=0}^{\pi/2} , \tag{111}$$

$$= \prod_{n=2}^{d} \frac{2(n-1)}{2(n-1)+p} . \tag{112}$$

For the special case $p = 4$, the general solution

$$\int_{\mathcal{U}(d)} |\langle 1| U |1\rangle|^p dU = \prod_{n=2}^{d} \frac{2(n-1)}{2(n-1)+p} \tag{113}$$

simplifies to $\prod_{n=2}^{d} \frac{2(n-1)}{2(n+1)} = \frac{2}{d(d+1)}$ as in agreement with Ref. 40. Note that in this way we have found a simple necessary criterion for testing if a set of matrices constitutes a unitary design. Namely, as there are no distinguished matrix elements and since $|\langle 1|U|1\rangle|^{2t} = \langle 1|U|1\rangle^t \langle 1|U^*|1\rangle^t$, it holds: A set of unitaries $\{U_i\}_N$ is a unitary t-design only if

$$\sum_{i=1}^{N} w_i |\langle k| U_i |l\rangle|^{2t} = \prod_{n=2}^{d} \frac{n-1}{n-1+t} \tag{114}$$

for all $k, l \in \{1, \ldots, d\}$, where w_i is the weighting of U_i ($w_i = \frac{1}{N}$ for unweighted designs). Further criteria can be constructed analogously.

B. Example 2

It is known that bilateral twirling $\int U \otimes U \rho U^\dagger \otimes U^\dagger dU$ of a state ρ on $\mathbb{C}^d \otimes \mathbb{C}^d$ results in a *Werner state*[27–29,41] which has the form

$$\rho_W = \frac{\mathbb{1} + \beta(\sum_{i,j=1}^{d} |ij\rangle \langle ji|)}{d(d+\beta)} , \tag{115}$$

where $-1 \leq \beta \leq 1$. Using a symbolic computation software, we explicitly and analytically twirled the maximally entangled state $|\Psi\rangle = \frac{1}{\sqrt{d}} \sum_{i=1}^{d} |i\rangle \otimes |i\rangle$ of dimensions $d = 2, 3, 4, 5$ utilizing Theorems 1 and 3,

$$\int_{\lambda_{k,l}=0}^{2\pi \ (k\geq l)} \int_{\lambda_{k,l}=0}^{\pi/2 \ (k<l)} U_C \otimes U_C |\Psi\rangle \langle \Psi| U_C^\dagger \otimes U_C^\dagger dU_d , \tag{116}$$

and alternatively with Theorems 2 and 4

$$\int_{\lambda_{k,l}=0}^{2\pi \ (k=l)} \int_{\lambda_{k,l}=0}^{\pi \ (k>l)} \int_{\lambda_{k,l}=0}^{\pi/2 \ (k<l)} U_C \otimes U_C |\Psi\rangle \langle \Psi| U_C^\dagger \otimes U_C^\dagger dU_d . \tag{117}$$

In all cases, this yielded a *Werner state* with $\beta = 1$, demonstrating once more the operationality and validity of our results. Note that our results also enable analytical twirling of multipartite qudit states.

C. Example 3

The entanglement of a bipartite qudit state $|\psi\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B = \mathbb{C}^d \otimes \mathbb{C}^d$ can be quantified via the (normalized) concurrence[42–45] determined by $C^2(|\psi\rangle) = \frac{d}{d-1}(1 - \mathrm{Tr}(\rho_B^2))$, where ρ_B is the reduced density matrix $\rho_B = \mathrm{Tr}_A(|\psi\rangle \langle \psi|)$. An interesting property of a quantum system is the *a priori entanglement*, i.e., a characteristic such as the generic probability that a state is entangled or the average amount of entanglement over all states in dependence of the dimension d. Here, we

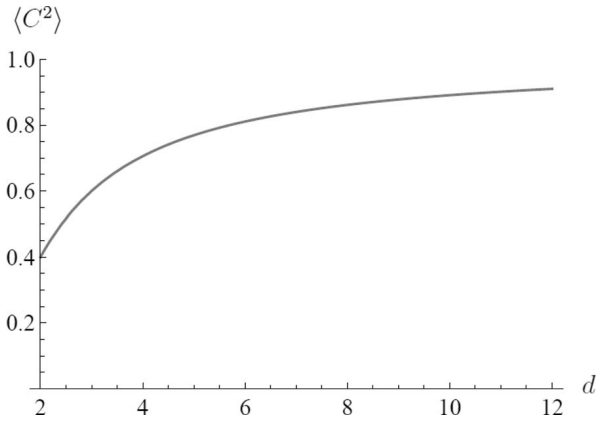

FIG. 4. The average entanglement (122) of a bipartite qudit system measured by the (squared) concurrence $C^2(|\psi\rangle)$ for the dimensions $d = 2, \ldots, 12$. The average $\langle C^2\rangle$ increases with the size of the Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B = \mathbb{C}^d \otimes \mathbb{C}^d$.

focus on the average

$$\langle C^2\rangle = \int_{\mathcal{U}(d^2)} C^2(U\,|\psi\rangle) dU\ , \tag{118}$$

where $|\psi\rangle$ is an arbitrary state of $\mathbb{C}^d \otimes \mathbb{C}^d$. If we express $|\psi\prime\rangle\langle\psi\prime| = U|\psi\rangle\langle\psi|U\dagger$ as $|\psi'\rangle\langle\psi'| = \sum_{i,j=1}^{d^2} u_i u_j^*\,|i\rangle\,\langle j|$, we obtain the reduced density matrix

$$\rho_B = \sum_{i,j=1}^{d} \left(\sum_{n=0}^{d-1} u_{i+nd} u_{j+nd}^* \right) |i\rangle\,\langle j|\ . \tag{119}$$

To solve the integral $\int \frac{d}{d-1}(1 - \mathrm{Tr}(\rho_B^2))dU$, we can associate each u_i with a matrix element of a $d^2 \times d^2$ unitary matrix. In this way, the average $\langle C^2\rangle$ reduces to a sum of integrals over the polynomials $I_4 = \int |\langle k|U|l\rangle|^4 dU$ and $I_{2,2} = \int |\langle k|U|l\rangle|^2 |\langle m|U|n\rangle|^2 dU$, where $\langle k|U|l\rangle$ and $\langle m|U|n\rangle$ denote distinct matrix elements. Now, taking account of (119), it is a simple combinatorial problem to show that in $\int \mathrm{Tr}(\rho_B^2)dU$ the term I_4 appears d^2 times and $I_{2,2}$ appears $2(d-1)d^2$ times. Hence,

$$\langle C^2\rangle = \frac{d}{d-1}(1 - d^2 I_4 - 2(d-1)d^2 I_{2,2})\ . \tag{120}$$

From (107), we already know that $I_4 = \frac{2}{d^2(d^2+1)}$ for integrals over $\mathcal{U}(d^2)$. It remains to determine $I_{2,2}$ for two arbitrary but distinct matrix elements $\langle k|U|l\rangle$ and $\langle m|U|n\rangle$. By computing

$$I_{2,2} = \int_{\mathcal{U}(d^2)} |\,\langle 1|\,U_C\,|1\rangle\,|^2 |\left\langle d^2\right|\,U_C\,|1\rangle\,|^2 dU_{d^2}\ , \tag{121}$$

analogously to (108)–(112) one finds with $|\left\langle d^2\right|\,U_C\,|1\rangle\,|^2 = \sin^2(\lambda_{1,d^2})$ that $I_{2,2} = \frac{1}{d^2(d^2+1)} = \frac{1}{2} I_4$. Consequently, the average entanglement of a bipartite qudit system is

$$\langle C^2\rangle = \frac{d(d-1)}{d^2+1}\ . \tag{122}$$

This result is graphically depicted in Figure 4. Physically interpreted it means that the higher dimensional the system is, the more likely it becomes to obtain a highly entangled state when picking a pure state of $\mathcal{H} = \mathbb{C}^d \otimes \mathbb{C}^d$ at random.

VII. SUMMARY

In this paper, we adopted the concept of the composite parameterization of the unitary group $\mathcal{U}(d)$ to the special unitary group $\mathcal{SU}(d)$. We showed that both parameterizations can be used equivalently to describe orthonormal vectors and subspaces with the minimal number of parameters.

The introduced parameterizations are completely factorized and therefore beneficial for numerical optimizations. We also determined the infinitesimal volume element in terms of the introduced parameters. We derived a general formula of the normalized Haar measure for both the unitary $\mathcal{U}(d)$ and the special unitary group $\mathcal{SU}(d)$ of arbitrary dimension. The found expressions give theoretical insights into the differential structure of $\mathcal{U}(d)$ and $\mathcal{SU}(d)$. Moreover, the Haar measure plays an important role in all kinds of unbiased randomizations. It was stressed that our results also constitute a framework for computing high-order group integrals. By means of our approach, we analytically solved several exemplary integrals and found that the solutions are in agreement with the literature. As integrals over unitary groups appear in various fields from particle physics to quantum optics to quantum information, it is to be expected that our results will find several interesting applications.

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APPENDIX A: SOME EXPLICIT EXPRESSIONS FOR $\mathcal{U}(d)$

$d = 2$:

$$\begin{aligned} U_C &= \exp\left(iP_2\lambda_{2,1}\right)\exp\left(iY_{1,2}\lambda_{1,2}\right)\exp\left(iP_1\lambda_{1,1}\right)\exp\left(iP_2\lambda_{2,2}\right) , \\ dU_2 &= \frac{1}{4\pi^3}\sin\lambda_{1,2}\cos\lambda_{1,2}\, d\lambda_{1,2}d\lambda_{2,1}d\lambda_{1,1}d\lambda_{2,2}. \end{aligned}$$

$d = 3$:

$$\begin{aligned} U_C &= \exp\left(iP_2\lambda_{2,1}\right)\exp\left(iY_{1,2}\lambda_{1,2}\right)\exp\left(iP_3\lambda_{3,1}\right)\exp\left(iY_{1,3}\lambda_{1,3}\right)\exp\left(iP_3\lambda_{3,2}\right) \\ &\quad\times\exp\left(iY_{2,3}\lambda_{2,3}\right)\exp\left(iP_1\lambda_{1,1}\right)\exp\left(iP_2\lambda_{2,2}\right)\exp\left(iP_3\lambda_{3,3}\right) , \\ dU_3 &= \frac{1}{4\pi^6}\sin\lambda_{1,2}\cos\lambda_{1,2}\sin\lambda_{1,3}\cos^3\lambda_{1,3}\sin\lambda_{2,3}\cos\lambda_{2,3} \\ &\quad\times d\lambda_{1,2}d\lambda_{2,1}d\lambda_{1,3}d\lambda_{3,1}d\lambda_{2,3}d\lambda_{3,2}d\lambda_{1,1}d\lambda_{2,2}d\lambda_{3,3}. \end{aligned}$$

$d = 4$:

$$\begin{aligned} U_C &= \exp\left(iP_2\lambda_{2,1}\right)\exp\left(iY_{1,2}\lambda_{1,2}\right)\exp\left(iP_3\lambda_{3,1}\right)\exp\left(iY_{1,3}\lambda_{1,3}\right)\exp\left(iP_4\lambda_{4,1}\right) \\ &\quad\times\exp\left(iY_{1,4}\lambda_{1,4}\right)\exp\left(iP_3\lambda_{3,2}\right)\exp\left(iY_{2,3}\lambda_{2,3}\right)\exp\left(iP_4\lambda_{4,2}\right)\exp\left(iY_{2,4}\lambda_{2,4}\right) \\ &\quad\times\exp\left(iP_4\lambda_{4,3}\right)\exp\left(iY_{3,4}\lambda_{3,4}\right)\exp\left(iP_1\lambda_{1,1}\right)\exp\left(iP_2\lambda_{2,2}\right)\exp\left(iP_3\lambda_{3,3}\right)\exp\left(iP_4\lambda_{4,4}\right) , \\ dU_4 &= \frac{3}{4\pi^{10}}\sin\lambda_{1,2}\cos\lambda_{1,2}\sin\lambda_{1,3}\cos^3\lambda_{1,3}\sin\lambda_{1,4}\cos^5\lambda_{1,4}\sin\lambda_{2,3}\cos\lambda_{2,3} \\ &\quad\times\sin\lambda_{2,4}\cos^3\lambda_{2,4}\sin\lambda_{3,4}\cos\lambda_{3,4}\, d\lambda_{1,2}d\lambda_{2,1}d\lambda_{1,3}d\lambda_{3,1}d\lambda_{1,4}d\lambda_{4,1} \\ &\quad\times d\lambda_{2,3}d\lambda_{3,2}d\lambda_{2,4}d\lambda_{4,2}d\lambda_{3,4}d\lambda_{4,3}\lambda_{1,1}d\lambda_{2,2}d\lambda_{3,3}d\lambda_{4,4}. \end{aligned}$$

APPENDIX B: SOME EXPLICIT EXPRESSIONS FOR $\mathcal{SU}(d)$

$d = 2$:

$$\begin{aligned} U_C &= \exp\left(iZ_{1,2}\lambda_{2,1}\right)\exp\left(iY_{1,2}\lambda_{1,2}\right)\exp\left(iZ_{1,2}\lambda_{1,1}\right) , \\ dU_2 &= \frac{1}{\pi^2}\sin\lambda_{1,2}\cos\lambda_{1,2}\, d\lambda_{1,2}d\lambda_{2,1}d\lambda_{1,1}. \end{aligned}$$

$d = 3$:

$$\begin{aligned} U_C &= \exp\left(iZ_{1,2}\lambda_{2,1}\right)\exp\left(iY_{1,2}\lambda_{1,2}\right)\exp\left(iZ_{1,3}\lambda_{3,1}\right)\exp\left(iY_{1,3}\lambda_{1,3}\right) \\ &\quad\times\exp\left(iZ_{2,3}\lambda_{3,2}\right)\exp\left(iY_{2,3}\lambda_{2,3}\right)\exp\left(iZ_{1,3}\lambda_{1,1}\right)\exp\left(iZ_{2,3}\lambda_{2,2}\right)\ , \\ dU_3 &= \frac{4}{\pi^5}\sin\lambda_{1,2}\cos\lambda_{1,2}\sin\lambda_{1,3}\cos^3\lambda_{1,3}\sin\lambda_{2,3}\cos\lambda_{2,3} \\ &\quad\times d\lambda_{1,2}d\lambda_{2,1}d\lambda_{1,3}d\lambda_{3,1}d\lambda_{2,3}d\lambda_{3,2}d\lambda_{1,1}d\lambda_{2,2}. \end{aligned}$$

$d = 4$:

$$\begin{aligned} U_C &= \exp\left(iZ_{1,2}\lambda_{2,1}\right)\exp\left(iY_{1,2}\lambda_{1,2}\right)\exp\left(iZ_{1,3}\lambda_{3,1}\right)\exp\left(iY_{1,3}\lambda_{1,3}\right)\exp\left(iZ_{1,4}\lambda_{4,1}\right) \\ &\quad\times\exp\left(iY_{1,4}\lambda_{1,4}\right)\exp\left(iZ_{2,3}\lambda_{3,2}\right)\exp\left(iY_{2,3}\lambda_{2,3}\right)\exp\left(iZ_{2,4}\lambda_{4,2}\right)\exp\left(iY_{2,4}\lambda_{2,4}\right) \\ &\quad\times\exp\left(iZ_{3,4}\lambda_{4,3}\right)\exp\left(iY_{3,4}\lambda_{3,4}\right)\exp\left(iZ_{1,4}\lambda_{1,1}\right)\exp\left(iZ_{2,4}\lambda_{2,2}\right)\exp\left(iZ_{3,4}\lambda_{3,3}\right), \\ dU_4 &= \frac{96}{\pi^9}\sin\lambda_{1,2}\cos\lambda_{1,2}\sin\lambda_{1,3}\cos^3\lambda_{1,3}\sin\lambda_{1,4}\cos^5\lambda_{1,4}\sin\lambda_{2,3}\cos\lambda_{2,3} \\ &\quad\times\sin\lambda_{2,4}\cos^3\lambda_{2,4}\sin\lambda_{3,4}\cos\lambda_{3,4}\,d\lambda_{1,2}d\lambda_{2,1}d\lambda_{1,3}d\lambda_{3,1}d\lambda_{1,4}d\lambda_{4,1} \\ &\quad\times d\lambda_{2,3}d\lambda_{3,2}d\lambda_{2,4}d\lambda_{4,2}d\lambda_{3,4}d\lambda_{4,3}\lambda_{1,1}d\lambda_{2,2}d\lambda_{3,3}. \end{aligned}$$

APPENDIX C: DIFFERENTIAL MATRIX REPRESENTATION FOR $\mathcal{U}(d)$

Adopting the matrix representation $[\lambda_{m,n}]$ introduced in Sec. III A to differentials, the normalized Haar measure may be written as

$$dU_d = \prod_{m,n=1}^{d}\Delta_{m,n}\ , \tag{C1}$$

with

$$\left[\Delta_{m,n}\right] = \begin{bmatrix} \frac{d\lambda_{1,1}}{2\pi} & -d(\cos^2(\lambda_{1,2})) & \cdots & -d(\cos^{2(d-1)}(\lambda_{1,d})) \\ \frac{d\lambda_{2,1}}{2\pi} & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & -d(\cos^2(\lambda_{d-1,d})) \\ \frac{d\lambda_{d,1}}{2\pi} & \cdots & \frac{d\lambda_{d,d-1}}{2\pi} & \frac{d\lambda_{d,d}}{2\pi} \end{bmatrix}. \tag{C2}$$

This notation is useful for the construction of a normalized Haar measure for problems which are independent of certain parameters $\lambda_{k,l}$ (see discussion in Sec. III A and Ref. 8, as well as *example 1*). Since in such cases the dependence on $\lambda_{k,l}$ and $d\lambda_{k,l}$ can be removed from the Haar measure, one can replace the corresponding entry $\Delta_{k,l}$ by a constant. If one sets $\Delta_{k,l} = 1$, then (C1) preserves the normalization of the reduced Haar measure. Moreover, this notation could lead to a better understanding of the differential geometry of $\mathcal{U}(d)$.

APPENDIX D: DIFFERENTIAL MATRIX REPRESENTATION FOR $\mathcal{SU}(d)$

Analogously, the normalized Haar measure on $\mathcal{SU}(d)$ may be written as

$$dU_d = \prod_{m,n=1}^{d}\Delta_{m,n}\ , \tag{D1}$$

with

$$\left[\Delta_{m,n}\right] = \begin{bmatrix} \frac{d\lambda_{1,1}}{2\pi} & -d(\cos^2(\lambda_{1,2})) & \cdots & -d(\cos^{2(d-1)}(\lambda_{1,d})) \\ \frac{d\lambda_{2,1}}{\pi} & \ddots & \ddots & \vdots \\ \vdots & \ddots & \frac{d\lambda_{d-1,d-1}}{2\pi} & -d(\cos^2(\lambda_{d-1,d})) \\ \frac{d\lambda_{d,1}}{\pi} & \cdots & \frac{d\lambda_{d,d-1}}{\pi} & 1 \end{bmatrix}. \tag{D2}$$

[1] These can be considered as generalizations of the Pauli matrix σ_y.
[2] The order of the product is $\prod_{i=1}^{N} A_i = A_1 \cdot A_2 \cdots A_N$.
[3] Note that the indices m and n again run from 1 to d except that there is no $\lambda_{d,d}$.
[4] Intuitively: When changing from the orthogonal coordinates $\{u_k\}$ to the non-orthogonal coordinates $\{\alpha_l\}$ the infinitesimal volume element transforms as $\prod_{k=1}^{d^2} du_k = \left|\det \frac{\partial(u_1,\ldots,u_{d^2})}{\partial(\alpha_1,\ldots,\alpha_{d^2})}\right| \prod_{l=1}^{d^2} d\alpha_l$ according to the Jacobian determinant.
[5] The independence of $|\det M_1|$ on $\lambda_{m,n}$ with $\min\{m,n\} \geq 2$ can also be confirmed by exploiting again the left and right invariance of the Haar measure.
[6] A basis for the vector space of operators $\mathbb{C}^d \times \mathbb{C}^d$ has d^2 elements. The constraint $\det U = 1$ on special unitary operators implies that the trace of any derivative $\partial U/\partial\alpha_l$ with respect to an arbitrary parameter is always zero. Traceless operators form a $d^2 - 1$ dimensional subspace of $\mathbb{C}^d \times \mathbb{C}^d$. As we have $d^2 - 1$ parameters $\{\alpha_l\}$ it is required to express the derivatives $\partial U/\partial\alpha_l$ in a basis of this subspace to obtain $d^2 - 1$ linearly independent column vectors.
[7] Note that these are the generalized diagonal Gell-Mann matrices (Ref. 38) in reversed order.
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Examining the dimensionality of genuine multipartite entanglement

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Abstract Entanglement in high-dimensional many-body systems plays an increasingly vital role in the foundations and applications of quantum physics. In the present paper, we introduce a theoretical concept which allows to categorize multipartite states by the number of degrees of freedom being entangled. In this regard, we derive computable and experimentally friendly criteria for arbitrary multipartite qudit systems that enable to examine in how many degrees of freedom a mixed state is genuine multipartite entangled.

Keywords Entanglement measures, witnesses, and other characterizations · Algebraic methods · Quantum information · Foundations of quantum mechanics · Formalism

1 Introduction

Ever since its discovery more than seventy years ago, quantum entanglement has been considered as the central essence of quantum theory, forcing us to rethink our view of reality, locality and causality. It impressively highlights the non-local-realistic and contextual character of nature and thereby provides insights into the very foundations of physics. Moreover, during the last two decades, it has become more and more clear that entanglement can serve as a resource for future information processing

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technologies, such as quantum cryptography, dense coding, quantum teleportation and quantum computing. It is even argued that entanglement plays a role in quantum phase transitions [1], ionization processes [2], high energy physics [3] and light-harvesting complexes [4].

When it comes to studying quantum phenomena in diverse systems one is regularly confronted with the problems of how to detect, characterize and quantify entanglement. With the exception of bipartite qubit systems, these problems are in general extremely hard to solve for systems of arbitrary number of parties and dimensions, i.e. multipartite qudits.

In the present paper we focus on a finer characterization of *genuine multipartite entanglement* [5] in multilevel systems. Genuine multipartite entangled states have been shown to be vital for fundamental tests of quantum physics [6–8] and find application in measurement-based quantum computing [9] and quantum secret sharing [10,11]. Although, this type of entanglement is not bounded on the dimensionality of the local systems, the use of systems with more than two levels, i.e. qudits, brings with it several advantages and deeper insights. For instance, it was found that quantum correlations are more robust against decoherence the more degrees of freedom are entangled [12,13]. Qudit entanglement also improves the security of quantum key distribution [14], and allows quantum secret sharing schemes [15], distributed protocols [16,17] and error-correcting codes [18] which cannot be realized with qubits. It is also to be expected that quantum computers that encode more than one qubit of information in each particle will require less resources and will thus be more efficient [19,20]. Furthermore, high-dimensional multipartite entanglement is essential for a complete understanding of quantum theory [21–25].

The aim of this paper is to provide practical and experimentally feasible criteria that allow to examine the dimensionality of genuine multipartite entanglement. The central problem is the following: Suppose we have realized a multipartite qudit scenario in the laboratory. How can we verify if a state is genuine multipartite entangled (GME) and how many degrees of freedom are involved in the entanglement?

For pure states this question is easily answered via the ranks of the reduced density matrices. However, for mixed states, as they appear in any real experiment, this is a nontrivial problem. Consider e.g. the mixed state $\rho_c = \frac{1}{2}\left|GHZ_3\right\rangle\left\langle GHZ_3\right| + \frac{1}{6}\sum_{i=0}^{2}\left|iii\right\rangle\left\langle iii\right|$, where $\left|GHZ_3\right\rangle = \frac{1}{\sqrt{3}}(\left|000\right\rangle + \left|111\right\rangle + \left|222\right\rangle)$ is a tripartite Greenberger-Horne-Zeilinger (*GHZ*) state entangled in three degrees of freedom. This state ρ_c is not truly three-dimensionally entangled since it can be decomposed into $\rho_c = \frac{1}{3}(\left|GHZ_{1,2}\right\rangle\left\langle GHZ_{1,2}\right| + \left|GHZ_{1,3}\right\rangle\left\langle GHZ_{1,3}\right| + \left|GHZ_{2,3}\right\rangle\left\langle GHZ_{2,3}\right|)$ with $\left|GHZ_{i,j}\right\rangle = \frac{1}{\sqrt{2}}(\left|iii\right\rangle + \left|jjj\right\rangle)$, which are each entangled in only two local degrees of freedom.

2 Definitions

Let us first give a precise definition of the dimensionality of multipartite entanglement—a multipartite generalization of the Schmidt rank [26–28] complementary to the tensor rank [29] that allows to characterize multipartite qudit states. This generalization

is important as the tensor rank is *not* the crucial characteristic that the many-body entangled qudit states in [15–25] have in common. This is mainly because in the multipartite case there is no simple connection between the tensor rank, k-separability and multilevel entanglement. For example, the states $|W\rangle = \frac{1}{\sqrt{3}}(|001\rangle + |010\rangle + |100\rangle)$, $|GHZ_3\rangle = \frac{1}{\sqrt{3}}(|000\rangle + |111\rangle + |222\rangle)$ and $\left|\Psi_{\text{bisep.}}\right\rangle = |0\rangle \otimes \frac{1}{\sqrt{3}}(|00\rangle + |11\rangle + |22\rangle)$ all have tensor rank 3. However, only $|GHZ_3\rangle$ is commonly regarded as multilevel-multipartite entangled. Hence, for a finer categorization of multipartite entanglement it is needed to specify novel characteristic quantities.

For a pure n-partite state $|\psi\rangle \in \mathcal{H} = \mathbb{C}^{d_1} \otimes \cdots \otimes \mathbb{C}^{d_n}$ consider the set of all reduced density matrices $\{\rho_A = Tr_B(|\psi\rangle\langle\psi|)\}$ regarding all bipartitions $\gamma = \{(A|B)\}$. Evidently, iff the state $|\psi\rangle$ is fully separable then the rank of all reduced density matrices ρ_A is 1. On the other hand, the state $|\psi\rangle$ contains entanglement iff there exists a ρ_A with $\text{rank}(\rho_A) > 1$. For a fixed bipartition $(A|B)$, the dimensionality of entanglement is determined by the Schmidt rank [26–28] which equals $\text{rank}(\rho_A)$. Hence, iff $\max\{\text{rank}(\rho_A)\} = f$ with $f \geq 2$ then the state $|\psi\rangle$ contains f-dimensional entanglement. We define a state to be f-dimensionally *genuine multipartite entangled* (GME) iff it is at least f-dimensionally entangled with respect to *all* bipartitions, that is $\min\{\text{rank}(\rho_A)\} = f$. This can be extended to mixed states in a natural way: A mixed state $\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$ is f-dimensionally entangled iff there exists no decomposition $\{p_i, |\psi_i\rangle\}$ into pure states $|\psi_i\rangle$ of dimensionality f_i all obeying $f_i < f$, but a decomposition into pure states satisfying $f_i \leq f$ for all i. A mixed state $\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$ is f-dimensionally GME iff any decomposition $\{p_i, |\psi_i\rangle\}$ of ρ contains at least one GME state $|\psi_i\rangle$ of dimensionality f or higher.

3 Dimensionality criteria

The problem of determining the dimensionality of multipartite entanglement for a given mixed state ρ is as complex as the separability problem, since it is practically impossible to vary over all pure state decompositions of ρ. For this reason it is imperative to find computable criteria for the detection of high-dimensional genuine multipartite entanglement. First steps in this direction have recently been made by Lim et al. [30] and Li et al. [31]. However, the criterion by Lim et al. is only able to discriminate 2-dimensional from 3-dimensional genuine multipartite entanglement in tripartite three-level systems. The criterion by Li et al. applies to arbitrary dimensionality and system size, but its noise resistance is rather unsatisfactory. Hence, further progress is needed here. Recently, a framework of criteria detecting genuine multipartite entanglement was introduced in [32–35]. Although it belongs to the strongest criteria for the detection of GME states without requiring semidefinite programming [36], it does not discriminate states of different dimensionality. In the present paper, we show how this powerful framework can be extended for verifying the presence of high-dimensional genuine multipartite entanglement in arbitrary mixed states.

Consider a density matrix ρ of an n-partite d-level system, i.e. a Hilbert space $\mathcal{H} = \left(\mathbb{C}^d\right)^{\otimes n}$. For a twofold copy $\rho^{\otimes 2}$ on $\mathcal{H}^{\otimes 2}$ we define for each bipartition $(A|B)$ of $\mathcal{H}$ a permutation operator $\mathcal{P}_A$ which permutes the subsystem A with its copy A', i.e.

$$\mathcal{H}^{\otimes 2} = \mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_{A'} \otimes \mathcal{H}_{B'}$$
$$\xrightarrow{\mathcal{P}_A} \mathcal{H}_{A'} \otimes \mathcal{H}_B \otimes \mathcal{H}_A \otimes \mathcal{H}_{B'}$$

For instance, for the bipartition $(\{1\}|\{2,\ldots,n\})$ and the vector $|k\rangle^{\otimes n} \otimes |l\rangle^{\otimes n} \in \mathcal{H}^{\otimes 2}$ the corresponding operator $\mathcal{P}_{\{1\}}$ acts like

$$\mathcal{P}_{\{1\}} |k\rangle^{\otimes n} \otimes |l\rangle^{\otimes n} = |l\rangle \otimes |k\rangle^{\otimes(n-1)} \otimes |k\rangle \otimes |l\rangle^{\otimes(n-1)} .$$

Using this abbreviation we introduce the quantity

$$Q_0 = \sum_{k\neq l}^{d-1} \left(|\langle k_n| \rho |l_n\rangle| - \sum_{\gamma} \sqrt{\langle k,l| \mathcal{P}_A^\dagger \rho^{\otimes 2} \mathcal{P}_A |k,l\rangle} \right) \tag{1}$$

with $|k_n\rangle = |k\rangle^{\otimes n}$ and $|k,l\rangle = |k\rangle^{\otimes n} \otimes |l\rangle^{\otimes n}$, where the $|k\rangle, |l\rangle$ are vectors of an orthonormal basis $\{|0\rangle, \ldots, |d-1\rangle\}$ of $\mathbb{C}^d$ and the sum runs over all bipartitions $\gamma = \{(A|B)\}$. Furthermore, we introduce the quantities ($m \in \{1,\ldots,\lfloor \frac{n}{2} \rfloor\}$)

$$Q_m = \frac{1}{m} \left[\sum_{k,l=0}^{d-2} \sum_{\sigma} \left(\underbrace{|\langle \alpha^k|\rho|\beta^l\rangle|}_{O^{k,l}_{\alpha,\beta}} - \sum_{\delta} \underbrace{\sqrt{\langle \alpha^k| \otimes \langle \beta^l| \mathcal{P}_\delta^\dagger \rho^{\otimes 2} \mathcal{P}_\delta |\alpha^k\rangle \otimes |\beta^l\rangle}}_{P^{k,l}_{\alpha,\beta}} \right) \right.$$
$$\left. - N_D \sum_{l=0}^{d-2} \sum_{\alpha} \underbrace{\langle \alpha^l|\rho|\alpha^l\rangle}_{D^l_\alpha} \right] \tag{2}$$

wherein $|\alpha^l\rangle \in \mathcal{H}$ are product vectors, where m of the n local systems contained in the set α are in the state $|l+1\rangle$ and remaining ones in $|l\rangle$, i.e. $|\alpha| = m$ and

$$|\alpha^l\rangle = \bigotimes_{i\in\alpha} |l+1\rangle_i \bigotimes_{i\notin\alpha} |l\rangle_i \ , \tag{3}$$

and the same holds for $|\beta^l\rangle$. We have

$$\sigma = \{(\alpha,\beta) : |\alpha \cap \beta| = m-1\} \tag{4}$$
$$N_D = (d-1)m(n-m-1). \tag{5}$$

The innermost sum depends on (α,β) and runs over[1]

$$\delta = \begin{cases} \alpha & \text{if } k = l \\ \{\delta \mid \delta \subset \overline{\alpha\backslash\beta}\} & \text{if } k < l \\ \{\delta \mid \delta \subset \overline{\beta\backslash\alpha}\} & \text{if } k > l \end{cases} \tag{6}$$

[1] Note that the empty set $\{\emptyset\}$ is always neglected.

where the complement (overline) is taken with respect to the set $\{1, \ldots, n\}$. Now, the main result of this paper is that if any of these functions Q_m fulfills

$$Q_m > f - 2 \quad (\text{where } f \in \{2, \ldots, d\}) \tag{7}$$

for a given density matrix ρ, then this state is at least f-dimensionally genuine multipartite entangled.

4 Proof

One standard strategy for detecting entanglement or distinguishing different types of entanglement is to introduce a quantity $Q(\rho)$ and to maximize it over all states of a specific type (e.g. k-separable states, states with particular Schmidt-rank, states of an entanglement class, etc.). Consequently, if for a particular state ρ this maximum is exceeded, it necessarily must be of a different kind. The main problem in deriving entanglement criteria in this way is the involved maximization. The complexity of this problem can be reduced by using quantities $Q(\rho)$ which are convex in ρ, because in this case the optimization has to be performed over all pure states only. Nevertheless, the difficulty of finding the global maximum remains.

In the present paper, a completely new approach is used. Namely, the convex quantities Q_m are constructed by incorporating the matrix elements of specific f-dimensionally GME states. This is done in a way such that by construction any other state of same or lower dimensionality cannot reach a certain bound. Thus, to prove that $Q_m \leq f - 1$ holds for all states which are entangled in equal or less than f degrees, no maximization has to be carried out.

First, consider the f-dimensionally genuine n-partite entangled *GHZ* state

$$\left|GHZ_f\right\rangle = \frac{1}{\sqrt{f}} \sum_{i=0}^{f-1} |i\rangle^{\otimes n} \ . \tag{8}$$

In density matrix form $\rho_{fGHZ} = \left|GHZ_f\right\rangle\left\langle GHZ_f\right|$, the only nonzero elements are $\langle k|^{\otimes n} \rho_{fGHZ} |l\rangle^{\otimes n} = \frac{1}{f}$. Each term $|\langle k_n| \rho |l_n\rangle|$ in (1) singles out the absolute value of an off-diagonal element of ρ_{fGHZ}, such that

$$\sum_{k \neq l} |\langle k_n| \rho_{fGHZ} |l_n\rangle| = 2\binom{f}{2}\frac{1}{f} = f - 1. \tag{9}$$

As can easily be confirmed, all terms $\sqrt{\langle k, l| \mathcal{P}_A^\dagger \rho_{fGHZ}^{\otimes 2} \mathcal{P}_A |k, l\rangle}$ vanish for any choice of k, l and any bipartition $(A|B)$ as the corresponding matrix elements are all zero. Thus, we have shown that $Q_0 = f - 1$ for ρ_{fGHZ}. In addition, it was proven in [32] that

$$|\langle k_n| \rho |l_n\rangle| - \sum_{\gamma} \sqrt{\langle k, l| \mathcal{P}_A^\dagger \rho^{\otimes 2} \mathcal{P}_A |k, l\rangle} \leq 0 \tag{10}$$

holds for all biseparable states. Hence, each of these terms (10) can only be larger than zero if the state ρ is genuine multipartite entangled in $|k\rangle$ and $|l\rangle$. Now, since in (1) the absolute values of all off-diagonal elements of ρ_{fGHZ} are added up, and since all terms which are subtracted from this sum are zero for ρ_{fGHZ}, it follows that $\left|GHZ_f\right\rangle$ is the only f-dimensionally GME pure state that reaches $Q_0 = f - 1$. Thus, any state that exceeds $f-1$ must at least be $(f+1)$-dimensionally GME, which proves (7) for $m = 0$.

Due to the way it is constructed, the function (1) is optimally suited to detect high-dimensional genuine multipartite entanglement in mixed states which are close to GHZ states. To show that the quantities Q_m serve their purpose (7) for $m > 0$, we introduce the f-dimensionally genuine multipartite entangled *m-Dicke state* ($m \in \{1, \ldots, \lfloor \frac{n}{2} \rfloor\}$)

$$|D_f^m\rangle := \frac{1}{\sqrt{(f-1)\binom{n}{m}}} \sum_{l=0}^{f-2} \sum_{\alpha} \bigotimes_{i\in\alpha} |l+1\rangle_i \bigotimes_{i\notin\alpha} |l\rangle_i \ , \tag{11}$$

where the inner sum runs over all α with $|\alpha| = m$ (see also [33]). Note that this includes a generalization $\left|W_f\right\rangle = |D_f^1\rangle$ of the prominent W state for qudits[2]. First, observe that for any fixed choice of $k = l$ in Q_m, (2) reduces to the inequalities from Refs. [32,33], i.e. in this case it is proven that $Q_m \leq 0$ holds for all biseparable states. On the other hand, by summing over all k and l in Q_m we add up the absolute value of specific off-diagonal elements $O_{\alpha,\beta}^{k,l}$ of the *m-Dicke state* $|D_f^m\rangle$. From these off-diagonal elements (determined by the proper set σ) there are corresponding diagonal elements (labeled $P_{\alpha,\beta}^{k,l}$) subtracted, which correspond to biseparable states having the same off-diagonal elements. For a subset of all those off-diagonal elements this suffices (as with the inequality based on Q_0), however, for some there are no corresponding diagonal elements belonging to a biseparable state. In order to guarantee that $Q_m \leq 0$ for all biseparable states one also needs to subtract the corresponding diagonal elements of the *Dicke state* (labeled D_α^l). Counting the cardinality of this subset is a purely combinatorial problem (similar to [33]) resulting in the factor N_D. By construction, this guarantees for fixed dimensionality, the maximal value of Q_m for the corresponding *Dicke state*, as in this case the sum of the off-diagonal elements is maximal, whereas all $P_{\alpha,\beta}^{k,l}$ are zero. By scaling this maximum with the constant $\frac{1}{m}$ we can unify all quantities Q_m in one consistent framework, i.e. the only f-dimensionally GME pure state that can attain $Q_m = f - 1$ is $|D_f^m\rangle$.

5 Detection strength

The introduced criteria allow to examine the dimensionality of multipartite entanglement in a noisy environment. Figure 1 shows the robustness for the states $|GHZ_d\rangle$ and $|W_d\rangle$ in the presence of white noise. We compared the illustrated thresholds

[2] Note that a different generalization of the W state was introduced in [37]. However, the state introduced therein is local-unitarily equivalent to the original W state, and therefore does not contain higher-dimensional entanglement.

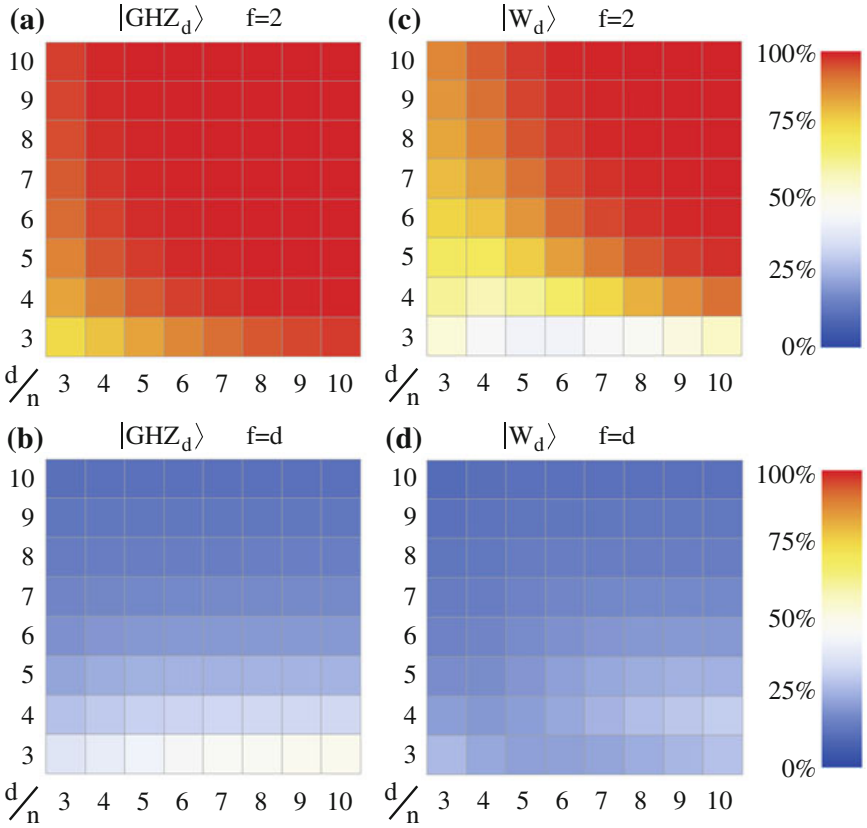

Fig. 1 (*Color online*) The noise resistance for the states $|GHZ_d\rangle$ and $|W_d\rangle$. The *scale* indicates up to which value of white noise a state is detected to be f-dimensionally genuine multipartite entangled (GME). **a** Up to the illustrated thresholds for p, the state $\rho = \frac{p}{d^n}\mathbb{1} + (1-p)\,|GHZ_d\rangle\langle GHZ_d|$ is detected to be GME, i.e. $Q_0 > 0$. **b** For noise p below the illustrated thresholds the state ρ is detected by $Q_0 > d-2$ to be truly d-dimensionally GME. **c**, **d** Illustrate these thresholds for the state $\rho = \frac{p}{d^n}\mathbb{1} + (1-p)\,|W_d\rangle\langle W_d|$ using $Q_1(\rho) > f-2$

with the thresholds of entanglement witnesses that follow from the fidelity of a state (see [31,27]), i.e. a state is d-dimensionally GME if $\langle GHZ_d|\,\rho\,|GHZ_d\rangle > \frac{d-1}{d}$ or $\langle W_d|\,\rho\,|W_d\rangle > \frac{n(d-1)-1}{n(d-1)}$, respectively. Here, we found that our criteria are strictly stronger for all $d > 2$ and $n > 2$—specifically, they outperform the noise robustness of previously known criteria [31] for *GHZ*-like states. E.g., the tripartite state

$$\rho = (1-p)\,|GHZ_3\rangle\langle GHZ_3| + p\frac{1}{27}\mathbb{1}, \tag{12}$$

is detected to be 3-dimensionally GME by $Q_0 > 1$ for $0 \leq p < 0.375$, whereas $\langle GHZ_3|\,\rho\,|GHZ_3\rangle > \frac{2}{3}$ merely detects the range $0 \leq p < 0.346$. For

$$\rho = (1-p)\,|W_3\rangle\langle W_3| + p\frac{1}{27}\mathbb{1} \tag{13}$$

the difference is even more significant: Using $Q_1 > 1$, we detect the range $0 \leq p < 0.265$ in comparison to $0 \leq p < 0.173$ following from $\langle W_3|\,\rho\,|W_3\rangle > \frac{5}{6}$. A further

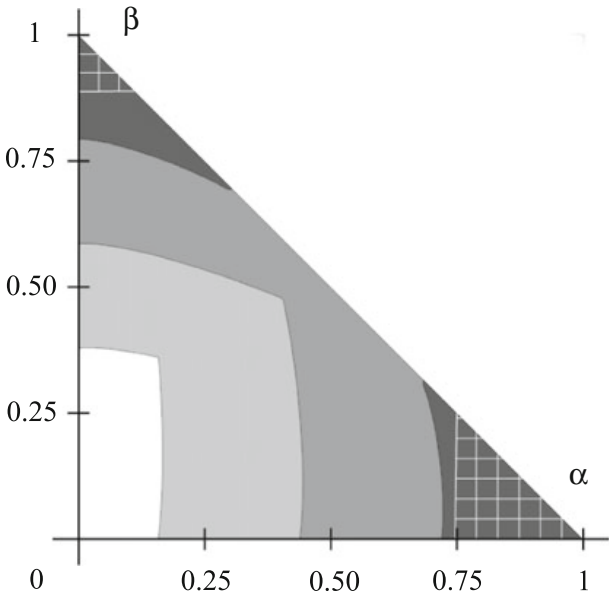

Fig. 2 Illustration of the detection strength of $Q_0, Q_1 > f - 2$ for the tripartite four-level state $\rho = \alpha\,|GHZ_4\rangle\langle GHZ_4| + \beta\,|W_4\rangle\langle W_4| + \frac{1-\alpha-\beta}{64}\mathbb{1}$. The *dark gray region* is detected to be 4-dimensionally GME (in comparison, fidelity-based criteria merely detect the *white meshed part* of this region to be 4-dimensionally GME). The *middle gray region* is detected to be at least 3-dimensionally GME, and the *light gray region* is detected to be at least 2-dimensionally GME

example of the detection strength is given in Fig. 2. As can be seen therein, the region of states detected by our criteria is considerably larger than the region revealed by fidelity-based witnesses. Finally, let us stress that the quantities Q_m are by construction optimally suited to detect f-dimensional GME states which are close to *GHZ*, *W* and *Dicke states*. If instead an unclassified input state is given one can improve the detection by maximizing the outcome of Q_m over local-unitary transformations. An appropriate optimization scheme can be found in [38–40].

6 Conclusion

Creating high-dimensional multipartite entangled states is one of the current challenges in experiments on quantum physics. In the present paper, we gave a precise mathematical characterization of such states and provided criteria for the dimensionality of genuine multipartite entanglement applicable to arbitrary multi-qudit systems. These criteria are easily computable since they do not rely on semidefinite programming or eigenvalue computations, but only on functions of density matrix elements. They are also advantageous in experiments, as they are rather robust against noise and to apply them it is not necessary to determine the entire density matrix of the system under consideration. In detail, due to the fact that the quantities Q_m only involve the matrix elements of *GHZ*, *W* and *Dicke states*, it is merely needed to determine these few entries of the density matrix, which can always be achieved via local measurements and corresponding correlations (see also the discussion in e.g. [32–35]). Consequently, they can be experimentally implemented with a reduced number of local observables, since the number of measurements for a full quantum state tomography scales exponentially in the number of parties n, i.e. is of the order $\mathcal{O}(d^{2n})$ [41], whereas the number of density matrix elements that occur in Q_m is only of the order $\mathcal{O}(d^2\binom{n}{m})$, that is polynomial in n (Note that the notation in terms of two-fold copies of a state is only a matter of

compactness, i.e. in experiments it is not necessarily needed to have two copies at a time). Finally, it is noteworthy that our results are even promising to be closely related to measures of genuine multipartite entanglement, as e.g. for multipartite qubits the quantity Q_0 yields a strong lower bound on the *gme-concurrence* [42].

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Measure of genuine multipartite entanglement with computable lower bounds

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We introduce an intuitive measure of genuine multipartite entanglement, which is based on the well-known concurrence. We show how lower bounds on this measure can be derived and also meet important characteristics of an entanglement measure. These lower bounds are experimentally implementable in a feasible way enabling quantification of multipartite entanglement in a broad variety of cases.

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I. INTRODUCTION

Entanglement is an essential component in quantum information and at the same time a central feature of quantum mechanics [1,2]. Its potential applications in quantum information processing vary from quantum cryptography [3] and quantum teleportation [4] to measurement-based quantum computing [5]. The use of entanglement as a resource bears not only on the question of how it can be detected, but also on how it can be quantified. For this purpose, several entanglement measures have been introduced, one of the most prominent of which is concurrence [1,2,6]. However, beyond bipartite qubit systems [6] and highly symmetric bipartite qudit states such as isotropic states and Werner states [7,8], there exists no analytic method to compute the concurrence of arbitrary high-dimensional mixed states. For a bipartite pure state $|\psi\rangle$ in a finite-dimensional Hilbert space $\mathcal{H}_1 \otimes \mathcal{H}_2 = \mathbb{C}^{d_1} \otimes \mathbb{C}^{d_2}$ the concurrence is defined as [9] $C(|\psi\rangle) = \sqrt{2(1-\mathrm{Tr}\,\rho_1^2)}$ where $\rho_1 = \mathrm{Tr}_2\rho$ is the reduced density matrix of $\rho = |\psi\rangle\langle\psi|$. For mixed states ρ the concurrence is generalized via the convex roof construction $C(\rho) = \inf_{\{p_i,|\psi_i\rangle\}} \sum_i p_i C(|\psi_i\rangle)$ where the infimum is taken over all possible decompositions of ρ, i.e., $\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$. This generalization is well defined; however, as it involves a nontrivial optimization procedure it is not computable in general. The concurrence is a useful measure with respect to a broad variety of tasks in quantum information that exploit entanglement between two parties. However, considering multipartite systems, a generalization of the concurrence is needed that strictly quantifies the amount of genuine multipartite entanglement—the type of entanglement that not only is the key resource of measurement-based quantum computing [10] and high-precision metrology [11] but also plays a central role in biological systems [12,13], quantum phase transitions [14,15], and quantum spin chains [16]. Although many criteria to detect genuine multipartite entanglement have been introduced (see, e.g., Refs. [17–32]), there is still no computable measure quantifying the amount of genuine multipartite entanglement present in a system. There are only a few quantities available for pure states (a set of possible measures is given in Ref. [33]), which, however, are in general incomputable for mixed states, and corresponding computable lower bounds have not been found so far. In this paper, we define a generalized concurrence (analogously to a measure proposed for pure states in Ref. [34]) for systems of arbitrarily many parties as an entanglement measure that distinguishes genuine multipartite entanglement from partial entanglement. Our main result is that we show that strong lower bounds on this measure can be derived by exploiting close analytic relations between this concurrence and recently introduced detection criteria for genuine multipartite entanglement.

II. GENUINE MULTIPARTITE ENTANGLEMENT

An n-partite pure state $|\psi\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \ldots \otimes \mathcal{H}_n$ is called biseparable if it can be written as $|\psi\rangle = |\psi_A\rangle \otimes |\psi_B\rangle$, where $|\psi_A\rangle \in \mathcal{H}_A = \mathcal{H}_{j_1} \otimes \ldots \otimes \mathcal{H}_{j_k}$ and $|\psi_B\rangle \in \mathcal{H}_B = \mathcal{H}_{j_{k+1}} \otimes \ldots \otimes \mathcal{H}_{j_n}$ under any bipartition of the Hilbert space, i.e., a particular order $\{j_1, j_2, \ldots, j_k | j_{k+1}, \ldots, j_n\}$ of $\{1,2,\ldots,n\}$ (for example, for a four-partite state, $\{1,3|2,4\}$ is a partition of $\{1,2,3,4\}$). An n-partite mixed state ρ is biseparable if it can be written as a convex combination of biseparable pure states $\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$, wherein the contained $\{|\psi_i\rangle\}$ can be biseparable with respect to different bipartitions (thus, a mixed biseparable state does not need to be separable with respect to any particular bipartition of the Hilbert space). If an n-partite state is not biseparable then it is called genuinely n-partite entangled.

If we denote the set of all biseparable states by $\mathcal{S}_2$ and the set of all states by $\mathcal{S}_1$ we can illustrate the convex nested structure of multipartite entanglement (see Fig. 1).

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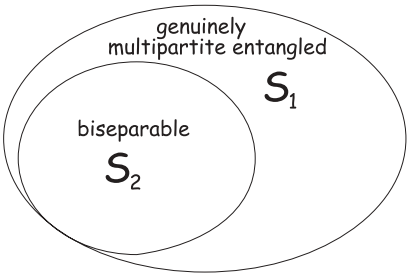

FIG. 1. Illustration of the convex nested structure of multipartite entanglement. The set of biseparable states $\mathcal{S}_2$ is convexly embedded within the set $\mathcal{S}_1$ of all states ($\mathcal{S}_2 \subset \mathcal{S}_1$).

A measure of genuine multipartite entanglement (GME) $E(\rho)$ should at least satisfy:

M1 $E(\rho) = 0 \; \forall \; \rho \in \mathcal{S}_2$ (zero for all biseparable states).

M2 $E(\rho) > 0 \; \forall \; \rho \in \mathcal{S}_1$ (detecting all GME states).

M3 $E(\sum_i p_i \rho_i) \leqslant \sum_i p_i E(\rho_i)$ (convex).

M4 $E(\Lambda_{LOCC}[\rho]) \leqslant E(\rho)$ [nonincreasing under local operations and classical communication (LOCC)].[1]

M5 $E(U_{local}\rho U_{local}^{\dagger}) = E(\rho)$ (invariant under local unitary transformations).

There are of course further possible conditions that are sometimes required (such as, e.g., additivity), but this set of conditions constitutes the minimal requirement for any entanglement measure. For a more detailed analysis of such requirements consult, e.g., Refs. [33,35].

III. CONCURRENCE FOR GENUINE *n*-PARTITE ENTANGLEMENT

Let us now introduce a measure of multipartite entanglement satisfying all necessary conditions (M1–M5) for being a multipartite entanglement measure.

Definition 1. For n-partite pure states $|\Psi\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \cdots \otimes \mathcal{H}_n$, where $\dim(\mathcal{H}_i) = d_i, i = 1,2,\ldots,n$ we define the GME-concurrence as

$$C_{GME}(|\Psi\rangle) := \min_{\gamma_i \in \gamma} \sqrt{2\left[1 - \mathrm{Tr}\left(\rho_{A_{\gamma_i}}^2\right)\right]}, \tag{1}$$

where $\gamma = \{\gamma_i\}$ represents the set of all possible bipartitions $\{A_i|B_i\}$ of $\{1,2,\ldots,n\}$. The GME-concurrence can be generalized for mixed states ρ via a convex roof construction, i.e.,

$$C_{GME}(\rho) = \inf_{\{p_i,|\psi_i\rangle\}} \sum_i p_i C_{GME}(|\psi_i\rangle), \tag{2}$$

where the infimum is taken over all possible decompositions $\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$. For example, for a tripartite pure state $|\psi\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \mathcal{H}_3$ there are three possible bipartitions $\gamma = \{\{1|2,3\},\{2|1,3\},\{3|1,2\}\}$. Consequently, the GME concurrence is $C_{GME}(\psi) = \min\{\sqrt{2[1-\mathrm{Tr}\,(\rho_1^2)]}, \sqrt{2[1-\mathrm{Tr}\,(\rho_2^2)]}, \sqrt{2[1-\mathrm{Tr}\,(\rho_3^2)]}\}$.

The definition of $C_{GME}(\rho)$ directly implies $C_{GME}(\rho) = 0$ for all biseparable states (M1) and $C_{GME}(\rho) > 0$ for all genuinely n-partite entangled states (M2). Convexity (M3) also follows directly from the fact that any mixture $\lambda\rho_1 + (1-\lambda)\rho_2$ of two density matrices ρ_1 and ρ_2 is at least decomposable into states that attain the individual infima. As the concurrence of any subsystem has been proven to be nonincreasing under LOCC (see, e.g., Ref. [9]), the minimum of all possible concurrences will of course still remain nonincreasing, thus proving (M4) also holds. Furthermore $\mathrm{Tr}(\rho^2)$ is invariant under local unitary transformations for every reduced density matrix irrespective of the decomposition, which proves that also condition (M5) holds. For pure states the GME-concurrence is closely related to the entanglement of the minimum bipartite entropy introduced for pure states in Ref. [34]. In contrast to the original definition using von Neumann entropies of reduced density matrices, we use linear entropies. In this way we can derive lower bounds even on the convex roof extension, which had not been considered before.

IV. LOWER BOUNDS ON THE GME-CONCURRENCE

As the computation of any proper entanglement measure is in general an NP-hard problem (see Ref. [36]), it is crucial for the quantification of entanglement that reliable lower bounds can be derived. These lower bounds should be computationally simple and also experimentally (locally) implementable to be of any use in practical applications. Let us now derive lower bounds on C_{GME} that meet these requirements. Consider inequality II from Ref. [17], which is satisfied by all biseparable states (such that its violation implies genuine multipartite entanglement):

$$\underbrace{\sqrt{\langle\Phi|\rho^{\otimes 2}\Pi_{\{1,2,\ldots,n\}}|\Phi\rangle} - \sum_{\gamma}\sqrt{\langle\Phi|\Pi_\gamma\rho^{\otimes 2}\Pi_\gamma|\Phi\rangle}}_{=:I[\rho,|\Phi\rangle]} \leqslant 0, \tag{3}$$

where $|\Phi\rangle$ is any state separable with respect to the two copy Hilbert spaces and $\Pi_{\{\alpha\}}$ is the cyclic permutation operator acting on the twofold copy Hilbert space in the subsystems defined by $\{\alpha\}$, i.e., exchanging the vectors of the subsystems $\{\alpha\}$ of the first copy with the vectors of the subsystems $\{\alpha\}$ of the second copy. A simple example would be $\Pi_{\{1\}}|\phi_1\phi_2\rangle \otimes |\psi_1\psi_2\rangle = |\psi_1\phi_2\rangle \otimes |\phi_1\psi_2\rangle$.

For the sake of comprehensibility let us show how to derive lower bounds for three qubits and then generalize the result (in the Appendix). If we consider the most general three-qubit pure state in the computational basis

$$\begin{aligned}|\psi\rangle = {} & a|000\rangle + b|001\rangle + c|010\rangle + d|011\rangle \\ & + e|100\rangle + f|101\rangle + g|110\rangle + h|111\rangle,\end{aligned} \tag{4}$$

the squared concurrences $C^2(\rho_\gamma) = 2[1 - \mathrm{Tr}\,(\rho_\gamma^2)]$ with respect to the three bipartitions read

$$C^2(\rho_1) = 4|ah - de|^2 + F_1, \tag{5}$$

$$C^2(\rho_2) = 4|ah - cf|^2 + F_2, \tag{6}$$

$$C^2(\rho_3) = 4|ah - bg|^2 + F_3, \tag{7}$$

[1] On a single copy. The property of being nonincreasing under LOCC in general cannot be required of any measure of genuine multipartite entanglement, as it has been shown (e.g., in Ref. [2]) that genuine multipartite entanglement can locally be distilled out of a biseparable state if more copies are available.

where F_i are nonnegative functions. The following relations thus hold:

$$C(\rho_1) \geqslant 2|ah - de| \geqslant 2|ah| - 2|de|, \tag{8}$$
$$C(\rho_2) \geqslant 2|ah - cf| \geqslant 2|ah| - 2|cf|, \tag{9}$$
$$C(\rho_3) \geqslant 2|ah - bg| \geqslant 2|ah| - 2|bg|, \tag{10}$$

and finally

$$\begin{aligned} &\min\{C(\rho_1), C(\rho_2), C(\rho_3)\} \\ &\quad \geqslant 2|ah| - 2\max\{|de|, |cf|, |bg|\} \\ &\quad \geqslant 2|ah| - 2(|de| + |cf| + |bg|) =: B. \end{aligned} \tag{11}$$

Now for any given mixed state the convex roof construction is bounded by

$$C_{GME}(\rho) \geqslant \inf_{\{p_i, |\psi_i\rangle\}} \sum_i p_i B_i. \tag{12}$$

For the choice $|\Phi\rangle = |000111\rangle$ and the abbreviation $\rho_{uvwxyz} := \langle uvw|\rho|xyz\rangle$, inequality (3) reads

$$\begin{aligned} I[\rho, |000111\rangle] = |\rho_{000111}| - \sqrt{\rho_{001001}\rho_{110110}} \\ - \sqrt{\rho_{010010}\rho_{101101}} - \sqrt{\rho_{100100}\rho_{011011}} \leqslant 0. \end{aligned} \tag{13}$$

Now

$$2|\rho_{000111}| \leqslant \inf_{\{p_i, |\psi_i\rangle\}} \sum_i p_i 2|a_i h_i|, \tag{14}$$

due to the triangle inequality, and

$$2\sqrt{\rho_{001001}\rho_{110110}} \geqslant \inf_{\{p_i, |\psi_i\rangle\}} \sum_i p_i 2|b_i g_i|, \tag{15}$$

holds due to the Cauchy-Schwarz inequality (and, of course, for all parts of the other bipartitions).

This leads to a lower bound on the convex roof construction

$$C_{GME}(\rho) \geqslant 2I[\rho, |000111\rangle]. \tag{16}$$

As $C_{GME}(\rho)$ is invariant under local unitary transformations, we can infer that indeed every $2I[\rho, |\Phi\rangle]$ constitutes a proper lower bound. By taking into account the set of all vectors $\{|\Phi\rangle\}$ we can thus define a computable lower bound, which itself has many favorable properties (satisfying M1, M3, M4, and M5):

$$C_{GME}(\rho) \geqslant \max_{|\Phi\rangle} 2I[\rho, |\Phi\rangle]. \tag{17}$$

As the lower bound is straightforwardly generalized (the structure of the proof essentially remains the same; see the Appendix for details), Eq. (17) is indeed a proper lower bound on (1) for any n-partite qudit state.

V. DISCUSSION

The detection quality of our obtained bounds on the GME-concurrence is illustrated in Fig. 2 for the family $\rho = c_1|\mathrm{GHZ}\rangle\langle\mathrm{GHZ}| + c_2|W\rangle\langle W| + \frac{1-c_1-c_2}{8}\mathbb{1}$ of three-qubit states, where

$$\begin{aligned} |\mathrm{GHZ}\rangle &= \tfrac{1}{\sqrt{2}}(|000\rangle + |111\rangle) \quad \text{and} \\ |W\rangle &= \tfrac{1}{\sqrt{3}}(|001\rangle + |010\rangle + |100\rangle) \end{aligned} \tag{18}$$

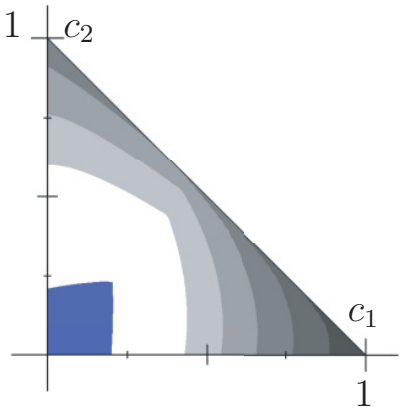

FIG. 2. (Color online) Contour plot of the lower bound $\max_{|\Phi\rangle} 2I[\rho, |\Phi\rangle]$ on the GME-concurrence for the set of three-qubit states $\rho = c_1|\mathrm{GHZ}\rangle\langle\mathrm{GHZ}| + c_2|W\rangle\langle W| + \frac{1-c_1-c_2}{8}\mathbb{1}$ given by convex mixtures of a GHZ state, W state, and the maximally mixed state. The grayscale is related to the bound $\max_{|\Phi\rangle} 2I[\rho, |\Phi\rangle]$ varying from 0 to 1 (where 0 is white), while the blue region (bottom left corner) denotes states that are positive under partial transposition with respect to all bipartitions. The optimization over all $\{|\Phi\rangle\}$ was realized using the composite parametrization of the unitary group (see Ref. [37]).

are the well-known genuinely multipartite entangled GHZ and W states, respectively. It can be seen that the bounds are nonzero for a considerable amount of multipartite entangled states, especially in the vicinity of the GHZ state.

In fact, our bounds are exact for GHZ-like states, i.e., states of the form $|g\mathrm{GHZ}\rangle = \alpha|0'\rangle^{\otimes n} + \beta|1'\rangle^{\otimes n}$ wherein $|0'\rangle \in \mathcal{H}_i$ and $|1'\rangle \in \mathcal{H}_i$ are arbitrary mutually orthogonal vectors. By expanding $|g\mathrm{GHZ}\rangle$ in terms of $|0'\rangle$ and $|1'\rangle$ analogously to (4) one finds $C(\rho_{A_{\gamma_i}}) = 2|\alpha\beta|\ \forall\ \gamma_i$, hence $C_{GME}(\rho) = 2|\alpha\beta|$. In order to prove the exactness of the bound we choose $|\phi\rangle = |0'\rangle^{\otimes n}|1'\rangle^{\otimes n}$ for inequality (3), which then yields $2I[|g\mathrm{GHZ}\rangle\langle g\mathrm{GHZ}|, |\phi\rangle] = 2|\alpha\beta|$. In fact we already know from the results of Ref. [17] that the inequality will detect a huge amount of genuinely multipartite entangled mixed states in arbitrary high-dimensional and multipartite systems. In all of these situations we thus also have a lower bound on the GME concurrence.

VI. EXPERIMENTAL IMPLEMENTATION

In order to be useful in practice, measures for multipartite entanglement need to be experimentally implementable by means of local observables (since all particles of composite quantum systems may not be available for combined measurements) without resorting to a full quantum state tomography (since the latter requires a vast number of measurements, which is unfeasible in practice). The bound (17) satisfies these demands, as for fixed $|\Phi\rangle$ its computation only requires at most the square root of the number of measurements needed for a full state tomography. Furthermore it can be implemented locally as explicitly shown in [18]. In an experimental situation where one aims at producing a certain state $|\psi\rangle$, it is now possible to choose the corresponding $|\phi\rangle$ and not only detect the state as being genuinely multipartite entangled, but also have a reliable statement about the amount of multipartite

entanglement the state exhibits. Even if the produced state deviates from the desired states, the criteria are astonishingly noise robust (as, e.g., analyzed in Ref. [17]), as for example a GHZ state mixed with white noise is shown to be genuinely multipartite entangled with a white noise resistance of ≈57%.

VII. CONCLUSION

We introduced a measure of genuine multipartite entanglement, which can be lower bounded by means of one of the currently most powerful detection criteria. These bounds are experimentally implementable and computationally very efficient, allowing us to not only detect, but also to quantify genuine multipartite entanglement in an experimental scenario. This has serious implications for applications where genuine multipartite entanglement is a crucial resource (as, e.g., in quantum computing [5] or cryptography [38]) and might allow us to give a good estimate of the relevance of genuine multipartite entanglement in other physical systems (as, e.g., in biological systems [13] or quantum spin chains [16]).

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APPENDIX

Let us finish by proving the lower bound for the general n-qudit case. For the most general pure n-qudit state $|\psi\rangle = \sum_{i_1,i_2,\ldots,i_n} c_{i_1,i_2,\ldots,i_n}|i_1 i_2 \cdots i_n\rangle$ the squared concurrences $C^2(\rho_\gamma) = 2[1 - \mathrm{Tr}(\rho_\gamma^2)]$ with respect to arbitrary bipartitions (γ) always take the form

$$C^2(\rho_\gamma) = 4|c_{00\ldots0}c_{11\ldots1} - c_{\alpha(\gamma)}c_{\beta(\gamma)}|^2 + F_\gamma, \tag{A1}$$

where F_γ are nonnegative functions (see, e.g., Refs. [33,39] for details on how to calculate the linear entropies of arbitrary subsystems). For every bipartition γ there exists one pair $\alpha(\gamma)$ and $\beta(\gamma)$ that can be retrieved from

$$\{\alpha(\gamma),\beta(\gamma)\} = \pi_\gamma\{00\ldots0,11\ldots1\} \tag{A2}$$

where π_γ permutes every number from the subset defined by γ from the first half of the joint set with the second. Thus

$$C(\rho_\gamma) \geqslant 2|c_{00\ldots0}c_{11\ldots1} - c_{\alpha(\gamma)}c_{\beta(\gamma)}| \tag{A3}$$

will hold also for every γ. Now for the GME-concurrence we can infer

$$\min_\gamma\{C(\rho_\gamma)\} \geqslant 2|c_{00\ldots0}c_{11\ldots1}| - \left(\sum_\gamma |c_{\alpha(\gamma)}c_{\beta(\gamma)}|\right) =: B. \tag{A4}$$

Now for any given mixed state the convex roof construction is bounded by

$$C_{GME}(\rho) \geqslant \inf_{\{p_i,|\psi_i\rangle\}} \sum_i p_i B_i. \tag{A5}$$

For the choice $|\Phi\rangle = |0\rangle^{\otimes n} \otimes |1\rangle^{\otimes n}$, inequality (3) reads

$$I[\rho,|\Phi\rangle] = |\rho_{00\ldots011\ldots1}| - \sum_\gamma \sqrt{\rho_{\alpha(\gamma)\alpha(\gamma)}\rho_{\beta(\gamma)\beta(\gamma)}} \leqslant 0. \tag{A6}$$

Now

$$2|\rho_{00\ldots011\ldots1}| \leqslant \inf_{\{p_i,|\psi_i\rangle\}} \sum_i p_i 2\left|c^i_{00(\cdots)0}c^i_{11(\cdots)1}\right|, \tag{A7}$$

due to the triangle inequality and

$$\sqrt{\rho_{\alpha(\gamma)\alpha(\gamma)}\rho_{\beta(\gamma)\beta(\gamma)}} \geqslant \inf_{\{p_i,|\psi_i\rangle\}} \sum_i p_i 2|c_{\alpha(\gamma)}c_{\beta(\gamma)}|, \tag{A8}$$

due to the Cauchy-Schwarz inequality.

This leads to a lower bound on the convex roof construction

$$C_{GME}(\rho) \geqslant 2I[\rho,|\Phi\rangle]. \tag{A9}$$

And again due to the local unitary invariance of $C_{GME}(\rho)$ this proves our lower bound for all $|\Phi\rangle$.

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Experimentally implementable criteria revealing substructures of genuine multipartite entanglement

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We present a general framework that reveals substructures of genuine multipartite entanglement. Via simple inequalities it is possible to discriminate different sets of multipartite qubit states. These inequalities are beneficial regarding experimental examinations as only local measurements are required. Furthermore, the number of observables scales favorably with system size. In exemplary cases we demonstrate the noise resistance and discuss implementations.

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I. INTRODUCTION

Quantum entanglement has been subject to intense studies in various directions for several decades and has been found in many different physical systems, including systems not consisting of ordinary matter and light (see, e.g., Refs. [1,2]). It gave rise to several concepts for new technologies such as quantum cryptography (see, e.g., Ref. [3]), quantum computation (e.g., Ref. [4]), or quantum teleportation (e.g., Ref. [5]). Despite these efforts, entanglement is still far from being completely understood (for an overview, see, e.g., Ref. [6]) and particularly in multipartite entanglement (see, e.g., Refs. [7,8]) there are many unanswered questions remaining. One of these open questions concerns the problem of classification of multipartite entanglement. This is usually addressed in terms of separability properties (which has been studied, e.g., in Refs. [9–11]) or, in more detail, in terms of density matrix decomposition equivalence classes. The focus of this work is the latter.

While for bipartite entanglement, states can be characterized comparatively easily by means of Schmidt numbers [12], multipartite entangled states have a much more complicated structure, which is only known explicitly for very special cases. For example, for three qubits, there are four distinct classes of states [13,14], namely separable ones, biseparable ones (i.e., states with two entangled particles which are separable from the third), and the two well-known classes of genuinely multipartite entangled states, the Greenberger-Horne-Zeilinger (GHZ) state and the W state (see Ref. [13]). For four qubits there are nine different classes (see Ref. [15]) and beyond that there is no known classification scheme.

Employing and classifying the substructure of (genuine) entanglement is of interest as current experiments are continuously improving in controlling larger and larger multipartite entangled systems, e.g., in quantum optics with photons (see, e.g., Refs. [16–18]) or with ions (see, e.g., Refs. [19,20]) or in circuit QED of superfluid systems (see, e.g., Refs. [21,22]). However, it is also important to be able to determinate the entanglement class as, e.g., the security of secrete sharing protocols rely on them (see Ref. [23]).

In this manuscript, we use the framework introduced in Ref. [24] in order to derive general inequalities, capable of distinguishing between different classes for multipartite qubit systems. So far, classes were usually defined with respect to stochastic local operations and classical communication (SLOCC) equivalence (for details see Refs. [25–29]), which captures whether given states can be converted into each other via stochastic local operations and classical communication. Here we pursue a different approach, defining certain equivalence classes that arise via local unitaries and permutations. This has the advantage that this class definition is Lorentz invariant (see Ref. [30]) and we are able to develop inequalities to distinguish between these classes in an experimentally feasible way. This manuscript is organized as follows: In Sec. II the basic terminology and definitions are introduced, so in Sec. III criteria for discriminating different classes of states can be presented, which is the main result of this work. These criteria are then tested and illustrated for a particular class of states in Sec. IV and thoroughly discussed in Sec. V.

II. CLASSIFYING MULTIPARTITE ENTANGLED STATES

Let us first repeat the definition for a multipartite state to be k-separable [6]. A pure n-partite state $|\Psi\rangle$ is called *k-separable* if it can be written as a product

$$|\Psi^k\rangle = |\phi_1\rangle \otimes |\phi_2\rangle \otimes \cdots \otimes |\phi_k\rangle, \quad k \leqslant n, \tag{1}$$

of k states $|\phi_i\rangle$, each of which corresponds to a single subsystem or a group of subsystems. If $k = n$, then the state is fully separable. If $k = 1$, i.e., there is no such form with at least two factors, then $|\Psi\rangle$ is 1-separable or genuinely n-partite entangled. For example, the well-known GHZ state $\frac{1}{\sqrt{2}}\{|000\rangle + |111\rangle\}$ and the W state $\frac{1}{\sqrt{3}}\{|001\rangle + |010\rangle + |100\rangle\}$ are genuinely multipartite entangled while, e.g., the state $\frac{1}{\sqrt{2}}\{|00\rangle + |11\rangle\}|0\rangle$ is 2-separable or biseparable.

For mixed states the definition of k separability is straightforward: A state is k separable if and only if the state can be

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decomposed into pure states

$$\varrho = \sum_i p_i \left|\Psi_i^k\right\rangle\left\langle\Psi_i^k\right|, \quad p_i > 0 \quad \text{and} \quad \sum_i p_i = 1, \tag{2}$$

wherein all contained pure states are at least k separable and at least one pure state is k separable (i.e., there exists no decomposition with $(k+1)$-separable states and no $(k-1)$-separable state is needed in the decomposition). Note that a mixed state can still be partially separable, even if the k subsystems cannot be split into two groups that are not entangled with each other. For example, the following tripartite state is biseparable (2-separable)

$$\begin{aligned} \varrho &= \sum_i p_i \rho_{12}^i \otimes \rho_3^i + \sum_i q_i \rho_{13}^i \otimes \rho_2^i + \sum_i r_i \rho_{23}^i \otimes \rho_1^i \\ \text{with} \quad & p_i, q_i, r_i > 0 \quad \text{and} \quad \sum_i p_i + \sum_j q_j + \sum_k r_k = 1, \end{aligned} \tag{3}$$

where ρ_{xy}^i are pure entangled bipartite states. Even though there is no bipartite splitting with respect to which the state is separable, it is considered biseparable since it can be prepared through a statistical mixture of bipartite entangled states. The nested structure of k separability is shown in Fig. 1.

For pure states the question of k separability can be answered by common separability criteria for bipartite systems, simply by considering all segmentations of the k-partite system into two parts. However, the same question becomes significantly more difficult to answer for mixed states ϱ. In Ref. [31] separability criteria for arbitrary k in form of simple inequalities have been introduced.

An equivalence class (with respect to density matrix decompositions) is defined as follows:

Definition 1. A class $\mathcal{C}(\{|\Psi_x^k\rangle\})$ is defined as the set of convex mixtures of local unitary equivalents and permutational equivalents of k-separable states $|\psi_j\rangle \in \{|\Psi_x^k\rangle\}$, excluding all higher separable states ($k' > k$) within that set

$$\begin{aligned} &\mathcal{C}\left(\left\{\left|\Psi_x^k\right\rangle\right\}\right) \\ &:= \left\{\sum_{i,j} p_i U_{\text{loc}}^i \Pi^i |\psi_j\rangle\langle\psi_j| {\Pi^i}^\dagger {U_{\text{loc}}^i}^\dagger\right\} \Bigg\backslash \bigcup_{i,k'>k} \mathcal{C}\left(\left\{\left|\Psi_i^{k'}\right\rangle\right\}\right). \end{aligned} \tag{4}$$

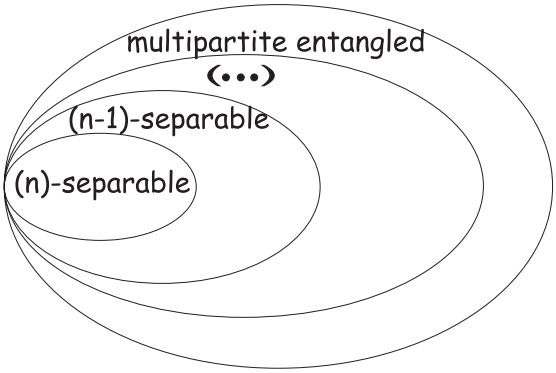

FIG. 1. Here the nested convex structure of k separability in multipartite systems is illustrated.

Here, the index x labels a defining property for the set $\{|\Psi_x^k\rangle\}$, e.g., the tensor rank, as in the following. The $U_{\text{loc}}^i = U_1^i \otimes U_2^i \otimes (\cdots) \otimes U_n^i$ are local unitary operators and Π^i are permutation operators exchanging arbitrary subspaces in $|\psi_j\rangle\langle\psi_j|$.

In this article we are interested in all classes of genuinely multipartite entangled states, i.e., $\mathcal{C}(\{|\Psi_x^1\rangle\})$. It is an open question how many of such equivalence classes are needed in general for a decomposition of a given ρ, as in Eq. (2). The task at hand is to identify all possible families of states $\{|\Psi_x^k\rangle\}$, which in a convex sum can build up a given density matrix ρ. For n qubits we can introduce at least three such classes for arbitrary n, which can be distinguished with the mathematical framework we introduce. These three classes are defined via generalizations of the famous GHZ state (see Ref. [32]), the W state (see Ref. [13]), and the Dicke state with two excitations (see Ref. [33]). In order to avoid confusion with the previous definition and to put them into a more general framework we label them according to their respective tensor rank (for more details on the tensor rank of multipartite states see, e.g., Ref. [34]). The above definition also includes all previous classification schemes, depending on the choice of $\{|\Psi_x^k\rangle\}$ (e.g., the classification from Ref. [14] with the two appropriate choices).

Definition 2. We define the class $\mathcal{C}(\{|\Psi_{(2)}^1\rangle\})$ of "double states" for n qubits (a generalization of the GHZ state [32]) via the set

$$\left\{\left|\Psi_{(2)}^1\right\rangle\right\} := \left\{|\psi\rangle \in \mathbb{C}^{2^n} : |\psi\rangle = \lambda_1 \bigotimes_{i=1}^n |x_i\rangle + \lambda_2 \bigotimes_{i=1}^n |\overline{x}_i\rangle\right\}, \tag{5}$$

where $|x_i\rangle$ are arbitrary normalized one-qubit states and $\langle\overline{x}_i|x_i\rangle = 0$ such that $|x_i\rangle$ and $|\overline{x}_i\rangle$ form orthonormal bases of each single-qubit system, $\lambda_1, \lambda_2 \in \mathbb{C} \setminus \{0\}$ and $|\lambda_1|^2 + |\lambda_2|^2 = 1$.

Definition 3. We define the class $\mathcal{C}(\{|\Psi_{(n)}^1\rangle\})$ of "n-tuple states" for n qubits (a generalization of the W state [13]) via the set

$$\left\{\left|\Psi_{(n)}^1\right\rangle\right\} := \left\{|\psi\rangle \in \mathbb{C}^{2^n} : |\psi\rangle = \sum_{i=1}^n \lambda_i |W_i\rangle\right\}, \tag{6}$$

where $|W_i\rangle = \bigotimes_{k\neq i} |x_k\rangle \otimes |\overline{x}_i\rangle$ and $\lambda_i \in \mathbb{C} \setminus \{0\}$, satisfying $\sum_i |\lambda_i|^2 = 1$.

Definition 4. We define the class $\mathcal{C}(\{|\Psi_{(n-1)}^1\rangle\})$ of "$(n-1)$-tuple states" for n qubits (equivalent to the Dicke state for n qubits [33] with two excitations) via the set

$$\left\{\left|\Psi_{(n-1)}^1\right\rangle\right\} := \left\{|\psi\rangle \in \mathbb{C}^{2^n} : |\psi\rangle = \sqrt{\frac{2}{n(n-1)}} \sum_{i<j} |D_{ij}\rangle\right\}, \tag{7}$$

where $|D_{ij}\rangle = \bigotimes_{k\neq i,j} |x_k\rangle \otimes |\overline{x}_i\rangle \otimes |\overline{x}_j\rangle$. In Ref. [34] it was shown that this state has tensor rank $(n-1)$.

Note that our definition of these classes differs from the one introduced in the context of SLOCC equivalence in Ref. [14], where the classes are defined to be nested convex such that $W \subset \text{GHZ}$, whereas $\mathcal{C}(\{|\Psi_{(n)}^1\rangle\}) \subset \mathcal{C}(\{|\Psi_{(2)}^1\rangle\})$ is not true. Also, in our definition there are more classes than in Ref. [14],

since, for example, the most general pure three-qubit state

$$|\Psi\rangle = \lambda_1|000\rangle + \lambda_2|111\rangle + \lambda_3|001\rangle + \lambda_4|010\rangle + \lambda_5|100\rangle \tag{8}$$

(see also Ref. [35]) is contained in neither of the classes defined above when $|\lambda_i| > 0\,\forall\, i$. This is discussed in more detail in Sec. V.

In the following we will show how we can distinguish our introduced classes of genuine multipartite entanglement by certain inequalities, followed by a section showing how these inequalities are experimentally implementable.

III. DISTINGUISHING CLASSES OF STATES

In the following we present our main results. All inequalities are proven in detail in the Appendix (Sec. VI).

*The "(**n**)-tuple state" inequality I(n).* The inequality

$$\mathrm{Re}\{\langle 0|^{\otimes n}\rho|1\rangle^{\otimes n}\} - \alpha(1 - \langle 0|^{\otimes n}\rho|0\rangle^{\otimes n} - \langle 1|^{\otimes n}\rho|1\rangle^{\otimes n}) \leqslant 0 \tag{I(n)}$$

is satisfied for all biseparable states and by all states of the class $\mathcal{C}(\{|\Psi^1_{(n)}\rangle\})$, where $\alpha = \frac{3}{2}$ for $n = 3$, $\alpha = 1$ for $n = 4$, and $\alpha = \frac{1}{2}$ for $n > 4$.

The "double state" inequality I(2). The inequality

$$\begin{aligned}
&\mathrm{Re}\left\{\sum_{i\neq j}\langle w_i|\rho|w_j\rangle + (-1)^{n+1}\langle \overline{w}_i|\rho|\overline{w}_j\rangle\right\} \\
&\quad - (n-2)\sum_i(\langle w_i|\rho|w_i\rangle + \langle \overline{w}_i|\rho|\overline{w}_i\rangle) \\
&\quad - \sum_{i\neq j}(\langle d_{ij}|\rho|d_{ij}\rangle + \langle \overline{d}_{ij}|\rho|\overline{d}_{ij}\rangle) \\
&\quad - \frac{n(n-1)}{2}(\langle 0|^{\otimes n}\rho|0\rangle^{\otimes n} + \langle 1|^{\otimes n}\rho|1\rangle^{\otimes n}) \leqslant 0 \qquad \text{(I(2))}
\end{aligned}$$

is satisfied for all biseparable states and by all states of the class $\mathcal{C}(\{|\Psi^1_{(2)}\rangle\})$, where $|d_{ij}\rangle = |0\rangle^{\otimes(i-1)} \otimes |1\rangle_i \otimes |0\rangle^{\otimes(j-i-1)} \otimes |1\rangle_j \otimes |0\rangle^{\otimes(n-j)}$, $|w_i\rangle = |0\rangle^{\otimes(i-1)} \otimes |1\rangle_i \otimes |0\rangle^{\otimes(n-i)}$ and an overline denotes orthonormality in all subsystems, e.g., $|\overline{d}_{ij}\rangle = |1\rangle^{\otimes(i-1)} \otimes |0\rangle_i \otimes |1\rangle^{\otimes(j-i-1)} \otimes |0\rangle_j \otimes |1\rangle^{\otimes(n-j)}$.

The "$(n-1)$-tuple state" inequality I$(n-1)$. The inequality

$$\begin{aligned}
&\mathrm{Re}\sum_{i\neq j}\{\langle w_i|\rho|w_j\rangle\} - (n-2)\sum_i(\langle w_i|\rho|w_i\rangle \\
&\quad - (n-2)\sum_{i\neq j}(\langle d_{ij}|\rho|d_{ij}\rangle) - \frac{n(n-1)}{2}(\langle 0|^{\otimes n}\rho|0\rangle^{\otimes n}) \leqslant 0
\end{aligned} \tag{I($n-1$)}$$

is satisfied for all biseparable states and by all states of the class $\mathcal{C}(\{|\Psi^1_{((n-1))}\rangle\})$.

As these inequalities constitute only necessary conditions, their yield depends strongly on the chosen basis. So in case of unknown input states it is necessary to optimize over all local unitary operators $U = U_1 \otimes U_2 \otimes \cdots \otimes U_n$ to obtain optimal results. A parametrization of unitary operators which is suited very well for this task can be found in Ref. [36]. In Fig. 2 we illustrate the substructure of multipartite entangled states, together with the corresponding inequalities, for three- and five-qubit states.

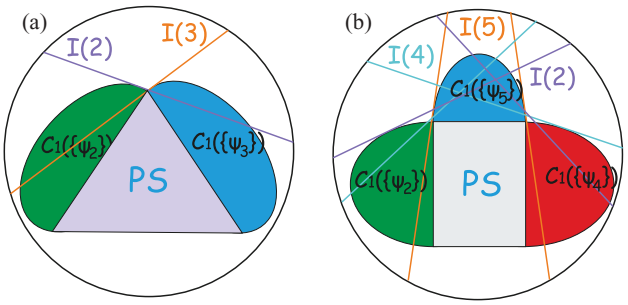

FIG. 2. (Color online) Here the structure of (a) three- and (b) five-qubit mixed states is illustrated. The three entanglement classes $\mathcal{C}(\{|\Psi^1_{(2)}\rangle\})$, $\mathcal{C}(\{|\Psi^1_{(n)}\rangle\})$, and $\mathcal{C}(\{|\Psi^1_{(n-1)}\rangle\})$ of course form convex sets together with the partially separable states, which can be excluded by our inequalities I(2), I(n), and I($n-1$) and inequality II from Ref. [24]. The partially separable states are subsumed as PS. The different sets are drawn completely disjoint, although it might still be possible that there is a nonvanishing overlap. Numerical analysis of tripartite systems suggests otherwise, but even if there was, it would not change any of the presented results. Also note that a two-dimensional picture will always fail to incorporate all essential properties of multipartite entanglement. This illustration should facilitate the understanding of how the inequalities work.

IV. EXPERIMENTAL IMPLEMENTATION

It is crucial for any criteria for large systems to be implementable experimentally without having to resort to quantum state tomography, i.e., in large systems it is beneficial if criteria are examinable without knowing all entries of a density matrix. This stems from the fact that a full state tomography for n qubits requires 2^{2n} measurement settings which for large n is unfeasible. It is also very important that the criteria are locally implementable, as in large systems global measurement operations become more complex and all particles may not be available for global manipulation.

All three criteria to distinguish the three defined subclasses of genuine multipartite entanglement are locally implementable in experiments. This can be shown as our inequalities can be rewritten in terms of local expectation values of Pauli operators. This directly follows from the fact that our inequalities consist of a linear combination of density matrix elements, where each of which can of course be expressed in terms of local expectation values. To that end let us first introduce a compact notation in order to provide the inequalities in an elegant way:

$$i_1 i_2 \cdots i_n := \langle \sigma_{i_1} \otimes \sigma_{i_2} \otimes (\cdots) \otimes \sigma_{i_n}\rangle \tag{9}$$

where $\sigma_1 := \mathbb{1}$.

In this notation the elements of density matrices can be written in a compact way, e.g., for three qubits

$$\mathrm{Re}\{\langle 000|\rho|111\rangle\} = xxx - yyx - yxy - xyy\,. \tag{10}$$

So for three qubits the "double state" inequality reads

$$(xxx - yyx - yxy - xyy) - 3(3 - zz1 - z1z - 1zz) \leqslant 0, \tag{11}$$

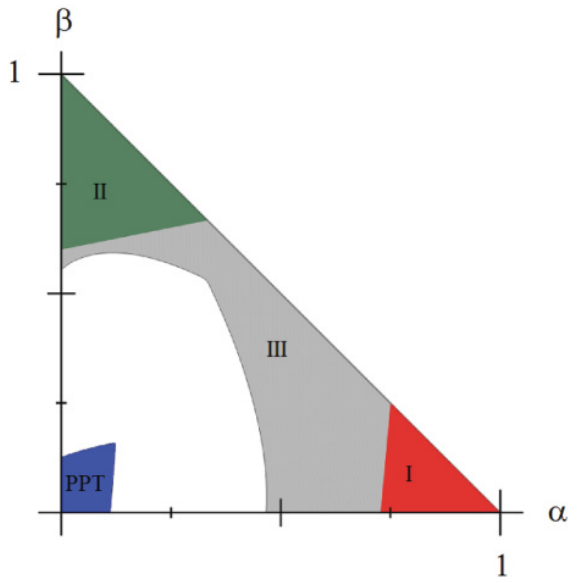

FIG. 3. (Color online) Here the entanglement classes for the four-qubit state $\rho = \alpha|\phi_1\rangle\langle\phi_1| + \beta|\phi_2\rangle\langle\phi_2| + \frac{1-\alpha-\beta}{16}\mathbb{1}$ are illustrated, with $|\phi_1\rangle = \frac{1}{\sqrt{2}}(|0000\rangle + |1111\rangle) \in \mathcal{C}\{|\Psi^1_{(2)}\rangle\}$ and $|\phi_2\rangle = \frac{1}{2}(|1000\rangle + |0100\rangle + |0010\rangle + |0001\rangle) \in \mathcal{C}\{|\Psi^1_{(4)}\rangle\}$. For the parameter region I (red) the state is not in $\mathcal{C}(\{|\Psi^1_{(4)}\rangle\})$, for region II (green) it is not in $\mathcal{C}(\{|\Psi^1_{(2)}\rangle\})$, and for region III (gray) it is genuinely multipartite entangled, as detected by the criteria introduced in Ref. [24]. The region labeled PPT (blue) contains all states which are positive under partial transposition for the two distinct bipartitions.

and the "three-tuple-state" inequality yields

$$\begin{aligned}&(1xx + xx1 + x1x + 1yy + y1y + yy1)\\&\quad - \tfrac{9}{32}(3 - zz1 - z1z - 1zz)\\&\quad - \tfrac{3}{16}(1 - 11z - 1z1 - z11) \leqslant 0,\end{aligned} \tag{12}$$

so we see that seven local measurement settings are required for the "double state" inequality and 12 for the "triple state" inequality as opposed to the 63 measurement settings required for a full state tomography. In this place we notice some correspondence to the class definition via SLOCC. The witness in Ref. [37] uses the same observables to distinguish between the W and GHZ class (however, in a different combination). The advantage of our criteria is that they generalize for systems with more parties in a straightforward way. In Fig. 3 we illustrate the membership to the various entanglement classes for an example of a family of four-qubit states.

V. DISCUSSION AND CONCLUSION

We have identified three classes of genuinely multipartite entangled states of n qubits and introduced criteria which enable a simple computational and an experimental discrimination between those classes. However, as shown in Refs. [14,15], these classes do not sufficiently characterize the set of all genuinely multipartite entangled states. In order to have a complete characterization one can use criteria to detect genuine multipartite entanglement (such as, e.g., Refs. [9,10,14,24]) to also include the complementing classes.

One possibility to define the complementing class is to write down the most general form of an n-qubit state:

$$|\psi_t\rangle := \sum_{i_1,i_2,\ldots,i_n} c_{i_1,i_2,\ldots,i_n}|i_1 i_2 \ldots i_n\rangle. \tag{13}$$

All n-qubit states are local unitarily equivalent to this state for some choice of $c_{i_1,i_2,\ldots,i_n}$. The equivalence class $\mathcal{C}(\{|\Psi^1_t\rangle\})$ contains all $\mathcal{C}(\{|\Psi^1\rangle\})$ for some choice of $c_{i_1,i_2,\ldots,i_n}$. So if we exclude the parameter choices for the three known classes, i.e., $\mathcal{C}(\{|\Psi^1_t\rangle\}) \setminus \{\mathcal{C}(\{|\Psi^1_{(2)}\rangle\}),\mathcal{C}(\{|\Psi^1_{(n)}\rangle\}),\mathcal{C}(\{|\Psi^1_{(n-1)}\rangle\})\}$, we have the complementing set containing all other genuinely multipartite entangled states. It is completely unknown in general how many inequivalent choices for $c_{i_1,i_2,\ldots,i_n}$ are possible for n-partite systems, but with our proposed framework it should be possible to design an inequality for any given class.

In summary, we have defined three different classes of genuine multipartite entanglement for n qubits, the double states (a generalization of GHZ states), the (n)-tuple states (a generalization of W states), and then $(n-1)$-tuple states (a generalization of certain Dicke states) which possess different physical properties and therefore provide different applications. These substructures of genuine entangled states are equivalence classes that arise via local unitaries and permutations. We have presented three simple computable inequalities, each of which is satisfied for all biseparable states and for the class of genuine multipartite entanglement that corresponds to the inequality. Therefore, any violation of the inequality detects that the given state is not of a certain class. This certainly can be used for different applications as, e.g., the success of secrete sharing protocols or quantum algorithms rely on certain class of entangled states. We have further shown that all presented criteria can be rewritten by local expectation values, thus are experimentally implementable and require far less measurement settings that full state tomography, i.e., scale favorable with the system size. Last but not least, we want to stress that we presented a framework which may be generalized to any n-partite qudit system, where until now there were no results concerning classification.

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APPENDIX

The general concept behind all upcoming proofs is a calculation of the inequalities for the most general pure state. As all inequalities are convex the validity for mixed states is automatically given. All inequalities consist of the real parts of a certain off-diagonal density matrix elements from which diagonal elements are subtracted. In order to prove the inequalities we will first show that certain real parts of the diagonal elements cancel each other, so we can then use them freely to complete negative squares with the real parts from the off-diagonal elements and thus prove the inequality.

1. Proof of the "double state" inequality

The "double state" inequality, (I(2)),

$$\begin{aligned}\sum_{i\neq j}\mathrm{Re}[(\langle w_i|\rho|w_j\rangle+(-1)^{n+1}\langle\overline{w}_i|\rho|\overline{w}_j\rangle)]\\ -\alpha\sum_i(\langle w_i|\rho|w_i\rangle+\langle\overline{w}_i|\rho|\overline{w}_i\rangle)\\ -\beta(\langle 00\cdots0|\rho|00\cdots0\rangle+\langle 11\cdots1|\rho|1\cdots11\rangle)\\ -\gamma\sum_{i\neq j}(\langle d_{ij}|\rho|d_{ij}\rangle+\langle\overline{d}_{ij}|\rho|\overline{d}_{ij}\rangle)\leqslant 0 \qquad \text{(A1)}\end{aligned}$$

is satisfied for all states of the form

$$|\psi_{(2)}\rangle=\lambda_1|x_1x_2\cdots x_n\rangle+\lambda_2|y_1y_2\cdots y_n\rangle, \qquad \text{(A2)}$$

where

$$|x_i\rangle=a_i|0\rangle+\overline{a_i}|1\rangle \qquad \text{(A3)}$$

$$|y_i\rangle=\overline{a_i}^*|0\rangle-a_i^*|1\rangle \qquad \text{(A4)}$$

for some $\alpha,\beta,\gamma>0$.

Proof 1. The individual scalar products yield

$$\langle w_i|\psi_{(2)}\rangle=\lambda_1\prod_{n\neq i}(a_n)\overline{a}_i-\lambda_2\prod_{n\neq i}(\overline{a^*}_n)a_i^*, \qquad \text{(A5)}$$

$$\langle\overline{w}_i|\psi_{(2)}\rangle=\lambda_1\prod_{n\neq i}(\overline{a}_n)a_i+(-1)^{n+1}\lambda_2\prod_{n\neq i}(a_n^*)\overline{a^*}_i, \qquad \text{(A6)}$$

$$\langle d_{ij}|\psi_{(2)}\rangle=\lambda_1\prod_{n\neq i,j}(a_n)\overline{a}_i\overline{a}_j+\lambda_2\prod_{n\neq i,j}(\overline{a^*}_n)a_i^*a_j^*, \qquad \text{(A7)}$$

$$\langle\overline{d}_{ij}|\psi_{(2)}\rangle=\lambda_1\prod_{n\neq i,j}(a_n)\overline{a}_i\overline{a}_j+(-1)^n\lambda_2\prod_{n\neq i,j}(\overline{a^*}_n)a_i^*a_j^*, \qquad \text{(A8)}$$

$$\langle 00\cdots0|\psi_{(2)}\rangle=\lambda_1\prod_n a_n+\lambda_2\prod_n\overline{a^*}_n, \qquad \text{(A9)}$$

$$\langle 11\cdots1|\psi_{(2)}\rangle=\lambda_1\prod_n\overline{a}_n+(-1)^n\lambda_2\prod_n a_n^*, \qquad \text{(A10)}$$

which results in

$$\begin{aligned}\langle w_i|\psi_{(2)}\rangle\langle\psi_{(2)}|w_j\rangle=\underbrace{|\lambda_1|^2\prod_{n\neq i,j}(|a_n|^2)\overline{a}_ia_i^*\overline{a^*}_ja_j}_{W_{ij}^0}+\underbrace{|\lambda_2|^2\prod_{n\neq i,j}(|\overline{a}_n|^2)\overline{a^*}_ia_i\overline{a}_ja_j^*}_{W_{ij}^1}\\ -\left(\lambda_1\lambda_2^*\prod_{n\neq i,j}(\overline{a}_na_n)\overline{a}_i^2a_j^2+\lambda_1^*\lambda_2\prod_{n\neq i,j}(\overline{a^*}_na_n^*)a^{*2}_i\overline{a^*}_j^2\right) \qquad \text{(A11)}\end{aligned}$$

and

$$\begin{aligned}\langle\overline{w}_i|\psi_{(2)}\rangle\langle\psi_{(2)}|\overline{w}_j\rangle=\underbrace{|\lambda_1|^2\prod_{n\neq i,j}(|\overline{a}_n|^2)\overline{a^*}_ia_i\overline{a}_ja_j^*}_{\overline{W}_{ij}^0}+\underbrace{|\lambda_2|^2\prod_{n\neq i,j}(|a_n|^2)\overline{a}_ia_i^*\overline{a^*}_ja_j}_{\overline{W}_{ij}^1}\\ +(-1)^{n+1}\left(\lambda_1\lambda_2^*\prod_{n\neq i,j}(\overline{a}_na_n)a_i^2\overline{a}_j^2+\lambda_1^*\lambda_2\prod_{n\neq i,j}(\overline{a^*}_na_n^*)\overline{a^*}_i^2a^{*2}_j\right) \qquad \text{(A12)}\end{aligned}$$

and

$$|\langle w_i|\psi_{(2)}\rangle|^2=|\lambda_1|^2\prod_{n\neq i}(|a_n|^2)|\overline{a}_i|^2+|\lambda_2|^2\prod_{n\neq i}(|\overline{a}_n|^2)|a_i|^2-2\mathrm{Re}\left[\lambda_1\lambda_2^*\prod_n(\overline{a}_na_n)\right] \qquad \text{(A13)}$$

$$|\langle\overline{w}_i|\psi_{(2)}\rangle|^2=|\lambda_1|^2\prod_{n\neq i}(|\overline{a}_n|^2)|a_i|^2+|\lambda_2|^2\prod_{n\neq i}(|a_n|^2)|\overline{a}_i|^2+(-1)^{n+1}2\mathrm{Re}\left[\lambda_1\lambda_2^*\prod_n(\overline{a}_na_n)\right] \qquad \text{(A14)}$$

and

$$|\langle 00\cdots0|\psi_{(2)}\rangle|^2=\underbrace{|\lambda_1|^2\prod_n(|a_n|^2)}_{|M_0|^2}+\underbrace{|\lambda_2|^2\prod_n(|\overline{a}_n|^2)}_{|M_1|^2}+2\mathrm{Re}\left[\lambda_1\lambda_2^*\prod_n(a_n\overline{a}_n)\right] \qquad \text{(A15)}$$

$$|\langle 11\cdots1|\psi_{(2)}\rangle|^2=\underbrace{|\lambda_1|^2\prod_n(|\overline{a}_n|^2)}_{|\overline{M}_0|^2}+\underbrace{|\lambda_2|^2\prod_n(|a_n|^2)}_{|\overline{M}_1|^2}+(-1)^n2\mathrm{Re}\left[\lambda_1\lambda_2^*\prod_n(a_n\overline{a}_n)\right] \qquad \text{(A16)}$$

and, finally,

$$|\langle d_{ij}|\psi_{(2)}\rangle|^2 = \underbrace{|\lambda_1|^2 \prod_{n\neq i,j}(|a_n|^2)|\overline{a}_i|^2|\overline{a}_j|^2}_{|D^0_{ij}|^2} + \underbrace{|\lambda_2|^2 \prod_{n\neq i,j}(|\overline{a}_n|^2)|a_i|^2|a_j|^2}_{|D^1_{ij}|^2} + 2\mathrm{Re}\left[\lambda_1\lambda_2^* \prod_n(\overline{a}_n a_n)\right] \tag{A17}$$

$$|\langle \overline{d}_{ij}|\psi_{(2)}\rangle|^2 = \underbrace{|\lambda_1|^2 \prod_{n\neq i,j}(|\overline{a}_n|^2)|a_i|^2|a_j|^2}_{|\overline{D^0}_{ij}|^2} + \underbrace{|\lambda_2|^2 \prod_{n\neq i,j}(|a_n|^2)|\overline{a}_i|^2|\overline{a}_j|^2}_{|\overline{D^1}_{ij}|^2} + (-1)^n 2\mathrm{Re}\left[\lambda_1\lambda_2^* \prod_n(\overline{a}_n a_n)\right]. \tag{A18}$$

This results for the real parts $R = 2\mathrm{Re}[\lambda_1\lambda_2^* \prod_n(\overline{a}_n a_n)]$ in

$$-n\alpha R + n\alpha(-1)^{n+1}R + \beta R + (-1)^n\beta R + n(n-1)\gamma R + (-1)^n n(n-1)\gamma R \tag{A19}$$

$$= R\{n\alpha[(-1)^{n+1} - 1] + \beta[1 + (-1)^n] + n(n-1)\gamma[1 + (-1)^n)]\}, \tag{A20}$$

which is zero for odd n. For even n and the choice $\alpha = \frac{n-2}{2}$, $\beta = \frac{n(n-2)}{4}$, and $\gamma = \frac{n-2}{4(n-1)}$ it yields

$$= R\left[n\frac{n-2}{2}(-2) + \frac{n(n-2)}{4}(2) + n(n-1)\frac{n-2}{4(n-1)}(2)\right] = 0. \tag{A21}$$

Using

$$\mathrm{Re}[\langle w_i|\psi_{(2)}\rangle\langle\psi_{(2)}|w_j\rangle] - \frac{n-2}{2(n-1)}(\langle w_i|\psi_{(2)}\rangle\langle\psi_{(2)}|w_i\rangle + \langle w_j|\psi_{(2)}\rangle\langle\psi_{(2)}|w_j\rangle)$$

$$= \frac{1}{n-1}\mathrm{Re}[\langle w_i|\psi_{(2)}\rangle\langle\psi_{(2)}|w_j\rangle] - \underbrace{\frac{n-2}{2(n-1)}|\langle w_i|\psi_{(2)}\rangle - \langle w_j|\psi_{(2)}\rangle|^2}_{X_{ij}} \tag{A22}$$

and

$$\mathrm{Re}[\langle \overline{w}_i|\psi_{(2)}\rangle\langle\psi_{(2)}|\overline{w}_j\rangle] - \frac{n-2}{2(n-1)}(\langle \overline{w}_i|\psi_{(2)}\rangle\langle\psi_{(2)}|\overline{w}_i\rangle + \langle \overline{w}_j|\psi_{(2)}\rangle\langle\psi_{(2)}|\overline{w}_j\rangle)$$

$$= \frac{1}{n-1}\mathrm{Re}[\langle \overline{w}_i|\psi_{(2)}\rangle\langle\psi_{(2)}|\overline{w}_j\rangle] - \underbrace{\frac{n-2}{2(n-1)}|\langle \overline{w}_i|\psi_{(2)}\rangle - \langle \overline{w}_j|\psi_{(2)}\rangle|^2}_{\overline{X}_{ij}} \tag{A23}$$

the inequality now reads

$$\sum_{i\neq j}\left\{\frac{1}{n-1}\mathrm{Re}\big[W^0_{ij} + W^1_{ij} + (-1)^{n+1}\big(\overline{W}^0_{ij} + \overline{W}^1_{ij}\big)\big] - (X_{ij} + \overline{X}_{ij}) - \frac{n-2}{4(n-1)}\big(\big|D^0_{ij}\big|^2 + \big|D^1_{ij}\big|^2 + \big|\overline{D}^0_{ij}\big|^2 + \big|\overline{D}^1_{ij}\big|^2\big)\right\}$$

$$- \frac{n(n-2)}{4}(|M^0|^2 + |M^1|^2 + |\overline{M^0}|^2 + |\overline{M^1}|^2) \leqslant 0 \tag{A24}$$

or, equivalently,

$$\sum_{i\neq j}\frac{1}{n-1}\left(\mathrm{Re}\big[W^0_{ij}\big] - \frac{n-2}{4}\big|D^0_{ij}\big|^2 - \frac{n-2}{4}|M^0|^2\right)$$

$$\sum_{i\neq j}\frac{1}{n-1}\left(\mathrm{Re}\big[W^1_{ij}\big] - \frac{n-2}{4}\big|D^1_{ij}\big|^2 - \frac{n-2}{4}|M^1|^2\right)$$

$$\sum_{i\neq j}\frac{1}{n-1}\left(\mathrm{Re}\big[\overline{W}^0_{ij}\big] - \frac{n-2}{4}\big|\overline{D}^0_{ij}\big|^2 - \frac{n-2}{4}|\overline{M}^0|^2\right)$$

$$\sum_{i\neq j}\frac{1}{n-1}\left(\mathrm{Re}\big[\overline{W}^1_{ij}\big] - \frac{n-2}{4}\big|\overline{D}^1_{ij}\big|^2 - \frac{n-2}{4}|\overline{M}^1|^2\right) \leqslant 0. \tag{A25}$$

Now we can use

$$\big|M^0 - D^0_{ij}\big|^2 = |M^0|^2 + \big|D^0_{ij}\big|^2 - 2\mathrm{Re}\big[W^0_{ij}\big], \tag{A26}$$

$$\big|M^1 - D^1_{ij}\big|^2 = |M^1|^2 + \big|D^1_{ij}\big|^2 - 2\mathrm{Re}\big[W^1_{ij}\big], \tag{A27}$$

$$\big|\overline{M}^0 + (-1)^{n+1}\overline{D}^0_{ij}\big|^2 = |\overline{M}^0|^2 + \big|\overline{D}^0_{ij}\big|^2 + (-1)^{n+1}2\mathrm{Re}\big[\overline{W}^0_{ij}\big], \tag{A28}$$

$$\big|\overline{M}^1 + (-1)^{n+1}\overline{D}^1_{ij}\big|^2 = |\overline{M}^1|^2 + \big|\overline{D}^1_{ij}\big|^2 + (-1)^{n+1}2\mathrm{Re}\big[\overline{W}^1_{ij}\big], \tag{A29}$$

which proves the inequality for $n \geqslant 4$. ■

Corollary 2.

$$\sum_{i\neq j}\mathrm{Re}[(\langle w_i|\rho|w_j\rangle+(-1)^{n+1}\langle\overline{w}_i|\rho|\overline{w}_j\rangle)]$$
$$-\alpha\sum_i(\langle w_i|\rho|w_i\rangle+\langle\overline{w}_i|\rho|\overline{w}_i\rangle)$$
$$-\beta(\langle 00\cdots0|\rho|00\cdots0\rangle+\langle 11\cdots1|\rho|1\cdots11\rangle)$$
$$-\gamma\sum_{i\neq j}(\langle d_{ij}|\rho|d_{ij}\rangle+\langle\overline{d}_{ij}|\rho|\overline{d}_{ij}\rangle)\leqslant 0 \tag{A30}$$

is satisfied for all biseparable states for some $\alpha,\beta,\gamma>0$.

Proof. The following inequality is satisfied by all biseparable states (as proven in Ref. [24]):

$$\sum_{i\neq j}\mathrm{Re}[\langle w_i|\rho|w_j\rangle]-\sum_{i\neq j}\sqrt{\langle 00\cdots0|\rho|00\cdots0\rangle\langle d_{ij}|\rho|d_{ij}\rangle}$$
$$-(n-2)\sum_i\langle w_i|\rho|w_i\rangle\leqslant 0 \tag{A31}$$

or, equivalently,

$$\sum_{i\neq j}\mathrm{Re}[\langle\overline{w}_i|\rho|\overline{w}_j\rangle]-\sum_{i\neq j}\sqrt{\langle 11\cdots1|\rho|11\cdots1\rangle\langle\overline{d}_{ij}|\rho|\overline{d}_{ij}\rangle}$$
$$-(n-2)\sum_i\langle\overline{w}_i|\rho|\overline{w}_i\rangle\leqslant 0 \tag{A32}$$

and

$$-\sum_{i\neq j}\mathrm{Re}[\langle\overline{w}_i|\rho|\overline{w}_j\rangle]-\sum_{i\neq j}\sqrt{\langle 11\cdots1|\rho|11\cdots1\rangle\langle\overline{d}_{ij}|\rho|\overline{d}_{ij}\rangle}$$
$$-(n-2)\sum_i\langle\overline{w}_i|\rho|\overline{w}_i\rangle\leqslant 0. \tag{A33}$$

Using

$$\sqrt{\langle 00\cdots0|\rho|00\cdots0\rangle\langle d_{ij}|\rho|d_{ij}\rangle}$$
$$\leqslant\tfrac{1}{2}(\langle 00\cdots0|\rho|00\cdots0\rangle+\langle d_{ij}|\rho|d_{ij}\rangle) \tag{A34}$$

we arrive at

$$\sum_{i\neq j}\mathrm{Re}[\langle w_i|\rho|w_j\rangle+(-1)^{n+1}\langle\overline{w}_i|\rho|\overline{w}_j\rangle]-\sum_{i\neq j}(\langle d_{ij}|\rho|d_{ij}\rangle+\langle\overline{d}_{ij}|\rho|\overline{d}_{ij}\rangle)-(n-2)\sum_i(\langle w_i|\rho|w_i\rangle+\langle\overline{w}_i|\rho|\overline{w}_i\rangle)$$
$$-\frac{n(n-1)}{2}(\langle 00\cdots0|\rho|00\cdots0\rangle+\langle 11\cdots1|\rho|11\cdots1\rangle)\leqslant 0, \tag{A35}$$

where we have to choose $\alpha=(n-2)$, $\beta=\frac{n(n-1)}{2}$, and $\gamma=1$. ■

Corollary 3.

$$\sum_{i\neq j}\mathrm{Re}[(\langle w_i|\rho|w_j\rangle+(-1)^{n+1}\langle\overline{w}_i|\rho|\overline{w}_j\rangle)]-\alpha\sum_i(\langle w_i|\rho|w_i\rangle+\langle\overline{w}_i|\rho|\overline{w}_i\rangle)$$
$$-\beta(\langle 00\cdots0|\rho|00\cdots0\rangle+\langle 11\cdots1|\rho|1\cdots11\rangle)-\gamma\sum_{i\neq j}(\langle d_{ij}|\rho|d_{ij}\rangle+\langle\overline{d}_{ij}|\rho|\overline{d}_{ij}\rangle)\leqslant 0 \tag{A36}$$

is satisfied by both biseparable states and $\mathcal{C}(\{|\Psi^1_{(2)}\rangle\})$ for $\alpha=(n-2)$, $\beta=\frac{n(n-1)}{2}$ and $\gamma=1$.

Proof. It is evident that inequality (A36) is satisfied for all biseparable states as proven in Proof 2. As α, β, and γ are larger than what is needed for all "double states," we can conclude that subtracting even more positive terms does not change the validity of inequality (A36) for these states. ■

2. *Proof of the "n-tuple state" inequality*

The "n-tuple state" inequality (I(n)) is satisfied by all states of the form

$$|\psi_{(n)}\rangle:=\sum_i\lambda_i|W_i\rangle, \tag{A37}$$

where

$$|W_i\rangle:=|x_1x_2\cdots x_{i-1}y_ix_{i+1}\cdots x_n\rangle \tag{A38}$$

and

$$|x_i\rangle=a_i\,|0\rangle+\overline{a_i}\,|1\rangle$$
$$|y_i\rangle=\overline{a_i}^*\,|0\rangle-a_i^*\,|1\rangle. \tag{A39}$$

Proof 2. First observe that

$$\langle 0|^{\otimes n}|\psi_{(n)}\rangle=\sum_i\lambda_i\,\overline{a}_i^*\left(\prod_{n\neq i}a_n\right),$$
$$\langle 1|^{\otimes n}|\psi_{(n)}\rangle=-\sum_i\lambda_i\,a_i^*\left(\prod_{n\neq i}\overline{a}_n\right), \tag{A40}$$

such that we obtain for the first term of the "n-tuple state" inequality with $\rho=\sum_{i,j}\lambda_i\lambda_j^*|W_i\rangle\langle W_j|$

$$\mathrm{Re}[\langle 0|^{\otimes n}\rho|1\rangle^{\otimes n}]$$
$$=-\mathrm{Re}\left[\prod_n a_n\overline{a}_n^*+\sum_{i\neq j}\lambda_i\lambda_j^*\,\overline{a}_i^{*2}a_j^2\left(\prod_{n\neq i,j}a_n\overline{a}_n^*\right)\right]. \tag{A41}$$

Let us introduce an index set $m_k=\{i_1i_2\cdots i_k\}$ and denote the complement by m_k^C. We can then with

$$\left|d_{m_k}\right\rangle:=|0\rangle_{m_k^C}^{\otimes n-k}|1\rangle_{m_k}^{\otimes k} \tag{A42}$$

rewrite the second term of the "n-tuple state" inequality by

$$\begin{aligned} &1-\langle 0|^{\otimes n}\rho|0\rangle^{\otimes n}-\langle 1|^{\otimes n}\rho|1\rangle^{\otimes n}\\ &=\sum_{k=1}^{n-1}\sum_{m_k}\langle d_{m_k}|\rho|d_{m_k}\rangle\\ &=\sum_{k=1}^{n-1}\sum_{m_k}\sum_{i,j}\lambda_i\lambda_j^*\,\langle d_{m_k}|W_i\rangle\langle W_j|d_{m_k}\rangle, \end{aligned} \tag{A43}$$

i.e., we have to calculate all diagonal terms minus the first and last one. We have two different cases ($m_k/i\ldots$ denotes the index set m_k without the index i)

$$\langle d_{m_k}|W_i\rangle=\begin{cases}-a_i^*\prod_{n\in m_k^c}(a_n)\prod_{l\in m_k/i}(\overline{a}_l), & \text{if}\quad i\in m_k\\ \overline{a}_i^*\prod_{n\in m_k^c/i}(a_n)\prod_{l\in m_k}(\overline{a}_l), & \text{if}\quad i\notin m_k\end{cases} \tag{A44}$$

and therefore four possibilities for the products

$$\langle W_j|d_{m_k}\rangle\langle d_{m_k}|W_i\rangle=\begin{cases}\prod_{n\in m_k^c}(|a_n|^2)\prod_{l\in m_k/i,j}(|\overline{a}_l|^2)a_i^*a_j\overline{a}_i^*\overline{a}_j, & \text{if}\quad i\in m_k,\ j\in m_k\\ -\prod_{n\in m_k^c/j}(|a_n|^2)\prod_{l\in m_k/i}(|\overline{a}_l|^2)a_i^*a_j\overline{a}_i^*\overline{a}_j, & \text{if}\quad i\in m_k,\ j\notin m_k\\ -\prod_{n\in m_k^c/i}(|a_n|^2)\prod_{l\in m_k/j}(|\overline{a}_l|^2)a_i^*a_j\overline{a}_i^*\overline{a}_j, & \text{if}\quad i\notin m_k,\ j\in m_k\\ \prod_{n\in m_k^c/\{i,j\}}(|a_n|^2)\prod_{l\in m_k}(|\overline{a}_l|^2)a_i^*a_j\overline{a}_i^*\overline{a}_j, & \text{if}\quad i\notin m_k,\ j\notin m_k\end{cases}. \tag{A45}$$

We expect that certain real parts cancel each other; in detail, we find that the following relation holds

$$X_{m_k}^{ij}:=\langle W_j|d_{m_k}\rangle\langle d_{m_k}|W_i\rangle=-\langle W_j|d_{m_{k'}}\rangle\langle d_{m_{k'}}|W_i\rangle \tag{A46}$$

if

$$k'=k+1 \tag{A47}$$

and

$$m_k\cup m'_{k+1}\setminus m_k\cap m'_{k+1}=\{i\}\,. \tag{A48}$$

This can be proven explicitly by computing the expressions. Now we can complete all corresponding $|\langle W_j|d_{m_k}\rangle|^2+|\langle W_i|d_{m_k}\rangle|^2$ to complete negative squares.

Explicitly we observe

$$\sum_i|\lambda_i|^2|\langle d_{\{i\}}|W_i\rangle|^2=\prod_n|a_n|^2 \tag{A49}$$

$$\sum_i|\lambda_i|^2|\langle d_{\{i\}^c}|W_i\rangle|^2=\prod_n|\overline{a}_n|^2 \tag{A50}$$

such that for the case $i=j$ we obtain the following negate square for the inequality under investigation

$$\begin{aligned} &-\sum_i|\lambda_i|^2\mathrm{Re}[\langle 0|^{\otimes n}W_i\rangle\langle W_i|1\rangle^{\otimes n}]-\alpha\Big(\sum_i|\lambda_i|^2|\langle d_{\{i\}}|W_i\rangle|^2+\sum_i|\lambda_i|^2|\langle d_{\{i\}^c}|W_i\rangle|^2\Big)\\ &=-\mathrm{Re}\Big[\prod_n a_n\overline{a}_n^*\Big]-\alpha\Big(\prod_n|a_n|^2+\prod_n|\overline{a}_n|^2\Big)=-\frac{1}{2}\Big|\prod_n a_n+\prod_n\overline{a}_n\Big|^2\leqslant 0, \end{aligned} \tag{A51}$$

where the last equation holds for $\alpha=\frac{1}{2}$. Thus we have proven that all terms with $i=j$ are negative.

For the terms $i\neq j$ we can proceed in a similar way

$$\begin{aligned} &\sum_{i,j}(-\mathrm{Re}[\lambda_i\lambda_j^*\,\langle 0|^{\otimes n}W_i\rangle\langle W_j|1\rangle^{\otimes n}]-\alpha(|\lambda_i|^2|\langle d_{\{ij\}}|W_i\rangle|^2+|\lambda_j|^2|\langle d_{\{ij\}^c}|W_j\rangle|^2))\\ &=\sum_{i,j}\Big\{-\mathrm{Re}\Big[\lambda_i\lambda_j^*\,\overline{a}_i^{*2}a_j^2\Big(\prod_{n\neq i,j}a_n\overline{a}_n^*\Big)\Big]-\alpha\Big(|\lambda_i|^2\Big|(-)a_i^*\overline{a}_j\prod_{n\neq i,j}a_n\Big|^2+|\lambda_j|^2\Big|a_i\overline{a}_j^*\prod_{n\neq i,j}\overline{a}_n\Big|^2\Big)\Big\}\\ &=\sum_{i,j}\Big[-\frac{1}{2}\Big|\lambda_i\,\overline{a}_i^*a_j\Big(\prod_{n\neq i,j}a_n\Big)+\lambda_j\,\overline{a}_ia_j^*\Big(\prod_{n\neq i,j}\overline{a}_n\Big)\Big|^2\Big]\leqslant 0, \end{aligned} \tag{A52}$$

where the last equation holds for $\alpha=\frac{1}{2}$ (note that as the sum goes over all i and j in any sum the role of i,j can be interchanged). Now we can combine both cases and the proof is complete. However, note that in the case $n=4$ the set $|d_{\{ij\}}\rangle$ and its complement are identical such that terms used to complete the negative squares for the case $i=j$ are not available for the case $i\neq j$, this we can compensate by choosing $\alpha=1$. Thus we have proven that the "n-tuple state" inequality for all n with $\alpha=\frac{1}{2}$ except for $n=4$, where one has to chose $\alpha=1$ holds for any state of the set $\mathcal{C}(\{|\Psi_{(n)}^1\rangle\})$.

That the inequality holds for biseparable states follows from inequality (II) presented in Ref. [24]. ■

3. *Proof of the "(n − 1)-tuple state" inequality*

The inequality

$$\sum_{i\neq j}\mathrm{Re}[(\langle w_i|\rho|w_j\rangle] - (n-2)\sum_i(\langle w_i|\rho|w_i\rangle) - \frac{n(n-1)}{2}(\langle 00\cdots 0|\rho|00\cdots 0\rangle) - (n-2)\sum_{i\neq j}(\langle d_{ij}|\rho|d_{ij}\rangle) \leqslant 0 \tag{A53}$$

is satisfied for all states of the form

$$|\psi_{(n-1)}\rangle = \sqrt{\frac{2}{n(n-1)}}\sum_{i<j}|D_{ij}\rangle, \tag{A54}$$

where

$$|D_{ij}\rangle = \bigotimes_{k\neq i,j}|x_k\rangle\otimes|y_i\rangle\otimes|y_j\rangle \tag{A55}$$

$$|x_i\rangle = a_i|0\rangle + \overline{a_i}|1\rangle \tag{A56}$$

$$|y_i\rangle = \overline{a_i}^*|0\rangle - a_i^*|1\rangle. \tag{A57}$$

Proof 3. To prove the inequality we first take a look at the individual products

$$\langle w_i|D_{xy}\rangle = \begin{cases} \overline{a}_i\overline{a}_x^*\overline{a}_y^*\prod_{k\neq i,x,y}a_k, & \text{if } i\neq x,y \\ -a_x^*\overline{a}_y^*\prod_{k\neq x,y}a_k, & \text{if } i=x \\ -\overline{a}_x^*a_y^*\prod_{k\neq x,y}a_k, & \text{if } i=y \end{cases} \tag{A58}$$

and

$$\langle d_{ij}|D_{xy}\rangle = \begin{cases} \overline{a}_i\overline{a}_j\overline{a}_x^*\overline{a}_y^*\prod_{k\neq i,j,x,y}a_k, & \text{if } i,j\neq x,y \\ -\overline{a}_j a_x^*\overline{a}_y^*\prod_{k\neq j,x,y}a_k, & \text{if } i=x,\ j\neq y \\ -\overline{a}_j\overline{a}_x^*a_y^*\prod_{k\neq j,x,y}a_k, & \text{if } i=y,\ j\neq x \\ -\overline{a}_i a_x^*\overline{a}_y^*\prod_{k\neq i,x,y}a_k, & \text{if } i\neq y,\ j=x \\ -\overline{a}_i\overline{a}_x^*a_y^*\prod_{k\neq i,x,y}a_k, & \text{if } i\neq x,\ j=y \\ a_x^*a_y^*\prod_{k\neq x,y}a_k, & \text{if } i=x,\ j=y \end{cases} \tag{A59}$$

Now the two products

$$|\langle\psi_{(n-1)}|w_i\rangle|^2 = \left|\sum_{x<y}\langle w_i|D_{xy}\rangle\right|^2 \tag{A60}$$

and

$$|\langle\psi_{(n-1)}|d_{ij}\rangle|^2 = \left|\sum_{x<y}\langle d_{ij}|D_{xy}\rangle\right|^2 \tag{A61}$$

again have real parts which cancel each other out:

$$\langle d_{ij}|D_{xy}\rangle\langle D_{x'y'}|d_{ij}\rangle = -\langle w_k|d_{mn}\rangle\langle d_{m'n'}|w_k\rangle \tag{A62}$$

if

$$\{ijijxyx'y'\}\setminus\{\{\{ij\}\cap\{xy\}\}\cup\{\{ij\}\cap\{x'y'\}\}\} \tag{A63}$$

$$= \{kkmnm'n'\}\setminus\{\{\{k\}\cap\{mn\}\}\cup\{\{k\}\cap\{m'n'\}\}\}, \tag{A64}$$

from which follows that the according squared terms may be used to complete negative squares with the first part of the inequality. The condition reads

$$\mathrm{Re}[\langle w_i|d_{xy}\rangle\langle d_{x'y'}|w_j\rangle] - \tfrac{1}{2}(|\langle d_{ab}|D_{mn}\rangle|^2 + |\langle d_{ab}|D_{m'n'}\rangle|^2) \tag{A65}$$

$$= -|\langle d_{ab}|D_{mn}\rangle + \langle d_{ab}|D_{m'n'}\rangle|^2 \tag{A66}$$

when

$$\{ijxyx'y'\}\setminus\{\{\{i\}\cap\{xy\}\}\cup\{\{j\}\cap\{x'y'\}\}\} \tag{A67}$$

$$= \{abcdmnm'n'\}\setminus\{\{\{ab\}\cap\{mn\}\}\cup\{\{cd\}\cap\{m'n'\}\}\} \tag{A68}$$

also, where the appropriate terms are not available one can use the corresponding $|\langle w_i|D_{xy}\rangle|^2$ from the inequality. By explicit, yet cumbersome, calculation one can in a straightforward way show that the inequality is indeed satisfied for all states of the class $\mathcal{C}(\{|\Psi^1_{((n-1))}\rangle\})$, analogously to the previous proofs. As this inequality is just the linearized version of inequality (III) from Ref. [24] it also holds for all biseparable states. ■

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Entanglement detection via mutually unbiased bases

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We investigate correlations among complementary observables. In particular, we show how to take advantage of mutually unbiased bases for the efficient detection of entanglement in arbitrarily high-dimensional, multipartite, and continuous-variable quantum systems. The introduced entanglement criteria are relatively easy to implement experimentally since they require only a few local measurement settings. In addition, we establish a link between the separability problem and the maximum number of mutually unbiased bases—opening an additional avenue in this long-standing open problem.

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I. INTRODUCTION

A key feature of quantum theory is the prediction of correlations that have no classical analog, i.e., correlations that differ fundamentally from Bertlmann's socks [1]. Whereas such quantum correlations were initially considered to be an artifact of the theory, it was later confirmed in several experiments that they actually exist in nature. They are a manifestation of the fact that composite quantum systems can be entangled, in the sense that they are not exclusively separable.

Nowadays, it is widely known that quantum entanglement enables numerous applications ranging from quantum cryptography to quantum computing. Although the theory of entanglement has been extensively studied within recent decades (for recent reviews, consult Refs. [2,3]), it is still an evolving research field with many open problems. One of these problems concerns the reliable and efficient detection of entanglement in experiments [4,5]. While for bipartite two-level systems it is possible to experimentally verify the presence of entanglement by making a few joint local measurements, the number of measurements needed for entanglement detection generally scales rather disadvantageously with the size of the system. The main challenge for high-dimensional multipartite systems is not only to develop mathematical tools for entanglement detection, but to find schemes whose experimental implementation requires minimal effort. In other words, the aim is to verify entanglement with as few measurements as possible, specifically without resorting to full state tomography.

Another fundamental concept of quantum theory is complementarity, which states that there exist observables that cannot be measured simultaneously. In the mathematical formalism, complementarity expresses itself through the fact that there are pairs of observables for which no common eigenbasis can be found. Consequently, if two observables are complementary then it is impossible to prepare a system such that the outcome of both is predictable with certainty. The extreme case of complementarity is when the eigenbases of two observables form a pair of mutually unbiased bases (MUBs) [6]. This is when all (normalized) eigenvectors of one observable have the same overlap with all eigenvectors of the other observable. Thus, if a system is in an eigenstate of a particular basis, then the measurement result in a corresponding mutually unbiased basis is completely random.

The question of how many MUBs exist for a given Hilbert space has been a lively topic of research (see [7] for a recent review). Although it is been known since 1989 [8] that for $\mathcal{H} = \mathbb{C}^d$ the number of MUBs is at most $d + 1$ and that such a *complete set* of MUBs exists whenever d is a prime power, the maximal number of MUBs remains open for all other dimensions. Even for the smallest non-prime-power dimension $d = 6$, the existence of a complete set remains an open problem, and current numerical [9–11] and analytical [12–16] evidence suggests that it is likely that there is none.

It is currently unclear if the (non)existence of a complete set of MUBs in non-prime-power dimensions has fundamental reasons or consequences. However, one should also look at MUBs from a pragmatic perspective; or as phrased by Bengtsson [17]: "the real MUB problem is not how many MUBs we can find. The real MUB problem is to find out what we can do with those that exist." Existing applications of MUBs are quantum state tomography [8,18–20], cryptographic protocols [21,22], and the mean king's problem [23,24]. In short, they are generally useful for finding and hiding (quantum) information.

In this paper, we present a different application of mutually unbiased bases. Namely, we link the concept of MUBs with the separability problem. We show that one can exploit the properties of MUBs to derive powerful entanglement detection criteria for arbitrarily high-dimensional systems. These criteria are well suited for the experimental verification of entanglement as they are experimentally accessible through measuring correlations between only a few local observables. In contrast to a full state tomography where the experimental effort can grow exponentially with the system size [25], our approach enables optimal entanglement detection using a number of measurement settings which scales only linearly with the dimensionality of the local subsystems. In fact, we also show that even two local MUB settings, in general, suffice for a comparably robust entanglement test. Furthermore, by considering the noise thresholds of our criteria we find an interesting theoretical connection between the separability of density matrices and the maximum number of MUBs. In

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particular, we provide an alternative proof that there cannot be more than $d+1$ MUBs in any dimension. We also consider extensions of our methodology for continuous variables and multipartite systems. These are discussed by the example of the two-mode squeezed state and the Aharonov state.

II. PRELIMINARIES

A set of orthonormal bases $\{\mathcal{B}_k\}$ for a Hilbert space $\mathcal{H}=\mathbb{C}^d$ where $\mathcal{B}_k=\{|i_k\rangle\}=\{|0_k\rangle,\ldots,|d-1_k\rangle\}$ is called mutually unbiased if and only if

$$|\langle i_k|j_l\rangle|^2=\frac{1}{d},\quad \forall\, i,j\in\{0,\ldots,d-1\},\tag{1}$$

holds for all basis vectors $|i_k\rangle$ and $|j_l\rangle$ that belong to different bases, i.e., $\forall\, k\neq l$. If two bases are mutually unbiased, their corresponding observables are complementary—a measurement of one of these observables reveals no information about the outcome of the other.

In dimension $d=2$, a set of three mutually unbiased bases is readily obtained from the eigenvectors of the three Pauli matrices σ_z,σ_x, and σ_y:

$$\mathcal{B}_1=\{|0_1\rangle,|1_1\rangle\}=\{|0\rangle,|1\rangle\},$$
$$\mathcal{B}_2=\{|0_2\rangle,|1_2\rangle\}=\left\{\frac{1}{\sqrt{2}}(|0\rangle+|1\rangle),\frac{1}{\sqrt{2}}(|0\rangle-|1\rangle)\right\},$$
$$\mathcal{B}_3=\{|0_3\rangle,|1_3\rangle\}=\left\{\frac{1}{\sqrt{2}}(|0\rangle+\mathbb{i}|1\rangle),\frac{1}{\sqrt{2}}(|0\rangle-\mathbb{i}|1\rangle)\right\}.$$

These three bases constitute a complete set since it is impossible to find an additional basis that is mutually unbiased to all of them.

In general, for prime-power dimensions $d=p^n$, there are several explicit methods to construct a complete set of $d+1$ MUBs making use of finite fields [8,26], the Heisenberg-Weyl group [27], generalized angular momentum operators [28], and identities from number theory [29]. For the special cases $d=2^n$ and $d=p^2$, it was shown that such sets can be constructed in a rather simple and experimentally accessible way [30,31].

The concept of mutually unbiased bases can also be extended to continuous-variable (CV) systems [7,32]. Here, the bases given by the (generalized) eigenstates of position and momentum operators provide a well-known example of MUBs. If one allows the right-hand side of Eq. (1) to vary between each pair of bases, a continuum of MUBs is available [7]. Requiring that all pairwise overlaps have the same modulus leads to a symmetric set of three MUBs for CV systems [32].

First, in order to relate MUBs with the separability problem, let us specify how correlations can be quantified. Consider a bipartite system where measurements on each of the two subsystems A and B have d different outcomes $\{0,\ldots,d-1\}$. If we can predict with certainty the outcome of a measurement on A when we know the outcome of a measurement on B (or vice versa) we call a system fully correlated. On the other hand, we call a system completely uncorrelated if the outcome of a measurement of one party tells us nothing about the other party, i.e., when the outcomes are completely random. Following this notion, it is possible to construct a correlation function for any two observables a,b on A,B. We denote the joint probability that the outcome of a is i and the outcome of b is j by $P_{a,b}(i,j)$. We define the correlation function

$$C_{a,b}=\sum_{i=0}^{d-1}P_{a,b}(i,i),\tag{2}$$

which we call the *mutual predictability*. It can be used to quantify the probability of predicting the measurement results of a knowing the outcome of b, and vice versa. Namely, if the observables a and b are fully correlated then the outcomes $\{i\}=\{0,\ldots,d-1\}$ can always be labeled in a way such that $C_{a,b}=1$. It is noteworthy that labels in general have no physical meaning. Thus, it is up to us what outcome we declare as $0,1,\ldots,$etc. However, the point is that when the observables a and b are completely uncorrelated we obtain $C_{a,b}=1/d$ no matter what labeling we choose.

In the quantum case, each observable a,b corresponds to an orthonormal basis $\{|i_a\rangle\}$ and $\{|i_b\rangle\}$. Here we have $P_{a,b}(i,j)=\langle i_a|\otimes\langle j_b|\rho|i_a\rangle\otimes|j_b\rangle$ where ρ is the state of the system, and thus the mutual predictability reads $C_{a,b}=\sum_{i=0}^{d-1}\langle i_a|\otimes\langle i_b|\rho|i_a\rangle\otimes|i_b\rangle$. Again, one obtains $C_{a,b}=1$ for fully correlated states when $\{|i_a\rangle\}$ and $\{|i_b\rangle\}$ are chosen appropriately with respect to ρ, and $C_{a,b}=1/d$ for completely uncorrelated states, independent of the chosen bases.

III. ENTANGLEMENT DETECTION: BIPARTITE QUDIT SYSTEMS

For a particular state ρ and measurement settings a,b the quantity $C_{a,b}$ tells us nothing about the separability of a state. For instance, we can have $C_{a,b}=1$ for all entangled pure states $|\psi\rangle$ which directly follows from the Schmidt decomposition. Any entangled state may be written in the form $|\psi\rangle=\sum_{i=0}^{r}\lambda_i|i_a^s\rangle\otimes|i_b^s\rangle$ with $1\leqslant r\leqslant d-1$ using the orthonormal Schmidt bases $\{|i_a^s\rangle\}$ and $\{|i_b^s\rangle\}$. Using observables a and b that correspond to these bases, we obviously obtain $C_{a,b}=1$. However, we also obtain $C_{a,b}=1$ for a classically correlated separable state $\rho_{CC}=\sum_{i=0}^{r}|\lambda_i|^2|i_a^s\rangle\langle i_a^s|\otimes|i_b^s\rangle\langle i_b^s|$ as it yields the same joint probabilities $P_{a,b}(i,i)$ when we use $\{|i_a^s\rangle\}$ and $\{|i_b^s\rangle\}$.

Hence, to detect entanglement, the mutual predictability $C_{a,b}$ has to be measured in at least two bases, a,b and a',b'. Let us consider a pure product state which we write as $|\psi\rangle_{\text{pro}}=|0_1\rangle\otimes|0_1\rangle$ in an arbitrary basis $\{|i_1\rangle\}$. For $\rho_{\text{pro}}=|\psi\rangle_{\text{pro}}\langle\psi|_{\text{pro}}$ one obtains $C_{1,1}=1$ if both parties use the basis $\{|i_1\rangle\}$. However, in a second basis $\{|i_2\rangle\}$ which is mutually unbiased to $\{|i_1\rangle\}$, the mutual predictability $C_{2,2}$ is completely lost: Since $\{|i_1\rangle\}$ and $\{|i_2\rangle\}$ are mutually unbiased we have that

$$P_{2,2}(i,i)=\langle i_2,i_2|\rho_{\text{pro}}|i_2,i_2\rangle\tag{3}$$
$$=\langle i_2,i_2\,|0_1,0_1\rangle\,\langle 0_1,0_1\,|i_2,i_2\rangle\tag{4}$$
$$=\underbrace{|\langle i_2\,|0_1\rangle|^2}_{1/d}\,\underbrace{|\langle i_2\,|0_1\rangle|^2}_{1/d}\tag{5}$$
$$=\frac{1}{d^2},\tag{6}$$

and consequently $C_{2,2}=\sum_{i=0}^{d-1}P_{2,2}(i,i)=1/d$.

Inspired by this result, let us consider the quantity $I_2=C_{1,1}+C_{2,2}$. As shown, with a pure product state we obviously can attain $I_2=1+\frac{1}{d}$ for a pair of MUBs. Similarly, we can

achieve $I_m = \sum_{k=1}^{m} C_{k,k} = 1 + \frac{m-1}{d}$ for a product state using m mutually unbiased bases $\mathcal{B}_k$ and corresponding terms $C_{k,k}$; because when the mutual predictability equals 1 in one basis then it is $1/d$ with respect to the other $m-1$ bases. The main result of this paper is that these values are upper bounds for separable states, i.e., for all separable states and any set of m mutually unbiased bases for A and B it holds that

$$I_m = \sum_{k=1}^{m} C_{k,k} \leqslant 1 + \frac{m-1}{d}. \tag{7}$$

In particular, for a complete set of MUBs we have

$$I_{d+1} = \sum_{k=1}^{d+1} C_{k,k} \leqslant 2. \tag{8}$$

Proof. For an arbitrary pure product state $|a\rangle \otimes |b\rangle \in \mathbb{C}^d \otimes \mathbb{C}^d$ we have

$$I_m = \sum_{k=1}^{m} C_{k,k} = \sum_{k=1}^{m} \sum_{i=0}^{d-1} |\langle i_k|a\rangle|^2 |\langle i_k|b\rangle|^2. \tag{9}$$

Here, the inequality of arithmetic and geometric means $(x_1 + x_2 + \cdots + x_n)/n \geqslant \sqrt[n]{x_1 x_2 \cdots x_n}$ for positive numbers implies that

$$\sum_{k=1}^{m} C_{k,k} \leqslant \frac{1}{2} \sum_{k=1}^{m} \sum_{i=0}^{d-1} (|\langle i_k|a\rangle|^4 + |\langle i_k|b\rangle|^4). \tag{10}$$

Now we can exploit the fact that for any pure state $|a\rangle \in \mathbb{C}^d$ and m mutually unbiased bases it holds that

$$\sum_{k=1}^{m} \sum_{i=0}^{d-1} |\langle i_k|a\rangle|^4 \leqslant 1 + \frac{m-1}{d}, \tag{11}$$

which was obtained in Ref. [33] as a generalization of the result established in Ref. [34]. Thus, Eq. (10) together with Eq. (11) prove the validity of (7) for all pure product states. Finally, since I_m is linear in the density matrix ρ it follows that (7) holds for all (mixed) separable states as pure states represent extreme points.

The quantities I_m together with the corresponding bounds for separable states can serve as criteria for entanglement detection in mixed states. However, what about the detection strength? Let us consider the d-dimensional isotropic states $\rho_I = \alpha |\phi_d^+\rangle\langle\phi_d^+| + \frac{1-\alpha}{d^2}\mathbb{1}$ with $|\phi_d^+\rangle = \frac{1}{\sqrt{d}} \sum_{i=0}^{d-1} |i\rangle \otimes |i\rangle$. These are known to be entangled for $\alpha > 1/(d+1)$ and separable for $\alpha \leqslant 1/(d+1)$ [35]. For an arbitrary basis choice $x \leftrightarrow \{|i_x\rangle\}$ in system A and $x^* \leftrightarrow \{|i_x\rangle^*\}$ in B the mutual predictability is always $C_{x,x^*} = \alpha + (1-\alpha)/d$ since ρ_I is $U \otimes U^*$ invariant [36]. Thus, using m mutually unbiased bases $\{\mathcal{B}_k\}$ for A and $\{\mathcal{B}_k^*\}$ for B we attain $I_m = m(\alpha + (1-\alpha)/d)$ which violates (7) for $\alpha > 1/m$. Consequently, entanglement allows for values $I_m > 1 + \frac{m-1}{d}$ which can be considered as an exact quantification of the statement that quantum correlations are more resistant against changes of the basis than ordinary correlations in separable states. As we also see the noise robustness of the criteria (7) increases with the number of MUBs (see Fig. 1). If there exists a complete set of $m = d+1$ MUBs the criterion (8) is necessary and sufficient for the separability of ρ_I as $\alpha = 1/(d+1)$ is the exact bound of separability.

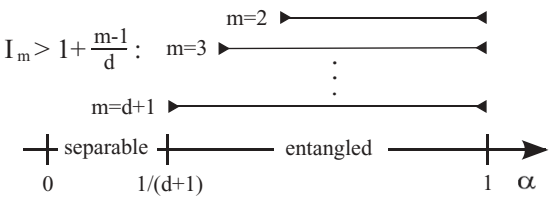

FIG. 1. Schematic illustration of the parameter regions detected by the criterion (7) for the d-dimensional isotropic states $\rho_I = \alpha |\phi_d^+\rangle\langle\phi_d^+| + \frac{1-\alpha}{d^2}\mathbb{1}$ in dependence on the number of mutually unbiased bases m. The detection strength improves with increasing m until for $m = d+1$ all entangled states are detected.

The significance of these results is manifold: First, the criterion (7) is surprisingly powerful. Each isotropic state is locally unitarily equivalent to any other maximally entangled state mixed with white noise [37]. By incorporating the corresponding local basis transformation that brings such a state into the isotropic form, we can detect all entanglement when d is of prime-power dimension. Remarkably, only two MUBs are needed for detecting entanglement up to a threshold of 50% noise. In comparison, Bell inequalities are often used as indicators of entanglement as they are simple to realize in experiments [2,4,5]. However, using two measurement settings for each party they merely reach a maximal noise threshold between 29.289% and 32.656% depending on the dimension d [38,39]. Notably, two MUBs suffice to verify all entangled pure states in arbitrary dimension, as is proven in Appendix A. Moreover, regarding experimental verification of entanglement, we are now in the position that we can customize the number of MUBs depending on what is experimentally feasible.

Second, we emphasize that with the presented concept we establish a direct link between the separability boundary and the maximum number of MUBs (illustrated in Fig. 1). Notice that if there were $m > d+1$ MUBs for a Hilbert space $\mathcal{H} = \mathbb{C}^d$, then we would have $I_m > 1 + \frac{m-1}{d}$ for separable states, namely, for isotropic states ρ_I with $1/m < \alpha \leqslant 1/(d+1)$. This, however, is not compatible with the statement of Eq. (7), and thus we have shown by contradiction that there cannot exist more than $d+1$ MUBs.

Last, it should be noted that our criteria are adaptable for arbitrary mixed states, i.e., for verifying entanglement in density matrices beyond the white noise scenario. In general, if one applies our criteria to an arbitrary unclassified state ρ one can improve the detection by maximizing the outcome of I_m over local unitaries (by seeking the optimal transformation $\rho \to U_A \otimes U_B \rho U_A^\dagger \otimes U_B^\dagger$) and permuting the order of the basis vectors in the mutually unbiased bases. Appropriate tools for this optimization can be found in Refs. [40,41]. An analysis of a broader class of states which is related to a geometric structure of the Hilbert-Schmidt space is given in Appendix B.

IV. ENTANGLEMENT DETECTION: CONTINUOUS VARIABLE STATES

The concepts introduced in the previous section are not limited to discrete systems but can easily be applied to continuous-variable states. As the noise robustness of the

criterion (7) increases with the number of MUBs, it is to expected that we can find quite strong entanglement detection criteria for CV systems since in this case there exist infinitely many MUBs [7]. From a theoretical point of view it would certainly be interesting to study the generalization of our concept for a continuum of MUBs. However, in the current paper we take the viewpoint of an pragmatic experimentalist who has access to only a limited number of complementary observables. Let us study the simplest case where one has access to only two mutually unbiased bases corresponding to position (x) and momentum (p) measurements of single particles. Consider the two-mode squeezed-state wave function [42]

$$\psi_S(x_1,x_2) = \sqrt{\frac{2}{\pi}}\exp[-e^{-2r}(x_1+x_2)^2/2 - e^{+2r}(x_1-x_2)^2/2], \quad (12)$$

$$\psi_S(p_1,p_2) = \sqrt{\frac{2}{\pi}}\exp[-e^{-2r}(p_1-p_2)^2/2 - e^{+2r}(p_1+p_2)^2/2], \quad (13)$$

depending on the squeezing parameter r, whose entanglement we would like to verify in an experiment by measuring joint probabilities. We use the mutual predictabilities $C_{x,x} = P_{x,x}(1,1) + P_{x,x}(2,2)$ of correlated positions,

$$P_{x,x}(1,1) = \int_{-\infty}^{0}\int_{-\infty}^{0} |\psi_S(x_1,x_2)|^2 dx_1 dx_2, \quad (14)$$

$$P_{x,x}(2,2) = \int_{0}^{\infty}\int_{0}^{\infty} |\psi_S(x_1,x_2)|^2 dx_1 dx_2, \quad (15)$$

and $C_{p,p} = P_{p,p}(1,2) + P_{p,p}(2,1)$ of anticorrelated momenta,[1]

$$P_{p,p}(1,2) = \int_{-\infty}^{0}\int_{0}^{\infty} |\psi_S(p_1,p_2)|^2 dp_1 dp_2, \quad (16)$$

$$P_{p,p}(2,1) = \int_{0}^{\infty}\int_{-\infty}^{0} |\psi_S(p_1,p_2)|^2 dp_1 dp_2. \quad (17)$$

Even though the correlations are measured quite imprecisely by dividing the state space into only two regions for each particle and observable (which can be regarded as a detector with very low resolution that produces only two distinguishable outcomes, equivalent to $d = 2$) this suffices to detect almost all entanglement in a squeezed state: Via the minimal realization of our approach, i.e., $C_{x,x} + C_{p,p} \leqslant 1.5$ for separable states, we detect entanglement if the squeezing parameter is $r > 0.3279$. This is already very close to the exact solution $r > 0$ [42]. Recall that this is done only by measuring correlations between positions x_1, x_2 and momenta p_1, p_2, that is, without full knowledge of the state. Note that, if experimentally possible, we are always allowed to add further MUBs and use a finer partitioning of the Hilbert space (in accordance with the detector resolution) to improve the detection strength. However, in several cases few (or even only two) MUBs are enough to experimentally verify the presence of entanglement.

[1]Note that correlations and anticorrelations are the same up to the labeling of the measurement outcomes.

V. DETECTION OF GENUINE MULTIPARTITE ENTANGLEMENT

It is characteristic for multipartite systems that entanglement can occur in various ways. Here, it can happen that some parts of the system are entangled, while at the same time, others are separable [2,3,43]. For this reason, the concept of k-separability has been introduced: A pure state $|\Psi\rangle$ of an n-partite system is called k-separable if it can be written as a tensor product of k vectors, i.e., $|\Psi\rangle = |\psi_1\rangle \otimes \cdots \otimes |\psi_k\rangle$. States that are n-separable do not contain any entanglement and are called *fully separable*. Of special interest are quantum states whose entanglement ranges over all n parties. Those are termed *genuine multipartite entangled* states [2] and cannot be factorized at all, that is, when $k = 1$. The generalization to mixed states is straightforward: A mixed state ρ is called k-separable if all pure-state decompositions $\rho = \sum_i p_i |\Psi_i\rangle\langle\Psi_i|$ require at least one $|\Psi_i\rangle$ which is at least k-separable according to the above definition.

While for pure states it is straightforward to examine if a state is genuinely multipartite entangled, it is demanding to answer this question for mixed states. The main problem here is that standard entanglement criteria which are applicable to bipartite systems generally fail for the verification of genuine multipartite entanglement. This is due to the fact that biseparable states ($k = 2$) can be entangled with respect to all bipartitions when they are mixed rather than pure: A typical example is a state of the form $\rho_{2\text{-sep}} = \frac{1}{3}(\rho_A \otimes \rho_{BC} + \rho_B \otimes \rho_{AC} + \rho_C \otimes \rho_{AB})$. Although this state is not genuinely tripartite entangled, it might not be separable with respect to any fixed bipartition of the system.

Along with the fact that there currently exist only few criteria for the detection of genuine multipartite entanglement in mixed states (see, e.g., Refs. [44–48]) comes another problem to deal with. Namely, most of the currently known criteria are not scalable, that is, in most cases the number of needed measurement settings grows exponentially with the number of parties. This is generally a serious obstacle to experimental implementations. In this section, we show that genuine multipartite entanglement can also be verified using few MUBs by adopting the previously introduced concept to the multiparticle scenario.

Let us discuss our approach by the example of an n-partite n-dimensional singlet state [49,50], known as the *Aharonov state* [51,52],

$$|\mathcal{S}_n\rangle = \frac{1}{\sqrt{n!}} \sum_{j,\ldots,l=0}^{n-1} \varepsilon_{j,\ldots,l} |j,\ldots,l\rangle, \quad (18)$$

where $\varepsilon_{j,\ldots,l}$ denotes the generalized Levi-Cività symbol. For example, for three qutrits it reads

$$|\mathcal{S}_3\rangle = \frac{1}{\sqrt{6}}(|012\rangle + |120\rangle + |201\rangle - |021\rangle - |102\rangle - |210\rangle). \quad (19)$$

The Aharonov state has two central properties. First, from a correlation point of view, it is completely anticorrelated. This

implies that if one performs measurements on $n-1$ parties and is aware of all outcomes then one can predict with certainty the outcome of the remaining party. Furthermore, this state is $U^{\otimes n}$ invariant, implying that these anticorrelations always hold when all of the n parties choose the same local basis [49,50]. With respect to the mentioned symmetries of the state, it is reasonable to introduce an n-particle anticorrelation function

$$A_{a,\ldots,z} = \sum_{j,\ldots,l=0}^{n-1} |\varepsilon_{j,\ldots,l}| P_{a,\ldots,z}(j,\ldots,l) \tag{20}$$

$$= \sum_{j,\ldots,l=0}^{n-1} |\varepsilon_{j,\ldots,l}| \langle j_a,\ldots,l_z|\rho|j_a,\ldots,l_z\rangle, \tag{21}$$

which is $A_{a,\ldots,z}=1$ if and only if all local measurement outcomes of the observables $\{a,\ldots,z\}$ are always unequal. Specifically, $A_{a,\ldots,z}=1$ for the Aharonov state when $a=\cdots=z$, i.e., when the same basis is chosen for all subsystems (as explained above). We build the linear combination

$$J_m = \sum_{a=1}^{m} A_{a,\ldots,a} \tag{22}$$

using m mutually unbiased bases. This quantity J_m is bounded by

$$J_m \leqslant 1 + \frac{m-1}{n} \tag{23}$$

for biseparable states.

Proof. Suppose we have a pure state $|\Psi_{2-\text{sep}}\rangle$ which is biseparable with respect to any bipartition $\{X|Y\}$. In general, such a state can reach $A_{a,\ldots,z}=1$ for a certain choice of observables $a,\ldots,z$. However, if we replace the local bases $\{a,\ldots,z\}$ by corresponding mutually unbiased bases $\{a,\ldots,z\}\to\{a',\ldots,z'\}$ then the predictability is lost, similarly to the bipartite qudit case (Sec. III). We thus obtain $A_{a',\ldots,z'} \leqslant 1/\min\{d_X,d_Y\}$ where d_X and d_Y are the dimensions of X and Y. Since $d=n$ is the minimum dimension over all bipartitions of the n-partite n-dimensional system it is guaranteed that $A_{a,\ldots,z}+A_{a',\ldots,z'} \leqslant 1+1/n$ holds for all biseparable states. Consequently, with m MUBs we arrive at (23), and since J_m is linear in the density matrix ρ it follows that any violation directly implies the existence of genuine multipartite entanglement in a (mixed) state.

Let us discuss the detection strength of the criterion (23) by the example of the Aharonov state in the presence of white noise, $\rho_{\text{aw}} = \alpha|\mathcal{S}_n\rangle\langle\mathcal{S}_n| + \frac{1-\alpha}{n^n}\mathbb{1}$. For the pure Aharonov state $|\mathcal{S}_n\rangle$ we have $A_{a,\ldots,a}=1$ for all a, and for white noise $\frac{1}{n^n}\mathbb{1}$ we have $A_{a,\ldots,a}=n!/n^n$. Thus, in total we obtain $J_m = m(\alpha+(1-\alpha)n!/n^n)$ which for

$$\alpha > \frac{n^n(m+n-1)-mnn!}{mn(n^n-n!)}, \tag{24}$$

leads to a violation of $J_m \leqslant 1+\frac{m-1}{n}$. Figure 2 illustrates the noise robustness of the criterion (23) in dependence on the number of used mutually unbiased bases m. As can be seen therein, while the concept used is rather simple, the derived criterion is remarkably powerful in detecting genuine multipartite entanglement in the vicinity of the Aharonov state. For protocols where this particular state is used as a resource (e.g. [49,53,54]) this could be exploited to test whether the state was correctly distributed between all parties. Note that there currently exists no comparable test for verifying genuinely multipartite entanglement in ρ_{aw} and that the actual noise threshold is unknown. Note furthermore that it is to be presumed that our concept can easily be adopted to other multipartite states by taking into account their symmetries and correlations. In many cases this should lead to criteria with a valuable experimental-effort-to-detection-strength ratio.

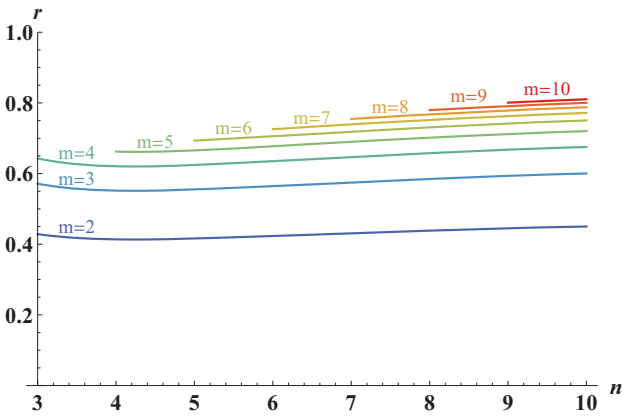

FIG. 2. (Color online) The noise robustness r of the criteria (23) for the n-partite Aharonov state in the presence of white noise, i.e., $\rho_{\text{aw}} = \alpha|\mathcal{S}_n\rangle\langle\mathcal{S}_n| + \frac{1-\alpha}{n^n}\mathbb{1}$. For $1-\alpha < r$ the state ρ_{aw} is detected to be genuinely multipartite entangled. The detection strength increases with the number of used mutually unbiased bases m.

VI. SUMMARY AND OUTLOOK

In conclusion we have established a connection between mutually unbiased bases and entanglement detection. We showed that MUBs allow for an intuitive way of constructing entanglement criteria for arbitrarily high-dimensional systems. These criteria are beneficial for experiments since they require only a few local measurements. By means of the isotropic and Bell-diagonal states (Appendix B), we demonstrated that our approach can yield necessary and sufficient criteria for separability if a complete set of MUBs is available for the local subsystems. In addition, we found that the number of MUBs can be related to the separability problem and provided an alternative proof that for a d-dimensional system there cannot exist more than $d+1$ MUBs.

Besides optimal detection through complete sets of MUBs, we showed that even using only two local complementary measurement settings it is possible to verify entanglement with a quite adequate robustness to noise. For experiments where the set of measurable observables is limited this may be of valuable help. For instance, for systems in high-energy physics investigated at accelerator facilities only a restricted observable space is available due to the laborious effort and technical limitations. However, e.g., for neutral entangled K mesons [55] one could realize two MUBs during the time evolution of the system, allowing for a direct test of entanglement via the introduced criteria. Two MUBs are also sufficient for detecting all entangled pure states of any two-qudit system (Appendix A) and allow for powerful

entanglement detection in continuous variables. Even the presence of genuine multipartite entanglement can be tested very effectively through correlations in MUBs, which we demonstrated by the example of the Aharonov state.

For prime-power dimensions, MUBs enable a complete state tomography. Consequently, local information and correlations with respect to MUBs should provide necessary and sufficient information to detect all entanglement in systems which are composed of subsystems with prime-power dimensionality. For such systems, it should be possible to develop a general framework of entanglement detection based on complementary observables. For qubit systems, such a framework should be equivalent to the concept of correlation tensors (see, e.g., Refs. [56–58]), as the decomposition of density matrices in terms of Pauli matrices is intrinsically linked to MUBs. However, a generalization of correlation tensors to higher-dimensional systems has so far been addressed only by means of the generators of the special unitary group [58–60]. Here, a theory in terms of MUBs should allow for an alternative method to investigate multilevel quantum correlations which is expected to be experimentally advantageous.

The presented scheme might also yield further results on systems with non-prime-power dimensions: Just as we have shown that an upper bound on the number of MUBs can be deduced from the separability problem via the isotropic states, it might also be possible to determine the actual number of MUBs using a certain state and/or system. Finally, as numerous quantum features such as discord [61], steering [62], and nonlocality (see Ref. [63] and references therein) give rise to particular correlations, it is conceivable that they can also be brought into relation with mutually unbiased bases, or even be directly formulated in terms of them.

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APPENDIX A: SUFFICIENCY OF TWO MUBS FOR PURE STATES

We show that two MUBs are sufficient to verify all entangled pure states of any bipartite qudit system $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B = \mathbb{C}^d \otimes \mathbb{C}^d$. Assume our objective is to prepare a particular pure state $|\Psi\rangle = \sum_{m,n=0}^{d-1} c_{m,n}|m\rangle \otimes |n\rangle$. In order to achieve that the mutual predictability is maximal, i.e.,

$$C_{1,1} = \sum_{i=0}^{d-1} \langle i_1| \otimes \langle i_1 \, |\psi\rangle \, \langle\psi \, |i_1\rangle \otimes |i_1\rangle = 1, \tag{A1}$$

we use the measurement bases $\{|i_1\rangle\}$ on A and B for which our target state takes on the Schmidt form $|\psi\rangle = \sum_{i=0}^{r} \lambda_i |i_1\rangle \otimes |i_1\rangle$ with $0 \leqslant r \leqslant d-1$, $\lambda_i \geqslant 0$, and $\sum_{i=0}^{r} \lambda_i^2 = 1$. For a second measurement of the mutual predictability $C_{2,2^*}$ we choose the (mutually unbiased) basis $\{|i_2\rangle\} = \{|0_2\rangle, \ldots, |d-1_2\rangle\}$ with $|i_2\rangle = \frac{1}{\sqrt{d}} \sum_{k=0}^{d-1} \omega^{ki} |k_1\rangle$ and $\omega = \exp(2\pi \mathbb{i}/d)$, determined by the discrete Fourier transform. For the composite basis vectors we have

$$|i_2\rangle \otimes |i_2\rangle^* = \frac{1}{d} \sum_{k,l=0}^{d-1} \omega^{(k-l)i} |k_1\rangle \otimes |l_1\rangle. \tag{A2}$$

This leads to

$$C_{2,2^*} = \sum_{i=0}^{d-1} \langle i_2| \otimes \langle i_2|^* \, |\psi\rangle \, \langle\psi \, |i_2\rangle \otimes |i_2\rangle^* \tag{A3}$$

$$= \sum_{i=0}^{d-1} |\langle\psi \, |i_2\rangle \otimes |i_2\rangle^*|^2 \tag{A4}$$

$$= \sum_{i=0}^{d-1} \left| \left[\sum_{n=0}^{r} \lambda_n \langle n_1| \otimes \langle n_1| \right] \left[\frac{1}{d} \sum_{k,l=0}^{d-1} \omega^{(k-l)i} |k_1, l_1\rangle \right] \right|^2. \tag{A5}$$

We see that the only relevant vectors are those with $k = l$, in which case we have $\omega^{(k-l)i} = 1$, and get

$$C_{2,2^*} = \sum_{i=0}^{d-1} \left| \frac{1}{d} \sum_{n=0}^{r} \lambda_n \right|^2. \tag{A6}$$

Here the squared absolute value $|\sum_{n=0}^{r} \lambda_n|^2$ can be rewritten as

$$C_{2,2^*} = \frac{1}{d} \left(\underbrace{\sum_{n=0}^{r} \lambda_n^2}_{1} + \sum_{m \neq n}^{r} \lambda_m \lambda_n \right) \tag{A7}$$

$$= \frac{1}{d} \left(1 + \sum_{m \neq n}^{r} \lambda_m \lambda_n \right). \tag{A8}$$

Thus, altogether we obtain

$$I_2 = C_{1,1} + C_{2,2^*} = 1 + \frac{1}{d} \left(1 + \sum_{m \neq n}^{r} \lambda_m \lambda_n \right). \tag{A9}$$

For any separable state $|\psi\rangle$ the Schmidt rank is 1, and consequently $\sum_{m \neq n}^{r} \lambda_m \lambda_n$ is zero since there is only one Schmidt coefficient λ_m which equals 1, whereas, we have $\sum_{m \neq n}^{r} \lambda_m \lambda_n > 0$ for any entangled state because they have Schmidt rank greater than or equal to 2, i.e., there are at least two nonzero Schmidt coefficients $\lambda_m \geqslant 0$. Consequently, two MUBs are sufficient to detect all entangled pure states, as all of them achieve $I_2 > 1 + \frac{1}{d}$.[2] ■

[2]Note that $I_2 > 1 + 1/d$ unambiguously implies the presence of entanglement regardless of which pairs of MUBs we use. However, just as for any entanglement verification scheme that does not require a full state tomography, we have to adjust our setup according to the expected state to achieve optimal detection.

APPENDIX B: ENTANGLEMENT DETECTION AND GEOMETRY

In Ref. [37], a special simplex of locally maximally mixed two-qudit states, also known as *Bell-diagonal states*, was introduced. This set of states is given by

$$\mathcal{W} = \left\{ \sum_{k,l=0}^{d-1} c_{k,l} P_{k,l} \,\middle|\, c_{k,l} \geqslant 0, \sum_{k,l=0}^{d-1} c_{k,l} = 1 \right\}, \tag{B1}$$

where $P_{k,l} = |\Omega_{k,l}\rangle\langle\Omega_{k,l}|$ are the projectors of d^2 mutually orthogonal Bell states, generated by applying the unitary Weyl operators

$$W_{k,l} = \sum_{s=0}^{d-1} \omega^{sk} |s\rangle\langle (s+l) \bmod d| \tag{B2}$$

with $\omega = \exp(2\pi \mathbb{i}/d)$ and $k,l \in \{0,\ldots,d-1\}$ on the maximally entangled state $|\Omega_{0,0}\rangle = \frac{1}{\sqrt{d}} \sum_{i=0}^{d-1} |i\rangle \otimes |i\rangle$, i.e.,

$$|\Omega_{k,l}\rangle = (W_{k,l} \otimes \mathbb{1})|\Omega_{0,0}\rangle. \tag{B3}$$

The isotropic states from Sec. III are also contained in this set. Here, for a complete set of MUBs, the quantity I_{d+1} from Eq. (8) reads

$$I_{d+1} = 1 + hd, \tag{B4}$$

where $h = \max\{c_{k,l}\}$ is the largest coefficient. Consequently, the region with $I_{d+1} \leqslant 2$ corresponds to the so-called *enclosure polytope* [37], whose facets are defined by the d^2 hyperplanes corresponding to optimal entanglement witnesses for all $\rho = \frac{1-\alpha}{d^2}\mathbb{1} + \alpha P_{k,l}$. It was shown that all states outside this polytope are entangled [37]. Hence, the quantity I_{d+1} based on the maximum number of MUBs reflects the geometric structure of the enclosure polytope, which itself shares the symmetries of the simplex $\mathcal{W}$.

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A geometric comparison of entanglement and quantum nonlocality in discrete systems

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Abstract

We compare entanglement with quantum nonlocality employing a geometric structure of the state space of bipartite qudits. The central object is a regular simplex spanned by generalized Bell states. The Collins–Gisin–Linden–Massar–Popescu–Bell inequality is used to reveal states of this set that cannot be described by local-realistic theories. Optimal measurement settings necessary to ascertain nonlocality are determined by means of a recently proposed parameterization of the unitary group $\mathcal{U}(d)$ combined with robust numerical methods. The main results of this paper are descriptive geometric illustrations of the state space that emphasize the difference between entanglement and quantum nonlocality. Namely, it is found that the shape of the boundaries of separability and Bell inequality violation are essentially different. Moreover, it is also shown that for mixtures of states sharing the same amount of entanglement, Bell inequality violations and entanglement measures are non-monotonically related.

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(Some figures in this article are in colour only in the electronic version)

1. Introduction

The fact that quantum physics contradicts local realism is one of the most seminal discoveries. In his pioneering work [1], Bell showed that the statistical behavior of a bipartite qubit system is irreconcilable with any local-realistic theory when the system is in a singlet state. He revealed that for such theories correlations are bounded by constraints which, however, can be violated if the setup is handled quantum physically. Since then much effort has been made to fully understand the origins and conditions that allow us to demonstrate and experimentally test this contradiction known as quantum nonlocality. Nowadays, a variety of so-called Bell

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inequalities are known. Recent Bell inequalities also cover systems with more than two degrees of freedom [2] and/or more than two parties [3–7].

However, the relation between entanglement and nonlocality is not completely clarified apart from the fact that Bell inequality violations are a consequence of the presence of entanglement [8–10]. The existence of entangled states that do not violate any Bell inequality [11] has raised several questions. First, how far can Bell inequalities be improved and is it possible for a given system to systematically derive the most powerful inequality or a set of those (see [12–15] for recent approaches)? Second, which entangled states allow a local-realistic description even if LOCC (local operators and classical communication) and POVMs (positive operator-valued measurements) are used and what are their characteristics? Besides that, a connection between the violation of a Bell inequality and the security of quantum cryptography was shown, attesting to the importance of further investigations [16, 17].

A nontrivial connection between nonlocality and entanglement was found by investigating the Collins–Gisin–Linden–Massar–Popescu–Bell (CGLMP) inequality [2]. In particular, it was shown that maximal violation is achieved with non-maximally entangled states [18, 19]. Similar features were also found in [20] for neutral K-mesons, which are two-level systems oscillating and decaying in time. For this system entangled in strangeness, though having only two degrees of freedom one finds no violation of the CHSH–Bell inequality if the system is prepared in the spin singlet state copiously produced in accelerator experiments [21]. A violation is only achieved if a non-maximally entangled state is used. Furthermore, a relation between Bell inequality violation and the violation of the $\mathcal{CP}$ symmetry ($\mathcal{C}$—charge conjugation, $\mathcal{P}$—parity) in particle physics was established [22, 23]. (It should be noted that this particular system in high energy physics is considerably different from systems not being affected by decay processes.) Another example demonstrating the fundamental difference between entanglement and nonlocality is given in [24]. Here, it is shown that the simulation of non-maximally entangled states via so-called nonlocal boxes (or Popescu–Rohrlich boxes) requires more resources than the simulation of a Bell state.

In this work we aim to study nonlocality and entanglement in the context of state space geometry. That is, we consider these properties using descriptive real vector representations for density matrices. Our main motivation is the fact that geometric considerations of the state space can provide deeper insights into quantum physics. They are also ideal to obtain an impression of the volumes related to certain properties or the strength of particular criteria. In case of a single qubit a geometric representation is given by the well-known three-dimensional Bloch-vector where the state space is called the Bloch-sphere. Regarding multipartite systems one usually tries to find representations where local properties and correlations can be separated in different quantities in order to avoid unwanted complexity caused by high dimensionality. Hence, when it comes to studying entanglement and nonlocality of a certain system it suffices to investigate representatives of equivalence classes of states which are equivalent with respect to local unitary transformations. In this way, for bipartite qubits it was found that correlations can be summarized in a three-dimensional vector lying within a regular tetrahedron [25, 26]. For the investigation of bipartite qudit systems we utilize a proposed generalization of this tetrahedron—a regular simplex spanned by mutually orthogonal maximally entangled states [27–29]. Our goal is to visualize and compare the geometries of the boundaries of entanglement and nonlocality of low-dimensional subsections of this set of states.

In order to do so, we choose certain classes of states for which via optimal entanglement witnesses we are able to exactly determine the boundary between separable and entangled states. For the same classes we then reveal all states that violate the CGLMP–Bell inequality. Determining, for a given state, whether it violates or obeys a certain Bell inequality is a high-dimensional nonlinear optimization problem which is difficult to solve even for

low-dimensional quantum systems. In section 3, we show how this problem can be solved utilizing an advantageous parameterization of the unitary group $\mathcal{U}(d)$ and robust numerical methods.

Our main results concerning the geometry of nonlocality and entanglement are given in section 5 for bipartite qubits and in section 7 for bipartite qutrits. In section 8, we extend our geometric considerations by incorporating a comparison between Bell inequality violation and an entanglement measure. Our results show that both quantities are so intrinsically different that not even for mixtures of states sharing the same amount of entanglement the relation is monotone.

2. Foundations of Bell inequalities

We begin by reviewing the foundations of Bell inequalities. Any local-realistic description of a bipartite system with d outcomes and n measurement apparatuses on each side implies the existence of d^{2n} probabilities

$$P(A_1 = j, \ldots, A_n = k; B_1 = l, \ldots, B_n = m) \geqslant 0 \tag{1}$$

with normalization

$$\sum_{j,\ldots,m=0}^{d-1} P(A_1 = j, \ldots, A_n = k; B_1 = l, \ldots, B_n = m) = 1 \tag{2}$$

determining the statistics of the observables $A_1, \ldots, A_n, B_1, \ldots, B_n$ which can take on the values $j, \ldots, k, l, \ldots, m \in \{0, \ldots, d-1\}$ [12, 30, 31]. As is known, probability distributions of this form cannot reproduce the statistical behavior of composite quantum systems $\mathcal{H}^{AB} = \mathbb{C}^d \otimes \mathbb{C}^d$ when the system is in a certain state and the observables are chosen appropriately. In order to reveal this, one constructs quantities I that consist of linear combinations of joint probabilities

$$P(A_a = x; B_b = y) = \sum_{j,\ldots,m=0 \text{ (except } x,y)}^{d-1} P(A_1 = j, \ldots, A_a = x, \ldots, A_n = k; B_1 = l, \ldots, B_b = y, \ldots, B_n = m)$$

and shows that they are bounded, i.e.

$$I \leqslant \Omega \tag{3}$$

if (1) and (2) are assumed. If this bound can be exceeded when the system is treated quantum physically, then the established inequality (3) is called a Bell inequality.

3. Determining nonlocal quantum states

States that cannot be described by a local-realistic theory are said to be nonlocal. One way of detecting nonlocality of a certain state ρ is to show that it violates a Bell inequality. The set of nonlocal states is complementary to the set of local states whose elements allow probability distributions of the form (1) with (2) for any number of apparatuses n. It should be noted that proving locality of a state is generally difficult since, in principle, it has to be shown that any Bell inequality is satisfied or an explicit local realistic description has to be found. Unfortunately, the problem of determining whether a particular Bell inequality is violated or obeyed for a given entangled state is also nontrivial.

In detail, to show that a certain state ρ possesses nonlocal correlations, one has to consider quantum mechanical joint probabilities

$$P^{\mathrm{QM}}(A_a = x;\, B_b = y) = \mathrm{Tr}(|x\rangle_{A_a}\langle x|_{A_a} \otimes |y\rangle_{B_b}\langle y|_{B_b} \cdot \rho) \tag{4}$$

where $\{|x\rangle_{A_a}\}$ and $\{|y\rangle_{B_b}\}$ are the orthonormal eigenvectors of the corresponding observables of Alice $\{A_1, \ldots, A_n\}$ and Bob $\{B_1, \ldots, B_n\}$. These probabilities are then inserted into the quantity I corresponding to a particular Bell inequality (3) which can then be rewritten in the form

$$I = \mathrm{Tr}(\mathcal{B}_I \rho) \tag{5}$$

wherein $\mathcal{B}_I$ is called the Bell operator [9].

In order to examine if the inequality is preserved or violated for a given ρ one has find observables that yield the maximum of I, i.e.

$$\max I = \max_{\{\mathcal{B}_I\}} \mathrm{Tr}(\mathcal{B}_I \rho). \tag{6}$$

This is in general a high-dimensional nonlinear constrained optimization problem for which analytic solutions are only known for a few special cases [32, 33]. Most often, the quantity I has to be maximized numerically for each given ρ.

Numerical tractability and reliability is closely related to the formulation and parameterization of the problem. Our problem can be brought into a computationally beneficial form in the following way: the outcome of I depends on the choice of the observables $\{A_a\}$ and $\{B_b\}$, i.e. the orthonormal bases $\{|k\rangle_{A_a}\}$ and $\{|k\rangle_{B_b}\}$. Since all orthonormal bases are local-unitarily related, our problem is equivalent to determining a set of unitary transformations $\{U_{A_a}\}$ and $\{U_{B_b}\}$ that maximize I. It is unknown whether or not there exists a restrictive set of unitaries that in all cases contains the global maximum: unbiased multiport beam splitters [2, 18, 34–36] containing only few parameters were shown to be too restrictive in general [37]. Consequently, we have to take into account all possible unitary transformations, i.e. the unitary group $\mathcal{U}(d)$. Regarding our problem we utilize the recently introduced 'composite parameterization' of $\mathcal{U}(d)$ [38] allowing an efficient variation. This parameterization is composed of elementary two-dimensional rotations and one-dimensional phase transformations. Explicitly, using one-dimensional projectors

$$P_l = |l\rangle\langle l| \tag{7}$$

and generalized anti-symmetric σ-matrices

$$\sigma_{m,n} = -\mathrm{i}|m\rangle\langle n| + \mathrm{i}|n\rangle\langle m|, \tag{8}$$

constructed with orthonormal basis vectors any unitary operator can be written as[1]

$$U_C = \left[\prod_{m=0}^{d-2}\left(\prod_{n=m+1}^{d-1}\exp(\mathrm{i}P_n\lambda_{n,m})\exp(\mathrm{i}\sigma_{m,n}\lambda_{m,n})\right)\right]\cdot\left[\prod_{l=0}^{d-1}\exp(\mathrm{i}P_l\lambda_{l,l})\right]. \tag{9}$$

The contained d^2 real parameters $\lambda_{m,n}$ lie within the ranges $\lambda_{m,n} \in [0, 2\pi]$ for $m \geqslant n$ and $\lambda_{m,n} \in \left[0, \frac{\pi}{2}\right]$ for $m < n$. Gathered in a $d \times d$ matrix

$$\begin{pmatrix} \lambda_{0,0} & \cdots & \lambda_{0,d-1} \\ \vdots & \ddots & \vdots \\ \lambda_{d-1,0} & \cdots & \lambda_{d-1,d-1} \end{pmatrix} \tag{10}$$

[1] The sequence of the product is $\prod_{i=0}^{N} A_i = A_0 \cdot A_1 \cdots A_N$.

these parameters are to be interpreted as follows: a diagonal entry $\lambda_{m,m}$ represents a global phase transformation for the vector $|m\rangle$, while an off-diagonal entry $\lambda_{m,n}$ represents an operation in the two-dimensional subspace spanned by $|m\rangle$ and $|n\rangle$: an upper right entry $\lambda_{m,n}$ is related to a rotation and the corresponding lower left entry $\lambda_{n,m}$ performs a relative phase shift. In our case we can exploit this structure to conveniently eliminate the d physically irrelevant phases that are related to bases in $\mathbb{C}^d$. That is, starting from the basis that was used to define U_C for the observables, one can remove the right part of the parameterization without discarding any solution, i.e. it suffices to consider the transformations

$$U_C = \left[\prod_{m=0}^{d-2}\left(\prod_{n=m+1}^{d-1}\exp(\mathrm{i}P_n\lambda_{n,m})\exp(\mathrm{i}\sigma_{m,n}\lambda_{m,n})\right)\right].$$

Optimal values for the parameters can now be determined via search algorithms such as differential evolution [39], simulated annealing [40] or the Nelder–Mead method [41]. With respect to this, the composite parameterization has various advantages compared to several other parameterizations. For instance, varying over $\mathcal{U}(d)$ by using arbitrary Hermitian operators H and computing $U = \exp(\mathrm{i}H)$ as done in [37] is computationally expensive [42], thus, inappropriate for high-dimensional problems. Computing U_C however is simple since it is only a product of the matrices $\exp(\mathrm{i}P_n\lambda_{n,m})\exp(\mathrm{i}\sigma_{m,n}\lambda_{m,n})$, which explicitly read

$$\begin{aligned}\cos(\lambda_{m,n})|n\rangle\langle n| + \sin(\lambda_{m,n})|n\rangle\langle m| - \mathrm{e}^{\mathrm{i}\lambda_{n,m}}\sin(\lambda_{m,n})|m\rangle\langle n| + \mathrm{e}^{\mathrm{i}\lambda_{n,m}}\cos(\lambda_{m,n})|m\rangle\langle m| \\ + \sum_{k\neq m,n}|k\rangle\langle k|.\end{aligned}$$

Also the feature that the product $\prod_{n=m+1}^{d-1}\exp(\mathrm{i}P_n\lambda_{n,m})\exp(\mathrm{i}\sigma_{m,n}\lambda_{m,n})$ leaves the subspace spanned by the basis vectors $\{|0\rangle,\ldots,|m-1\rangle\}$ invariant for a fixed m (see [38]) improves the speed of the computation for large d. Efficiently, we multiply matrices that are smaller than $d\times d$ and in each step $m\to m+1$ the dimension is increased by 1. Another reason to use this particular parameterization, besides its computational benefits, is the fact that the parameters can directly be related to experimental setups; that is, the upper right entries of (10) correspond to settings of beam splitters and the lower left entries to phase shifters.

4. The CGLMP–Bell inequality

A relevant Bell inequality for bipartite systems of dimension $d\times d$ is the CGLMP inequality [2]. For $n=2$ observables on each side A_1, A_2 and B_1, B_2 it was shown that

$$\begin{aligned}I_d = \sum_{k=0}^{\lfloor d/2\rfloor-1}\left(1-\frac{2k}{d-1}\right)\{&+[P(A_1=B_1+k)+P(B_1=A_2+k+1)\\&+P(A_2=B_2+k)+P(B_2=A_1+k)]\\&-[P(A_1=B_1-k-1)+P(B_1=A_2-k)\\&+P(A_2=B_2-k-1)+P(B_2=A_1-k-1)]\}\end{aligned}\tag{11}$$

with $P(A_a=(B_b+k)\bmod d)=\sum_{j=0}^{d-1}P(A_a=(j+k)\bmod d, B_b=j)$ bounded by 2 for local-realistic theories. This inequality can be seen as a generalization of the well-known CHSH–Bell inequality [43] since for $d=2$ they are equivalent. The CGLMP–Bell inequality was proven to correspond to facets of local-realistic correlations implied by (1) and (2) for $n=2$ observables and therefore belongs to the class of tight Bell inequalities [31]. Some known results on the CGLMP inequality can be used to test the power and reliability of our

proposed algorithm. As shown in [2] with a supposed set of optimal observables[2] one can attain the values

$$I_d = \frac{2}{d^2} \sum_{k=0}^{[\frac{d}{2}]-1} \left(1 - \frac{2k}{d-1}\right) \left(\frac{1}{\sin^2\left(\frac{\pi}{d}\left(k+\frac{1}{4}\right)\right)} - \frac{1}{\sin^2\left(\frac{-\pi}{d}\left(k+\frac{3}{4}\right)\right)} \right) \tag{12}$$

for the maximally entangled state $\frac{1}{\sqrt{d}} \sum_{s=0}^{d-1} |s\rangle \otimes |s\rangle$. By maximizing I_d over all observables, i.e. the $4(d^2 - d)$ involved parameters $\lambda_{m,n}$ as described in the previous section using the Nelder–Mead method, we have been able to confirm these values up to dimension $d = 40$ with an accuracy of 10^{-6}. Thus, the maximum of I_d increases with dimension d and lies within $I_2 = 2.828\,43$ for $d = 2$ and $I_d = 2.969\,81$ which is reached for large d. For all investigated dimensions the algorithm has required only a few runs to find the value given by (12) due to the robustness of the Nelder–Mead method. Similar approaches utilizing other parameterization also confirm (12); however, since they are computationally less tractable they do not reach $d = 40$ but only $d = 5$ as in [37, 44] or $d = 9$ as in [45]. Note that there are also techniques for deriving upper bounds on I_d [46] using semi-definite programming [47] which can be used for small d to prove that the found values are indeed global maxima. By maximizing the largest eigenvalue of $\mathcal{B}_{I_d}$ we could also confirm the results in [18, 44], namely that for $d \geqslant 3$ the maximal violation of the CGLMP inequality is attained with non-maximally entangled states.

5. The state space geometry of entanglement and CHSH–Bell inequality violation for bipartite qubits

Now, we come to the main issue of this paper, namely comparing entanglement and quantum nonlocality using geometric representations of the state space. For a single qubit such a representation is given by the three-dimensional Bloch vector (for generalized Bloch vectors see [48]). In a similar way, any density matrix of a bipartite qubit system can be written as

$$\rho = \frac{1}{4} \left(\mathbb{1} \otimes \mathbb{1} + \vec{a} \cdot \vec{\sigma} \otimes \mathbb{1} + \mathbb{1} \otimes \vec{b} \cdot \vec{\sigma} + \sum_{m,n=1}^{3} c_{mn} \sigma_m \otimes \sigma_n \right) \tag{13}$$

with two three-dimensional real vectors $\vec{a}$ and $\vec{b}$ related to local properties and a real 3×3 matrix c_{mn} related to correlations. With regard to studying entanglement and nonlocality, we are not interested in the local properties of the system. Hence, local unitary transformations $U_A \otimes U_B$ can be used to diagonalize the matrix c_{mn} (for more details on this and the following steps see [25, 26]). The diagonal entries can be regarded as components of a three-dimensional real vector $\vec{c}$. Due to the non-negativity condition $\rho \geqslant 0$ the components of this vector must obey the inequalities[3]

$$\begin{aligned} 1 + c_1 + c_2 - c_3 &\geqslant 0, \\ 1 - c_1 - c_2 - c_3 &\geqslant 0, \\ 1 + c_1 - c_2 + c_3 &\geqslant 0, \\ 1 - c_1 + c_2 + c_3 &\geqslant 0. \end{aligned}$$

These constraints restrict $\vec{c}$ to lie within a regular tetrahedron spanned by the projectors of the four well-known Bell states $|\Psi^+\rangle$, $|\Psi^-\rangle$, $|\Phi^+\rangle$ and $|\Phi^-\rangle$. This tetrahedron represents the core of the state space we are interested in and for it, we determine the regions that are entangled or nonlocal, respectively.

[2] There exists no analytic proof that they are optimal.

[3] These are necessary conditions for non-negativity. They are also sufficient when $\vec{a} = 0$ and $\vec{b} = 0$.

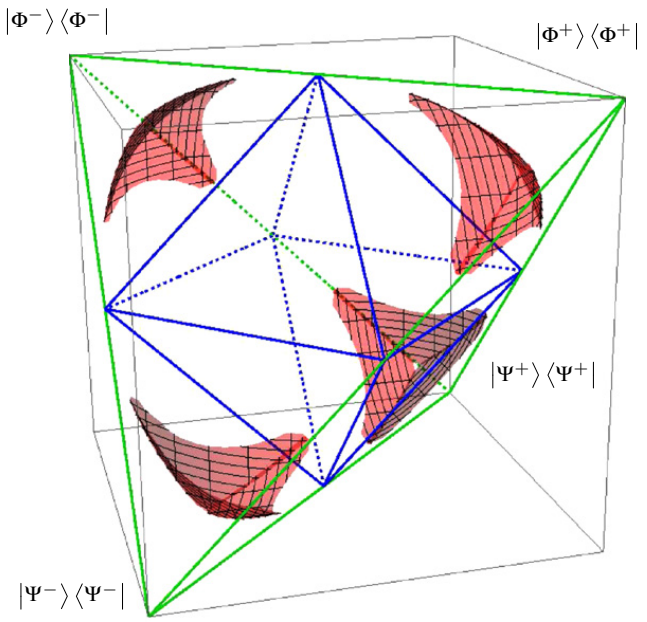

Figure 1. Illustration of the tetrahedron (green) spanned by the four Bell states located in the corners of the cube. By means of the PPT criterion one finds that all states outside this octahedron (blue) are entangled. States beyond the meshed surfaces (red) violate the CHSH–Bell inequality.

For $d = 2$ it was proven that the PPT (positive under partial transposition [49]) criterion is necessary and sufficient, i.e. iff all eigenvalues of a partially transposed density matrix are non-negative, then the state is separable (for $d \geqslant 3$ it is only a necessary criterion). By means of this criterion one finds that all states outside the octahedron spanned by the points $\vec{c}_{1/2} = (0, 0, \pm 1)$, $\vec{c_{3/4}} = (0, \pm 1, 0)$ and $\vec{c_{5/6}} = (0, 0, \pm 1)$ are entangled. For $\vec{a} = 0$ and $\vec{b} = 0$ this is necessary and sufficient for entanglement.

Now, we complete this geometric picture introduced in [25, 26] by adding the geometry of quantum nonlocality. States of the tetrahedron that violate the CHSH–Bell inequality (CGLMP inequality for $d = 2$) can be determined analytically. According to the criterion given in [32] the maximal attainable value for I_2 is $2\sqrt{\lambda_1 + \lambda_2}$, where λ_1 and λ_2 are the two largest eigenvalues of the matrix U_ρ having the components $u_{mn} = \sum_{k=1}^{3} c_{km} c_{kn}$. Consequently, since in our case c_{mn} is a diagonal matrix with the entries c_1, c_2 and c_3 the Bell inequality is violated iff at least one of the three inequalities

$$c_1^2 + c_2^2 > 1,$$
$$c_1^2 + c_3^2 > 1,$$
$$c_2^2 + c_3^2 > 1$$

holds. This means that each of the inequalities defines a cylinder with radius 1 and if a density matrix lies outside of 1, it is nonlocal. The union of the exterior regions of these three cylinders belongs to the set of nonlocal states. The tetrahedron including the boundaries of separability and CHSH violation is visualized in figure 1. It descriptively demonstrates that not all entangled states violate the CHSH inequality. Note that it is also known that all entangled bipartite qubit states can be distilled and therefore do contain so-called hidden nonlocality [50].

6. The state space geometry of bipartite qudits—the magic simplex $\mathcal{W}$

A generalization of the tetrahedron for bipartite qudit systems for arbitrary dimension d was introduced in [27, 28]. Analogously to the qubit case, a regular simplex can be constructed using mutually orthogonal generalized Bell states. This so-called magic simplex is given by the set of states

$$\mathcal{W} = \left\{ \sum_{k,l=0}^{d-1} c_{k,l} P_{k,l} \;\middle|\; c_{k,l} \geqslant 0, \sum_{k,l=0}^{d-1} c_{k,l} = 1 \right\}, \tag{14}$$

where $P_{k,l} = |\Omega_{k,l}\rangle\langle\Omega_{k,l}|$ are the projectors of d^2 Bell-type states generated by applying the Weyl operators

$$W_{kl} = \sum_{s=0}^{d-1} \mathrm{e}^{\frac{2\pi \mathrm{i}}{d} sk} |s\rangle\langle (s+l) \bmod d| \tag{15}$$

with $k, l \in \{0, \ldots, d-1\}$ on the maximally entangled state

$$|\Omega_{0,0}\rangle = \frac{1}{\sqrt{d}} \sum_{s=0}^{d-1} |s\rangle \otimes |s\rangle, \tag{16}$$

i.e.

$$|\Omega_{k,l}\rangle = (W_{k,l} \otimes \mathbb{1})|\Omega_{0,0}\rangle. \tag{17}$$

The simplex is a convex set located in a (d^2-1)-dimensional hyperplane in a d^2-dimensional real vector space of Hermitian operators spanned by the operators $\{P_{k,l}\}$. Unlike as for two qubits, where every state ρ has a representative in the tetrahedron, for $d \geqslant 3$ not every ρ on $\mathbb{C}^d \otimes \mathbb{C}^d$ can be related to an element of the simplex [27, 28]. However, the derived class of states is of special importance in quantum key distribution [51] and entanglement distillation protocols [52]. Moreover, these states are frequently studied in the context of (bound) entanglement [29, 53–56] and entanglement measures [57, 58] due to their interesting features. A detailed discussion on the properties of $\mathcal{W}$ and on how it is embedded in the state space can be found in [27, 28]. For the subsequent investigations let us note that local (anti-)unitary transformations $U_A \otimes U_B$ mapping $\mathcal{W}$ onto itself are related to symmetries of $\mathcal{W}$, since equivalence classes

$$[\rho] = \left\{ \rho' \in \mathcal{W} \middle| \rho' = U_A \otimes U_B \; \rho \; U_A^\dagger \otimes U_B^\dagger \right\}$$

share the same properties with respect to separability and (non)locality. The set of all symmetries can be represented with a discrete classical phase space, see figure 2. From theorem 9 of [28] one can infer that states with components $\{c_{k,l}\}$ and $\{c'_{k',l'}\}$, respectively, belong to the same equivalence class iff there exists a phase space transformation of the form

$$\begin{pmatrix} k \\ l \end{pmatrix} = \begin{pmatrix} m & n \\ p & q \end{pmatrix} \begin{pmatrix} k' \\ l' \end{pmatrix} + \begin{pmatrix} j \\ r \end{pmatrix} \qquad M := \begin{pmatrix} m & n \\ p & q \end{pmatrix} \tag{18}$$

with $\det M = 1$ or $\det M = d-1$ such that $c_{k,l} = c'_{k,l}$ with $m, n, p, q, j, r \in \mathbb{Z}$.

Quantum nonlocality has so far not been investigated for the magic simplex $\mathcal{W}$. In this paper we aim to determine the states of the magic simplex $\mathcal{W}$ that violate the CGLMP–Bell inequality by using the novel approach introduced in section 3. In particular, we want to exactly specify the implied boundaries, i.e. states ρ that obey

$$\max_{\{\mathcal{B}_{I_d}\}} \mathrm{Tr}(\mathcal{B}_{I_d} \; \rho) = 2.$$

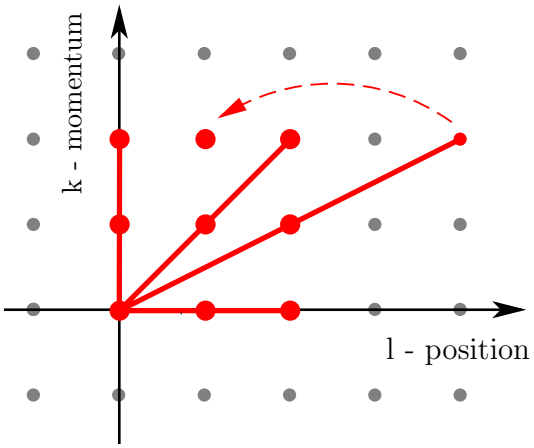

Figure 2. Illustration of the finite discrete classical phase space for $d = 3$ of the simplex $\mathcal{W}$. All possible complete lines through the point $(0, 0)$ for $d = 3$ are drawn, representing one class of states which have the same geometry concerning separability and (non)locality. Lines can be completed by points with $k, l \notin \{0, \ldots, d-1\}$ because of the periodicity of the Weyl operators implying $P_{k,l} = P_{k+m\cdot d, l+n\cdot d}$ for all $n, m \in \mathbb{Z}$.

For arbitrary families of states this is in general difficult since it has to be done iteratively in small regions until a required precision is reached. However, for the considered classes of states one can exploit that the trace of the CGLMP–Bell operator vanishes, i.e. $\mathrm{Tr}(\mathcal{B}_{I_d}) = 0$ which is a consequence of the specific form of the CGLMP–Bell inequality: the quantity I_d (11) is composed of the probabilities $P(A_a = (B_b + k) \bmod d) = \sum_{j=0}^{d-1} P(A_a = (j + k) \bmod d, B_b = j)$ and when it is rewritten as $\mathrm{Tr}(\mathcal{B}_{I_d}\rho)$, every $P(A_a = x, B_b = y)$ corresponds to a one-dimensional projector $|x\rangle_{A_a}\langle x|_{A_a} \otimes |y\rangle_{B_b}\langle y|_{B_b}$ which has trace 1. Since there are equally many projectors with positive and negative prefactors in every term of the sum in (11) and due to the linearity of the trace, it follows that $\mathrm{Tr}(\mathcal{B}_{I_d}) = 0$.

Consequently, for states of the form $\rho = \frac{1-\nu}{d^2}\mathbb{1}_{d^2} + \nu\tau$, i.e. a particular state τ mixed with uncolored noise $\frac{1}{d^2}\mathbb{1}_{d^2}$, we can exploit that

$$\begin{aligned}\max_{\{\mathcal{B}_{I_d}\}} \mathrm{Tr}(\mathcal{B}_{I_d}\rho) &= \max_{\{\mathcal{B}_{I_d}\}} \mathrm{Tr}\left(\mathcal{B}_{I_d}\left[\frac{1-\nu}{d^2}\mathbb{1}_{d^2} + \nu\ \tau\right]\right)\\ &= \max_{\{\mathcal{B}_{I_d}\}} \mathrm{Tr}(\mathcal{B}_{I_d}\nu\ \tau)\\ &= \nu \max_{\{\mathcal{B}_{I_d}\}} \mathrm{Tr}(\mathcal{B}_{I_d}\ \tau),\end{aligned} \tag{19}$$

which implies that if the maximal value of $\max I_d(\tau) = \max_{\mathcal{B}_{I_d}} \mathrm{Tr}(\mathcal{B}_{I_d}\tau)$ is known, then the parameter value $\nu = 2/\max I_d(\tau)$ for ρ yields a state on the boundary of CGLMP–Bell inequality violation.

In order to compare our new results on the geometry of quantum nonlocality with the geometry of entanglement we use several results and techniques of precedent publications on the magic simplex $\mathcal{W}$. For a detailed discussion of how to decide separability for the simplex states via the PPT criterion, matrix realignment, optimal entanglement witnesses and entanglement measures we refer the reader to [27–29, 53, 56, 58].

7. The state space geometry of entanglement and CGLMP–Bell inequality violation for bipartite qutrits

In the following we investigate and illustrate low-dimensional sections of the $\mathcal{W}$-simplex for bipartite qutrits ($d = 3$). As a first example consider the so-called isotropic states

$$\rho = \frac{1-\alpha}{9}\mathbb{1}_9 + \alpha P_{k,l}. \tag{20}$$

The phase space transformation rules (18) imply that all such one-parameter states with arbitrary $k, l \in \{0, \ldots, 2\}$ but the same α have the same properties in terms of separability/entanglement and (non)locality. Any state of this form is separable for $\frac{1}{4} \geqslant \alpha \geqslant 0$ and entangled for $\alpha > \frac{1}{4}$ (see [59] and references therein). Using (19) and the compliance of our numerical results with (12) we find that the CGLMP–Bell inequality is violated for $\alpha > \frac{1}{2}(6\sqrt{3} - 9)$.

Next, consider the two-parameter families of states of the form

$$\rho = \frac{1-\alpha-\beta}{9}\mathbb{1}_9 + \alpha P_{k,l} + \beta P_{m,n} \tag{21}$$

with arbitrary $k, l, m, n \in \{0, \ldots, 2\}$. Any such state is local-unitarily equivalent to the state $\rho = \frac{1-\alpha-\beta}{9}\mathbb{1}_9 + \alpha P_{0,0} + \beta P_{0,1}$. For this set of states the PPT boundary reads

$$8\alpha^2 + 8\beta^2 - 11\beta\alpha + 2\alpha + 2\beta - 1 = 0,$$

which was derived by setting the eigenvalues of the partially transposed matrix ρ^{T_B} to zero. There are also bound entangled states in this set. They can be found through optimal entanglement witnesses yielding the boundaries [58]

$$4\alpha^2 - 5\alpha + 40\beta^2 + (17\alpha - 14)\beta + 1 = 0 \qquad \text{and}$$
$$4\beta^2 - 5\beta + 40\alpha^2 + (17\beta - 14)\alpha + 1 = 0.$$

The boundary of the CGLMP–Bell violation was obtained by computing $\max I_3(\rho)$ for 200 equally spaced points on the boundaries of positivity $\left(\alpha = \frac{\beta-1}{8}, \beta = \frac{\alpha-1}{8}\right.$ and $\left.\beta = 1 - \alpha\right)$. Again, (19) was exploited to determine the values of α and β corresponding to states on the boundary, i.e. $\max_{\mathcal{B}_{I_d}} \mathrm{Tr}(\mathcal{B}_{I_d}\rho) = 2$. The result is graphically illustrated in figure 3. The illustration suggests that the boundary of CGLMP–Bell inequality violation describes a circle for $\alpha, \beta > 0$ and a line if one of the parameters is negative, i.e. $\alpha < 0$ or $\beta < 0$. Note that this abrupt change in the shape only appears for the boundary of CGLMP–Bell inequality violation but not for the boundary of separability. Conjectures on the exact specifications of these boundaries are contained in the considerations of the three-parameter families of states

$$\rho = \frac{1-\alpha-\beta-\gamma}{9}\mathbb{1} + \alpha P_{k,l} + \beta P_{m,n} + \gamma P_{p,q} \tag{22}$$

as the special case $\gamma = 0$. Theorem 3 of [27] implies that, depending on whether the index pairs $\{(k, l), (m, n), (p, q)\}$ form a line or not (in the sense of the discrete classical phase space, figure 2), this three-parameter family of states is either local-unitarily equivalent to the state

$$\rho_{\text{line}}(\alpha, \beta, \gamma) = \frac{1-\alpha-\beta-\gamma}{9}\mathbb{1}_9 + \alpha P_{0,0} + \beta P_{0,1} + \gamma P_{0,2} \tag{23}$$

or

$$\rho_{\text{off-line}}(\alpha, \beta, \gamma) = \frac{1-\alpha-\beta-\gamma}{9}\mathbb{1}_9 + \alpha P_{0,0} + \beta P_{0,1} + \gamma P_{1,0}. \tag{24}$$

The class of line states are graphically illustrated in figure 4, and a particular slice of the off-line states is visualized in figure 5(*b*).

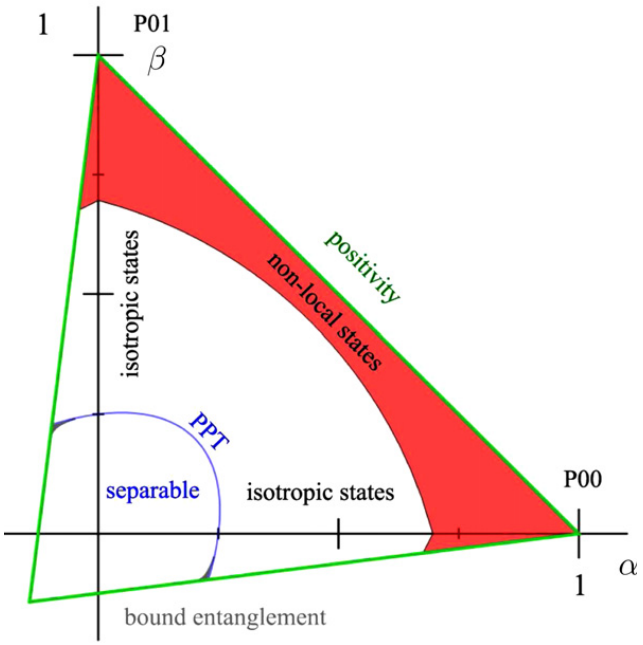

Figure 3. Illustration of the state $\rho = \frac{1-\alpha-\beta}{9}\mathbb{1}_9 + \alpha P_{0,0} + \beta P_{0,1}$. All states lie within the (green) triangle which corresponds to the border of positivity. The (blue) ellipse corresponds to the PPT border, i.e. all PPT states lie inside. As shown in [27] if one parameter is negative, there is also a small (gray, filled) region of bound entanglement. States ρ in the (red) filled area violate the CGLMP–Bell inequality ($\max I_3(\rho) > 2$). Interestingly, the geometry given by the CGLMP–Bell operator changes its shape (from a circle to a line) at the transition from positive to negative parameters.

For the states $\rho_{\text{line}}(\alpha, \beta, \gamma)$ the PPT boundary is

$$8\alpha^2 + 8\beta^2 + 8\gamma^2 + 2\alpha + 2\beta + 2\gamma - 11\alpha\beta - 11\alpha\gamma - 11\beta\gamma - 1 = 0.$$

As stated in [58] further (bound) entangled states can be revealed using optimal entanglement witnesses which for the boundary of separability written in implicit form yield

$$40\alpha^2 + \alpha(17\beta + 17\gamma - 14) + 4\beta^2 + \gamma(4\gamma - 5) - \beta(19\gamma + 5) + 1 = 0,$$

and the equations one gets via permutations with respect to α, β, γ. The boundary of CGLMP–Bell violation is deduced via (19) from the values $\max I_3(\rho)$ of 1000 equally spaced states on the boundaries of positivity ($\alpha = \frac{\beta+\gamma-1}{8}$ (and all parameter permutations of this term) and $\gamma = 1 - \alpha - \beta$). The resulting points apparently describe a spherical surface which meets the boundaries of positivity and PPT at the point $\alpha = \beta = \gamma = \frac{1}{3}$. This sphere appears to be intersected by planes in the vicinity of the isotropic states, figure 4.

When taking into account symmetries and the fact that (12) yields the boundary parameter $\frac{1}{2}(6\sqrt{3}-9)$ for the isotropic states one can suppose a sphere with radius $r = \frac{1}{156}(413\sqrt{3}-558)$ and center at $\alpha = \beta = \gamma = \frac{1}{156}(-361 + 186\sqrt{3})$. These specifications coincide with the numerical data up to the order 10^{-6}.

For $\rho_{\text{line}}(\alpha, \beta, \gamma)$ the measurement settings given in [2] combined with local unitary transformations constituted by the Weyl operators yield the illustrated intersecting planes given by the possible parameter permutations of the function

$$\gamma = \tfrac{1}{2}(\alpha + \beta + 6\sqrt{3} - 9). \tag{25}$$

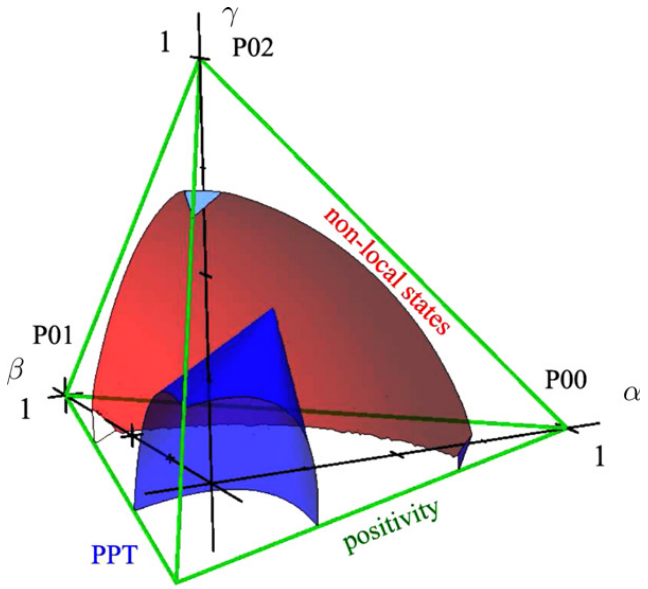

Figure 4. Illustration of a three-dimensional state subspace given by bipartite qutrit line states $\rho_{\text{line}}(\alpha, \beta, \gamma)$, equation (23). As for bipartite qubit states, figure 1, all states have to be within a (green) tetrahedron (positivity condition). The boundary of PPT states forms a (blue) cone and thus all states beyond this surface are entangled. The tip of the cone touches the surface of positivity at $\alpha = \beta = \gamma = \frac{1}{3}$. States ρ beyond the shaded (light red/blue) surface violate the CGLMP–Bell inequality ($\max I_3(\rho) > 2$). Again, the geometric form changes from a sphere to a plane when one or more parameters become negative.

To see this one can use the local-unitarily equivalent state $\rho = \frac{1-\alpha-\beta-\gamma}{9}\mathbb{1}_9 + \alpha P_{0,0} + \beta P_{1,0} + \gamma P_{2,0}$ and write $\text{Tr}(\mathcal{B}_{I_3}\rho) = \alpha\,\text{Tr}(\mathcal{B}_{I_3}P_{0,0}) + \beta\,\text{Tr}(\mathcal{B}_{I_3}P_{1,0}) + \gamma\,\text{Tr}(\mathcal{B}_{I_3}P_{2,0})$.[4] Here, the measurement bases in [2] yield $\text{Tr}(\mathcal{B}_{I_3}P_{0,0}) = \frac{4}{6\sqrt{3}-9}$ and $\text{Tr}(\mathcal{B}_{I_3}P_{1,0}) = \text{Tr}(\mathcal{B}_{I_3}P_{2,0}) = \frac{-2}{6\sqrt{3}-9}$. Thus, by setting $\text{Tr}(\mathcal{B}_{I_3}\rho) = 2$ we obtain (25) up to a parameter permutation, which in practice can be realized using a local-unitarily modified Bell operator $W_{k,l}^\dagger \otimes \mathbb{1}_3\ \mathcal{B}_{I_3}\ W_{k,l} \otimes \mathbb{1}_3$ since $\text{Tr}(\mathcal{B}_{I_3}P_{k,l}) = \text{Tr}\left(\mathcal{B}_{I_3}\ W_{k,l} \otimes \mathbb{1}_3\ P_{0,0}\ W_{k,l}^\dagger \otimes \mathbb{1}_3\right) = \text{Tr}\left(\left(W_{k,l}^\dagger \otimes \mathbb{1}_3\ \mathcal{B}_{I_3}\ W_{k,l} \otimes \mathbb{1}_3\right) P_{0,0}\right)$. For parameter regions in the vicinity of the isotropic states where one parameter is positive and two parameters are equal or less than zero the approach of section 3 does not lead to a better result than that.

For the remaining family of off-line states, equation (24), the geometric form of the boundary of CGLMP–Bell violation has a more complex shape. An uncovered suggestion on the exact form has therefore not been made. Figure 5(*b*) gives an impression of the fact that the boundaries of PPT, as well as CGLMP–Bell violation have a different shape for the different types of states. For instance, in contrast to the class of line states where there is only one state $\alpha = \beta = \gamma = \frac{1}{3}$ on the boundary of positivity $1 - \alpha - \beta - \gamma = 0$ that does not violate the CGLMP–Bell inequality, for the second type $\rho_{\text{off-line}}$ there is a whole region of states for $1-\alpha-\beta-\gamma = 0$ that obeys the CGLMP–Bell inequality. Moreover, in comparison, the entire region of nonlocal states in figure 5(*b*) is smaller than in that figure 5(*a*). For entanglement, one finds the opposite, which is a intriguing result. It is rather counterintuitive because the

[4] Note that it is not an error that the values for $P_{1,0}$ and $P_{2,0}$ differ from that of $P_{0,0}$. Different states, even though they are local-unitarily equivalent require different measurement settings.

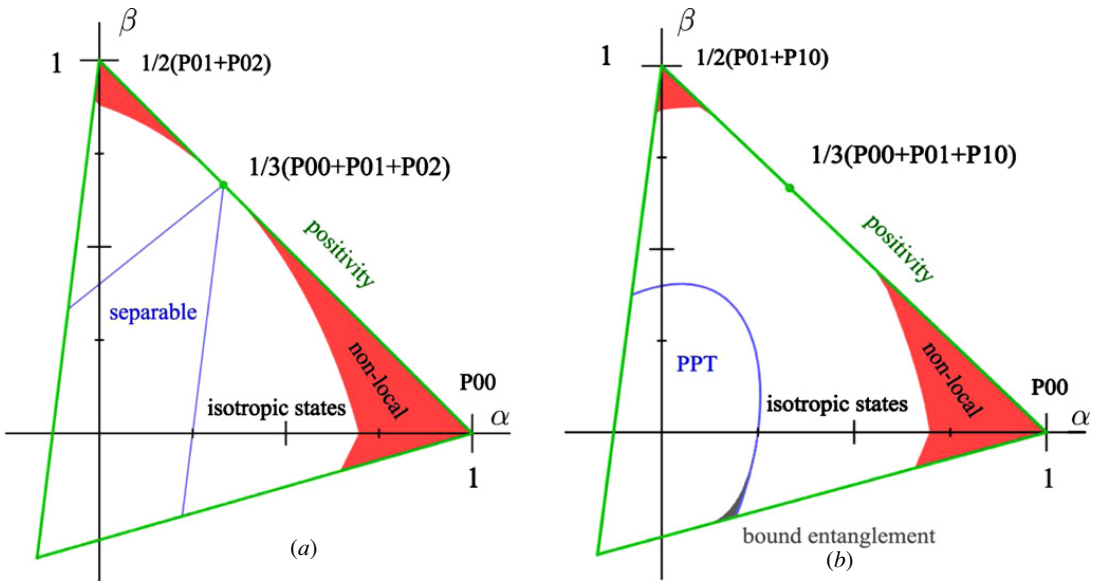

Figure 5. Comparison of the class of line states $\rho_{\text{line}}\left(\alpha, \frac{\beta}{2}, \frac{\beta}{2}\right)$, equation (23), with the class of off-line states $\rho_{\text{off line}}\left(\alpha, \frac{\beta}{2}, \frac{\beta}{2}\right)$, equation (24). In the first case, one finds that there is no bound entanglement and that the separable states form a polygon. In the second case, the boundary given by the PPT criterion is curved (blue) and bound entanglement is found for $\beta < 0$ (gray, filled region). The region of nonlocal states (filled, red region) is smaller in case the third Bell state does not belong to the line formed by the other two Bell states of the mixture.

region of separable states of the subset

$$\rho_{\text{line}}\left(\alpha, \frac{\beta}{2}, \frac{\beta}{2}\right) \tag{26}$$

already is larger than the PPT region of the same subset of off-line states

$$\rho_{\text{off}-\text{line}}\left(\alpha, \frac{\beta}{2}, \frac{\beta}{2}\right) \tag{27}$$

which in addition also contains bound entanglement for $\beta < 0$.

8. Entanglement measures versus Bell inequality violations

In [57, 60], an entanglement measure for multipartite qudit systems was introduced, as well as a method how optimal bounds can be derived for it. Here we apply this measure to bipartite qutrits.

For any bipartite qutrit state $\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$, entanglement can be quantified via

$$\mathcal{E}(\rho) := \inf_{\{p_i, |\psi_i\rangle\}} \sum_i p_i \, \{S(\text{Tr}_A |\psi_i\rangle\langle\psi_i|) + S(\text{Tr}_B |\psi_i\rangle\langle\psi_i|)\} \tag{28}$$

$$= 2 \inf_{\{p_i, |\psi_i\rangle\}} \sum_i p_i \, S(\text{Tr}_A |\psi_i\rangle\langle\psi_i|), \tag{29}$$

where S is any Renyi entropy. In our case we use the linear entropy $S_L(\rho) = \frac{3}{2}(1 - \text{Tr}\,\rho^2)$. In general the infimum, i.e. the optimal decomposition, is not known. The derivation of lower

bounds on the measure are based on the observation that the linear entropy can be rewritten as [38, 57]

$$\frac{4}{3}S_L(\rho_A) = \sum_{k_A<l_A}\sum_{k_B<l_B} \mathrm{Tr}(|\psi\rangle\langle\psi|\sigma_{k_A,l_A}\otimes\sigma_{k_B,l_B}(|\psi\rangle\langle\psi|)^*\sigma_{k_A,l_A}\otimes\sigma_{k_B,l_B}) \tag{30}$$

$$=: C_m^2(|\psi\rangle\langle\psi|) \tag{31}$$

using the anti-symmetric σ-matrices (8). $C_m^2(|\psi\rangle\langle\psi|)$ is called the m-concurrence and is an entanglement measure for pure states in its own right. The m-concurrence is generalized to mixed states via the convex roof construction (29) to

$$\begin{aligned} C_m^2(\rho) &:= \inf_{\{p_i,|\psi_i\rangle\}}\sum_i p_i C_m^2(|\psi_i\rangle\langle\psi_i|) \\ &= \inf_{\{p_i,|\psi_i\rangle\}}\sum_i p_i \sum_{k_A<l_A}\sum_{k_B<l_B} \mathrm{Tr}(|\psi_i\rangle\langle\psi_i|\sigma_{k_A,l_A}\otimes\sigma_{k_B,l_B}(|\psi_i\rangle\langle\psi_i|)^*\sigma_{k_A,l_A}\otimes\sigma_{k_B,l_B}). \end{aligned} \tag{32}$$

This expression has the lower bound

$$C_m^2(\rho) \geqslant \sum_{k_A<l_A}\sum_{k_B<l_B} \inf_{\{p_i,|\psi_i\rangle\}}\sum_i p_i \mathrm{Tr}(|\psi_i\rangle\langle\psi_i|\sigma_{k_A,l_A}\otimes\sigma_{k_B,l_B}(|\psi_i\rangle\langle\psi_i|)^*\sigma_{k_A,l_A}\otimes\sigma_{k_B,l_B}),$$

for which the contained individual infima are known as (see [61, 62])

$$\inf_{\{p_i,|\psi_i\rangle\}}\sum_i p_i \mathrm{Tr}(|\psi_i\rangle\langle\psi_i|\sigma_{k_A,l_A}\otimes\sigma_{k_B,l_B}(|\psi_i\rangle\langle\psi_i|)^*\sigma_{k_A,l_A}\otimes\sigma_{k_B,l_B}) = X^2_{k_A,l_A,k_B,l_B}, \tag{33}$$

with

$$X_{k_A,l_A,k_B,l_B} := \max\left[2\max\left[\left\{x^i_{k_A,l_A,k_B,l_B}\right\}\right] - \sum_i x^i_{k_A,l_A,k_B,l_B}, 0\right] \tag{34}$$

where $\left\{x^i_{k_A,l_A,k_B,l_B}\right\}$ are the square roots of the eigenvalues of

$$\rho\ \sigma_{k_A,l_A}\otimes\sigma_{k_B,l_B}\ \rho^*\ \sigma_{k_A,l_A}\otimes\sigma_{k_B,l_B}. \tag{35}$$

The derived bound in general depends on in which basis the state ρ is written and is thus not invariant under local unitaries [38]. Consequently, the optimal lower bound for a state ρ is given by the maximum over all $\rho' = U_A\otimes U_B\ \rho\ U_A^\dagger\otimes U_B^\dagger$. This problem can be reduced to a 12-parameter optimization problem analogously to section 3. Note that there are also algorithms to numerically derive tight upper bounds on the convex roof [63]; thus, we know for which classes of states the exact value of the measure is obtained.

Now, consider the class of line states with two equally weighted Bell states according to (26). We evaluated the introduced bounds on a grid of (α, β) points with a step size of 0.02 and found that they are exact (up to numerical precision) for this particular class of states. The numerical data can be represented with an accuracy of 10^{-6} by the expressions

$$C_m^2\left(\rho_{\text{line}}\left(\alpha,\frac{\beta}{2},\frac{\beta}{2}\right)\right) = \frac{1}{27}\max\{0, 8\alpha-\beta-2\}^2 \qquad \text{for } \alpha \geqslant \frac{1}{4}+\frac{\beta}{8},$$

$$C_m^2\left(\rho_{\text{line}}\left(\alpha,\frac{\beta}{2},\frac{\beta}{2}\right)\right) = \frac{2}{27}\max\{0, 5\beta-4\alpha-2\}^2 \qquad \text{for } \alpha < \frac{1}{4}+\frac{\beta}{8},$$

for the m-concurrence C_m^2. The contour plot (figure 6) shows that all states lying on lines parallel to the boundaries of separability contain the same amount of entanglement. In

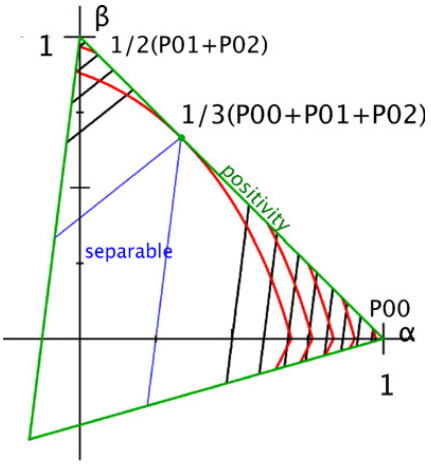

Figure 6. Comparison of the contour plots of the m-concurrence $C_m^2(\rho)$ with Bell inequality violation given by $\max I_3(\rho)$ for the line states $\rho_{\text{line}}\left(\alpha, \frac{\beta}{2}, \frac{\beta}{2}\right)$. The black lines parallel to the boundaries of separability correspond to the amount of entanglement, while the red curves correspond to the degree of Bell inequality violation. The fact that both quantities cannot be monotonically related can easily be seen by walking along one of the red lines on the right side, i.e. $\alpha \geqslant \frac{1}{4} + \frac{\beta}{8}$. For instance, starting from one of the points where a red curve intersects the upper green boundary of positivity, the amount of entanglement increases first until $\beta = 0$ but when β becomes negative it decreases again.

comparison to this, the strength of CGLMP–Bell inequality violation is not related to the distance to the separable states. Figure 6 is an illustrative example that Bell inequality violations and the entanglement measures are non-monotonically related. Another example is illustrated in figure 7 where the amount of entanglement of states on the border of CGLMP–Bell inequality violation ($\max I_3(\rho) = 2$) and of positivity are plotted. Both results demonstrate that there exists no monotone function relating the Bell inequality violation to the amount of entanglement. For pure states this was already known; however, the surprising thing is that the same statement is also true for mixtures of states that all share the same amount of entanglement, i.e. $\{P_{k,l}\}$.

9. Summary

We presented the first detailed state space analysis of a Bell inequality in the context of geometry: the analysis necessitated to ascertain whether a Bell inequality is violated or obeyed for a given quantum state ρ. In order to solve this, we used a novel composite parameterization of the unitary group $\mathcal{U}(\mathrm{d})$ and robust numerical methods (section 3). Using this we achieved compliance with the orthonormality constraints and reduced the numerical search to $d^2 - d$ real parameters for each involved observable. Our tests for the CGLMP inequality (section 4) showed that our method works with good numerical precision and that the used parameterization is beneficial with respect to numerical tractability. In section 5 we began our geometric state space considerations concerning entanglement and nonlocality. We derived a regular tetrahedron spanned by the four Bell states for bipartite qubits. For this tetrahedron, the sets of entangled and CHSH inequality violating states were determined with analytic methods. The graphical illustration of the tetrahedron (figure 1) provides a descriptive example that not all entangled states violate the CHSH inequality. In section 6 we considered the state

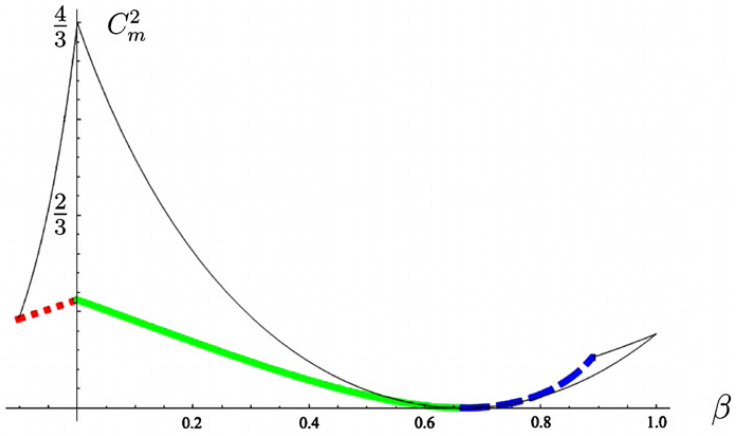

Figure 7. These curves show the amount of entanglement for the line state $\rho\left(\alpha, \frac{\beta}{2}, \frac{\beta}{2}\right)$, equation (23), in dependence of β (compare with figure 5(*a*)). The solid thin (black) curve is the amount of entanglement for all states lying on the boundary of positivity. The other graphs show the amount of entanglement for the boundary of CGLMP–Bell inequality violation. In detail, the dotted (red) graph illustrates the amount of entanglement for $\beta < 0$. The solid thick (green) graph illustrates the amount of entanglement in the range $\beta = 0$ to the separable state $\rho\left(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}\right)$ along the curved CGLMP boundary, while the dashed (blue) graph illustrates the region $\beta \geqslant \frac{2}{3}$.

space geometry for the more general case of bipartite qudits. We focused on a generalization of the tetrahedron—the so-called magic simplex $\mathcal{W}$—a class of states which is of special interest for quantum key distribution and entanglement distillation protocols. We gave a short review of the properties and symmetries of $\mathcal{W}$ which are related to a classical discrete phase space (figure 2). In section 7 we determined the nonlocal states of the simplex for the special case of bipartite qutrits ($d = 3$) using the proposed numerical method. Here, we exploited a particular property of states containing uncolored noise (19) to further reduce the numerical effort. The boundaries of CGLMP–Bell inequality violation and separability were visualized for the class of the so-called line states and for the class of the so-called off-line states in figure 3 to figure 5. As could be seen in all cases, both boundaries are not simply related by a constant shift or scaling factor but rather are fundamentally different. In section 8 we considered the relation between entanglement measures and Bell inequality violations. We determined the exact value of the m-concurrence [57, 60] for a particular class of line states with two equally weighted parameters. Comparing the strength of CGLMP–Bell inequality violation with the amount of entanglement, we geometrically demonstrated that both quantities are non-monotonically related.

In summary, we have seen that geometric considerations of the state space are an insightful way of studying the manifestations of entanglement. As we have shown, these approaches are suitable for revealing fundamental differences between entanglement and quantum nonlocality.

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Statement of contribution

I hereby certify that Mag. Christoph Ari Spengler is the major contributor and main author of the journal publications:

[P1] J. Phys. A: Math. Theor. **43**, 385306 (2010).
[P2] J. Math. Phys. **53**, 013501 (2012).
[P3] Quantum Inf. Process., DOI: 10.1007/s11128-012-0369-8 (2012).
[P6] Phys. Rev. A **86**, 022311 (2012).
[P7] J. Phys. A: Math. Theor. **44**, 065304 (2011).

As a co-author, he made a contribution of at least 25% to the publications:

[P4] Phys. Rev. A **83**, 062325 (2011).
[P5] Phys. Rev. A **83**, 022328 (2011).

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Talks and Conferences

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04/2012	**Young Researchers in Mathematics (YRM 2012)** University of Bristol, U.K. Contributed talk: '*Composite parameterization and Haar measure for all unitary and special unitary groups*'
10/2011	**Brno-Vienna-Bratislava Nonlocal Seminar** Masaryk University Brno, Czech Republic Contributed talk: *'Examining the dimensionality of genuine multipartite entanglement'*
06/2011	**8th Central European Quantum Information Processing Workshop (CEQIP 2011)** Znojmo, Czech Republic Contributed talk: '*Composite parameterization and Haar measure for all unitary and special unitary groups*'

05/2011 **Seminar der Mathematischen Physik**
University of Vienna
Invited talk (Jakob Yngvason): '*Composite parameterization and Haar measure for all unitary and special unitary groups'*

02/2011 **Seminar on *Quantum Information Processing and Communication***
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Invited talk (Jozef Gruska and Jan Bouda):
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01/2011 **14th Workshop on Quantum Information Processing (QIP2011)**
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Contributed poster (winner of the 'People`s Choice Poster Award'):
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11/2010 **Vienna Central European Seminar : Complex Stochastic Dynamics**
University of Vienna

09/2010 **CoQuS II kick-off workshop**
University of Vienna
Contributed posters:
'A composite parameterization of unitary groups, density matrices and subspaces'
'The state space geometry of the CGLMP–Bell inequality'

08/2010 **Annual Meeting of the Austrian Physical Society**
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07/2010 **Workshop on Quantum Algorithms, Computational Models, and Foundation of Quantum Mechanics**
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07/2010 **10th Canadian Summer School on Quantum Information**
University of British Columbia, Vancouver, Canada

06/2010 **Workshop in honour of Reinhold Bertlmann :**
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06/2010 **7th Central European Quantum Information Processing**
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09/2009 **Vienna Symposium on the Foundations of Modern Physics**
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06/2009 **Vienna-Theory-Lunch Seminar**
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Contributed talk: '*Quantum nonlocality and its state space geometry'*

09/2008 **Annual Meeting of the Austrian Physical Society** (FAKT Session)
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