Inseparability criteria in finite Hilbert spaces

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Zusammenfassung

Was ist Verschränkung? Diese Frage beschäftigt nun seit mehr als 70 Jahren die Physiker und hat eine Diskussion ausgelöst, die ihres gleichen sucht. Vor allem in den letzten zwei Jahrzehnten, angetrieben von den technologischen Fortschritten in der experimentellen Physik, hat diese Diskussion eine Vielzahl von neuen Erkenntnissen geliefert. Wir wissen heute, dass Verschränkung eine neuartige, ausschließlich quantenmechanische Ressource ist, die es uns erlaubt, viele Aufgaben zu bewerkstelligen, die mit den Methoden der klassischen Theorien nicht oder sehr ineffizient zu behandeln sind. Zum Beispiel sind die Quantenkryptographie, die Quantenteleportation und der Quantencomputer die direkten Anwendungen dieser neuen Ressource. Und doch, obwohl so viele Erfolge erzielt wurden, bleibt die Frage – Was ist Verschränkung? – nach wie vor nicht ausreichend beantwortet. Einer der wichtigsten Gründe dafür ist die Tatsache, dass keine anwendbaren Inseparabilitätskriterien bekannt sind, mit deren Hilfe die separablen von den verschränkten quantenmechanischen Zuständen unterschieden werden können (die Unterscheidung zwischen separablen und verschränkten Zuständen wird auch als Separabilitätsproblem bezeichnet). Das zentrale Ziel der vorliegenden Dissertation ist deshalb, eben solche Inseparabilitätskriterien zu entwickeln.

Um dieses Ziel zu erreichen, bilden wir zunächst das Separabilitätsproblem auf ein Problem aus der konvexen Geometrie ab, nämlich der Suche nach einer Hyperebene, die zwei konvexe Mengen von einander trennt. Dabei bedienen wir uns der Darstellung der hermitischen Operatoren als Vektoren im Hilbert-Schmidt Vektorraum. In dieser Darstellung leiten wir eine Klasse von Ungleichungen ab, deren Verletzung, ähnlich wie bei den Bellschen Ungleichungen, ein eindeutiger Hinweis dafür ist, dass Verschränkung vorliegt. Mit einigen wenigen Ausnahmen entspricht unsere geometrische Vorgehensweise zur Suche von Inseparabilitätskriterien den Methoden basierend auf den so genannten Zeugenoperatoren (witness operators). Doch gerade diese kleinen Abweichungen zu den existierenden Verfahren erlauben es uns, einen optimalen Zeugenoperator zu finden und somit eine bisher noch offene Frage

zu beantworten. Unter der Berücksichtigung der Tatsache, dass die Existenz eines optimalen Zeugenoperators einem notwendigen und hinreichenden Inseparabilitätskriterum entspricht, wird deshalb auch das Separabilitätsproblem gelöst.

Bei der Suche nach anwendbaren Inseparabilitätskriterien verfolgen wir zwei verschiedene Strategien. Zunächst beschreiben wir ein hinreichendes Kriterium, welches *einfach* zu überprüfen ist. Dieses Kriterium basiert auf der Singulärwertzerlegung (SVD) des Dichteoperators und kann Verschränkung nachweisen, ohne dass komplizierte Optimierungsprobleme gelöst werden müssen. Wir demonstrieren, dass dieses SVD-Kriterium inseparable Zustände detektieren kann, für welche das Peres-Horodecki Verfahren, ein anderes einfach zu berechnendes Inseparabilitätskriterium, versagt. Infolgedessen können wir durch eine Kombination der beiden Verfahren die Mengen der verschränkten Zustände, welche einfach zu detektieren sind, signifikant vergrößern. Die zweite Strategie besteht darin, ein *notwendiges und hinreichendes* Kriterium zu entwickeln. Zu diesem Zweck stellen wir ein Optimierungsproblem vor und beweisen, dass dessen positive Lösung einer eineindeutigen Signatur für Verschränkung entspricht. Zum Lösen dieses Optimierungsproblems bedienen wir uns der Methoden von Operations Research und entwickeln einen Algorithmus, der diese Aufgabe erfüllt. Dieser kann auf modernen Computern implementiert werden und kann das Separabilitätsproblem in Hilberträumen mit bis zu 1000 Dimensionen behandeln. Unter einer Annahme, welche durch viele numerische Tests bestätigt wurde, liefert dieser Algorithmus im Falle von inseparablen Zuständen immer einen optimalen Zeugenoperator. Im Falle von separablen Zuständen liefert der Algorithmus die explizite Zerlegung des entsprechenden Dichteoperators als konvexe Summe über reine Produktzustände, was per Definition ein Beweis für die Separabilität ist. Unter Ausnutzung der geometrischen Darstellung können wir außerdem zeigen, dass beide Kriterien operational sind. Das heißt, sie können als eine Summe über Erwartungswerte von lokalen hermitischen Operatoren geschrieben werden, welche in Experimenten beobachtbar sind. Im letzten Teil der vorliegenden Dissertation zeigen wir, dass die beiden Kriterien, welche zunächst nur in zweiteiligen Quantensystemen gelten, auch auf Quantensysteme mit mehr als zwei Untersystemen erweiterbar sind.

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1 Introduction

> Our mind, by virtue of a certain finite, limited capability, is by no means capable of putting a question to Nature that permits a continuous series of answers. The observations, the individual results of measurements, are the answers of Nature to our discontinuous questioning.
>
> Erwin Schrödinger

As soon as the concept of entanglement was introduced a controversy about its correct interpretation has originated. Today, more than 70 years later, the problem has not been completely resolved. For Albert Einstein entanglement was a *spooky action at a distance* and a proof that quantum theory cannot be considered complete. In the famous paper [1] with Boris Podolski and Nathan Rosen he started the discussion about the nature of entanglement. Erwin Schrödinger, who invented the word entanglement, described a gedanken experiment [2–4] to clarify its meaning and introduced the Schrödinger cat, which can be dead and alive at the same time, to the world of physics. For him entanglement was *the characteristic trait of quantum mechanics* [5]. For yet another founding father of quantum mechanics, namely Niels Bohr, entanglement was the manifestation of the principle of *complementarity* in quantum mechanics [6]. These three ingenious scientists were not able to agree on a common answer to the question – ***What is entanglement?*** – and therefore assigned the task of finding a satisfying answer to the next generation of physicists.

In 1952 David Bohm presented his approach [7, 8] known as the *hidden variable theory* (or local realistic theory, LRT) to resolve the problem of spookiness that Einstein had associated with entanglement and had led him to believe that quantum theory is incomplete. Bohm thought that he could remedy Einstein's paradox by introducing unknown deterministic microscopic parameters. Moreover, he was convinced that his *interpretation leads to precisely the same results for*

all physical processes as does the usual interpretation [7] of quantum mechanics. Hence the question whether entanglement is a real property of nature remained unanswered.

In 1964, it was John Bell who derived [9] an upper limit, known as Bell's inequality, on the strength of correlations for any theory with hidden variables. This inequality can be violated by entangled states that are described within the framework of quantum mechanics. Bell also proposed an experimental setup with maximally entangled states and thereby provided a framework to decide which of the two paradigms is correct: Quantum theory or the theory of hidden variables. Thus for the first time entanglement was not only of purely theoretical interest but also linked to an observation.

However, it took another twenty years before the experimentalists were able to perform a measurement [10] based on Bell's proposition. With the help of these experiments they could prove that quantum mechanics provides the correct description of the processes that occur in nature. In addition for the first time it was possible to give a generally accepted interpretation of entanglement as quantum correlations that violate Bell's inequalities and are stronger than correlations allowed by theories of hidden variables. For a period of nearly twenty years it was believed that this interpretation is universal and that the violation of Bell's inequalities provides a necessary and sufficient criterion for the detection of entanglement in a quantum system.

In the early nineties however examples of entangled states were found [11–13] which do not violate Bell's inequalities and hence the next round of discussion about the interpretation of entanglement was started which today is still as fascinating as it was twenty years ago. This discussion inspired a tremendous theoretical [14–17] and technological [18–23] progress over the last few decades and yielded a much deeper understanding of quantum mechanics [24–26] than its pioneers Einstein, Schrödinger and Bohr had ever imagined. We are now able to coherently prepare, manipulate, and measure individual quantum systems, as well as create entangled quantum systems [27–29] in a controlled way. In addition parallel to these developments, entanglement has begun to be recognized as a novel resource that may be used to perform tasks that are either impossible or very inefficient at the classical level. For example, quantum cryptography [30–33], quantum teleportation [34–37] and quantum computation [38–40]

are direct applications of this novel resource. These applications stimulated the development of modern quantum information science [41]. Thousands of publications have been written on the subject of entanglement and it's applications. For example the Cornell based preprint server yields the error message *Warning: search aborted at 1000 due to number of matches. Please use more restricted search criteria* if one uses the word *entanglement* as the search parameter. Despite the fact that the spectrum of answers is incredibly large the question – ***What is entanglement?*** – has still not been completely answered. One of the most important reasons for this, is the fact that we still don't have an applicable criterion to decide whether a quantum system is entangled or not. The aim of the present thesis is to provide such a criterion.

2 Short overview

> Quantum theory provides us with a striking illustration of the fact that we can fully understand a connection though we can only speak of it in images and parables.
>
> Werner Heisenberg

In the present chapter we first introduce the definitions and notation which we will use in the following parts of this thesis. Then we give a short overview about existing inseparability criteria and discuss their properties. Finally, we define the central problem of this work.

2.1 Definitions and notation

In the following we consider two quantum systems which are labeled A and B. They will also be given names of persons: Alice and Bob. Each system has a finite Hilbert space $\mathcal{H}_A$ and $\mathcal{H}_B$ respectively which are arranged such that

$$N_A \equiv \dim \mathcal{H}_A \leq N_B \equiv \dim \mathcal{H}_B. \tag{2.1}$$

The entire Hilbert space can thus be written as the direct product

$$\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B, \quad N \equiv \dim \mathcal{H} = N_A N_B. \tag{2.2}$$

We respectively use normal letters to denote pure quantum states in the local systems

$$|a\rangle \in \mathcal{H}_A \quad \text{and} \quad |b\rangle \in \mathcal{H}_B \tag{2.3}$$

and capital letters to represent quantum states of the entire Hilbert space

$$|\Psi\rangle \in \mathcal{H}. \tag{2.4}$$

In general we assume that the state vectors $|\psi\rangle$ are normalized

$$\langle\psi|\psi\rangle = 1 \tag{2.5}$$

and we will explicitly mention all exceptions to this rule. The orthonormal bases of the Hilbert spaces

$$\{|n\rangle \in \mathcal{H}_A,\, n = 1 \ldots N_A\}, \tag{2.6}$$

$$\{|n\rangle \in \mathcal{H}_B,\, n = 1 \ldots N_B\} \tag{2.7}$$

and

$$\{|\Psi_n\rangle \in \mathcal{H},\, n = 1 \ldots N\} \tag{2.8}$$

are arbitrary but fixed and all basis changes will be noted explicitly. Due to the fact that the entire Hilbert space $\mathcal{H}$ is composed of two Hilbert spaces its basis can be chosen to be

$$\{|n\rangle \otimes |m\rangle \equiv |nm\rangle \in \mathcal{H},\ n = 1 \ldots N_A,\, m = 1 \ldots N_B\} \tag{2.9}$$

where the tensor product sign $\otimes$ is omitted in all subsequent equations. Thus any pure state $|\Psi\rangle \in \mathcal{H}$ can be written as

$$|\Psi\rangle = \sum_{n=1}^{N_A} \sum_{m=1}^{N_B} \Psi_{nm} |nm\rangle \tag{2.10}$$

with the complex coefficients

$$\Psi_{nm} = \langle nm|\Psi\rangle. \tag{2.11}$$

We use the hat symbol, for example $\hat{O}$, to denote operators which act on the Hilbert space. In order to describe mixed quantum states we introduce the density operator $\hat{\rho}$ which is Hermitian, non-negative and normalized. Such a density operator can be spectrally decomposed as

$$\hat{\rho} = \sum_{n=1}^{N} \rho_n |\Psi_n\rangle\langle\Psi_n| \tag{2.12}$$

where $|\Psi_n\rangle$ denotes an eigenvector with the non-negative eigenvalue ρ_n. Further-

more the normalization condition requires that

$$\mathrm{Tr}\{\hat{\rho}\} \equiv \sum_{n=1}^{N} \rho_n = 1 \tag{2.13}$$

where $\mathrm{Tr}\{\cdot\}$ denotes the trace over the entire Hilbert space.

In the case of two composed quantum systems we distinguish between two classes of quantum states, the class of separable (or not entangled) states and the class of inseparable (or entangled) states. A quantum state is separable [42] if and only if its corresponding density operator $\hat{\rho}_{sep}$ can be written as a convex sum

$$\hat{\rho}_{sep} \equiv \sum_{n=1}^{\infty} p_n |a_n b_n\rangle\langle a_n b_n| \tag{2.14}$$

where $|a_n\rangle \in \mathcal{H}_A$ and $|b_n\rangle \in \mathcal{H}_B$ are arbitrary but normalized and $p_n \geq 0$. Conversely, $\hat{\rho}_{ent}$ is inseparable if it cannot be written in this form. Physically, a state described by a separable density operator can always be prepared locally by Alice producing $|a_n\rangle$ with probability p_n and Bob correspondingly producing $|b_n\rangle$ with the same probability. Hence, entangled states are those states that cannot be created by means of local operations.

Thus the natural and fundamental question arises whether it is possible to distinguish between entangled and separable states or more precisely, if one can find a criterion to determine whether a given density operator $\hat{\rho}$ is separable or not. This highly nontrivial question is also known as the problem of separability [42] and has not been solved in a satisfactory manner yet. However, for special cases, partial solutions to this problem exist and in the following section we will present some of them.

2.2 Inseparability criteria

The purpose of this section is to briefly catalog some important concepts commonly used for the characterization of entanglement. It is impossible to give a complete overview about all existing inseparability criteria and therefore we focus our attention only on the criteria which are used in the following parts of this work.

2.2.1 Entanglement of pure states

For a given pure state $|\Psi\rangle$ of a bipartite quantum system living on a Hilbert space $\mathcal{H}$, a suitable entanglement measure $E(|\Psi\rangle)$ exists and can be quantified by the von Neumann entropy of the reduced density matrix $\hat{\rho}_A = \mathrm{Tr}_B\{|\Psi\rangle\langle\Psi|\}$

$$E(|\Psi\rangle) \equiv -\mathrm{Tr}\{\hat{\rho}_A \ln \hat{\rho}_A\} \tag{2.15}$$

where $\mathrm{Tr}_B\{\cdot\}$ denotes the trace over the subsystem B. If we take into account that every pure state $|\Psi\rangle$ has a Schmidt decomposition, as shown in appendix A.4.1, i.e. that in appropriately chosen orthonormal bases $\{|a_k\rangle \in \mathcal{H}_A\}$ and $\{|b_k\rangle \in \mathcal{H}_B\}$ it can be represented as

$$|\Psi\rangle = \sum_{k=1}^{K} s_k |a_k b_k\rangle \tag{2.16}$$

where $s_k \leq 1$ denote positive and uniquely determined Schmidt factors, we can give an equivalent definition of the entanglement measure

$$E(|\Psi\rangle) = -\mathrm{Tr}\{\hat{\rho}_A \ln \hat{\rho}_A\} = -\mathrm{Tr}\{\hat{\rho}_B \ln \hat{\rho}_B\} = -\sum_n s_n^2 \ln s_n^2. \tag{2.17}$$

We see that $E(|\Psi\rangle)$ is always non-negative and in particular we observe that $E(|\Psi\rangle)$ vanishes only if one of the Schmidt factors is equal to one and all others vanish. Thus only a product state is a separable pure state, which is equivalent to the definition of separability given by Eq. (2.14). We also observe that $E(|\Psi\rangle)$ is maximal if all Schmidt factors of the state $|\Psi\rangle$ are equally distributed and the upper bound of the sum corresponds to the minimum $N_A = \min\{N_A, N_B\}$ of the dimensionality of the Hilbert spaces $\mathcal{H}_A$ and $\mathcal{H}_B$. In the following we will call

$$|\Psi_{\max}\rangle = \frac{1}{\sqrt{N_A}} \sum_{k=1}^{N_A} |a_k b_k\rangle \tag{2.18}$$

the maximally entangled state.

Hence, in the case of pure quantum states the von Neumann entropy yields a *necessary* and *sufficient* inseparability criterion. In the case of mixed states however, the question whether a given state $\hat{\rho}$ is entangled or not, is in general very hard to answer. In the next subsections we give a short overview of the existing inseparability criteria for mixed quantum states.

2.2.2 Bell inequalities

In his famous work [9] Bell showed that quantum correlations between spatially separated physical systems can be stronger than correlations allowed by the so-called local realistic theories (LRT) which are also known as the hidden variable theories. Bell presented inequalities which are violated by certain entangled states so that quantum mechanics cannot be regarded as a LRT. The original Bell inequality, which is based on the perfect anti-correlations of the singlet state

$$|\Psi\rangle = \frac{1}{\sqrt{2}}\left(|01\rangle - |10\rangle\right), \tag{2.19}$$

was later extended by Clauser, Horne, Shimony, and Holt (CHSH) [43] to a more general inequality for two observers, where each of them has the choice of two measurement settings with two outcomes. In the following we use the CHSH formulation.

In a local theory measurement outcomes cannot depend on the choice of the measurement of another space like separated observer, while in a realistic theory the results of any measurement are predetermined, regardless of whether the measurement is carried out or not. Thus, if we consider an experiment which determines the correlations in a given system by the sum

$$C = |\langle A_1 B_1\rangle + \langle A_2 B_1\rangle + \langle A_1 B_2\rangle - \langle A_2 B_2\rangle| \tag{2.20}$$

where $\langle A_i B_j\rangle$ denotes the expectation value of two dichotomic observables[1], then in the case of a LRT the correlation function is bounded by two

$$C_{LRT} \leq 2, \tag{2.21}$$

as shown in [43]. This is valid for any choice of the dichotomic observables $\{A_i\}$ and $\{B_j\}$. The inequality above is called the Bell-CHSH inequality.

For a quantum mechanical description we have to replace the observables A_i and B_j by Hermitian operators $\hat{A}_i$ and $\hat{B}_j$ with eigenvalues $+1$ and -1. Furthermore, the state of the system is described by a density operator $\hat{\rho}$. The corresponding

[1] Dichotomic observables describe an experimental apparatus which has two outcomes labeled $+1$ and -1.

correlation function is then given by

$$C_{QM} = \left| \left\langle \hat{A}_1 \otimes \hat{B}_1 \right\rangle_{\hat{\rho}} + \left\langle \hat{A}_1 \otimes \hat{B}_2 \right\rangle_{\hat{\rho}} + \left\langle \hat{A}_2 \otimes \hat{B}_1 \right\rangle_{\hat{\rho}} - \left\langle \hat{A}_2 \otimes \hat{B}_2 \right\rangle_{\hat{\rho}} \right| \tag{2.22}$$

with the expectation values

$$\left\langle \hat{A}_i \otimes \hat{B}_j \right\rangle_{\hat{\rho}} = \mathrm{Tr}\left\{ \hat{A}_i \otimes \hat{B}_j \hat{\rho} \right\}.$$

As shown in [44, 45] the upper bound of this correlation function is $2\sqrt{2}$, i.e.

$$C_{QM} \leq 2\sqrt{2}, \tag{2.23}$$

and it can only be reached by a maximally entangled state, Eq. (2.18). Moreover, it is shown that in the case of separable density operators the Bell-CHSH inequalities cannot be violated, that is, only entangled states have correlations which are stronger than the correlations allowed by classical mechanics. By using these results we are able to formulate the following inseparability criterion:

> A density operator $\hat{\rho}$ is entangled if there exist two dichotomic Hermitian operators $\hat{A}_1$ and $\hat{A}_2$ which act on Hilbert space $\mathcal{H}_A$ and two dichotomic Hermitian operators $\hat{B}_1$ and $\hat{B}_2$ which act on $\mathcal{H}_B$ such that the correlation function, Eq. (2.22), exceeds two.

However, there exist non separable states which do not violate the Bell-CHSH inequalities, as shown in [11]. Hence, this is only a sufficient inseparability criterion. The big advantage of Bell-CHSH inequalities lies in the fact that the expectation values of the dichotomic Hermitian operators and therefore the correlation function C_{QM} can be observed in an experiment. Such experiments have been performed in 1981 [10] to prove Bell's theorem.

2.2.3 Peres-Horodecki criterion

The Peres-Horodecki criterion is based on the partial transpose operation which is defined as follows. Let

$$\hat{\rho} = \sum_{n,m=1}^{N_A} \sum_{p,q=1}^{N_B} \rho_{nm}^{pq} |n\rangle\langle m| \otimes |p\rangle\langle q| \tag{2.24}$$

be the decomposition of a density operator in arbitrary bases $\{|n\rangle \in \mathcal{H}_A\}$ and $\{|n\rangle \in \mathcal{H}_B\}$ of Alice and Bob. The partial transpose with respect to Alice is then given by

$$\hat{\rho}^{\mathrm{PTA}} \equiv \sum_{n,m=1}^{N_A} \sum_{p,q=1}^{N_B} \rho_{nm}^{pq} |m\rangle\langle n| \otimes |p\rangle\langle q|. \tag{2.25}$$

The Peres-Horodecki criterion claims that a given density operator $\hat{\rho}$ is inseparable if its partial transpose $\hat{\rho}^{\mathrm{PTA}}$ is not a valid density operator. That is, one of the eigenvalues of $\hat{\rho}^{\mathrm{PTA}}$ is negative. Furthermore, for low dimensional quantum systems with

$$N_A = \dim \mathcal{H}_A = 2 \quad \text{and} \quad N_B = \dim \mathcal{H}_B = 2, 3 \tag{2.26}$$

or simply 2×2 and 2×3 systems this criterion is *necessary* and *sufficient*. This means that $\hat{\rho}$ is separable *if and only if* $\hat{\rho}^{\mathrm{PTA}}$ is a non-negative operator. The proofs for these statements can be found in [12, 13, 46]. However, for larger systems there are states for which the Peres-Horodecki criterion fails and hence is only a sufficient criterion. The big advantage of the Peres-Horodecki criterion lies in the fact, that it is easy to check. One only has to calculate eigenvalues of a matrix. However, unlike the Bell inequalities the partial transposition is a physically strange operation. Transposition can be understood as time inversion, so partial transposition means that e.g. Alice inverses time while Bob does not. As a consequence, it is impossible to perform an experiment which is equivalent to the Peres-Horodecki criterion.

2.2.4 Witness operators

A very general approach to analyze the entanglement of a given density operator is based on the so-called entanglement witnesses which are designed directly for distinguishing between separable and entangled states [42]. A Hermitian operator $\hat{W}$ is called an entanglement witness if it has a positive expectation value with

respect to *all* separable states

$$\mathrm{Tr}\left\{\hat{\rho}_{sep}\hat{W}\right\} \geq 0, \tag{2.27}$$

while there exists at least one state $\hat{\rho}$ such that

$$\mathrm{Tr}\left\{\hat{W}\hat{\rho}\right\} < 0. \tag{2.28}$$

The negative expectation value is hence a signature of entanglement. The importance of entanglement witnesses stems from the fact that a given density operator is separable if and only if there exists a witness operator that detects it [42]. This statement is equivalent to a *necessary* and *sufficient* inseparability criterion in a Hilbert space with arbitrary many dimensions. Thus, if one was able to construct all possible entanglement witnesses one would have solved the problem of separability. Unfortunately it is not known how to construct entanglement witnesses for a given inseparable state in a deterministic way. Therefore the inseparability criterion based on the witness operators is of minor importance for practical purposes. It turns out, as shown in [47], that the Bell-CHSH inequalities and the Peres-Horodecki criterion can be regarded as witness operators and hence, in the case of 2×2 and 2×3 quantum systems it is possible to construct an optimal witness operator. Moreover, due to fact that witness operators are Hermitian they provide a useful tool for the experimental detection of entanglement [48].

2.3 Outlook

With the help of the definitions in section 2.1 we are now in the position to formulate the central problem treated in the present work, which is the problem of separability [42]:

> Find an applicable criterion to determine whether a given density operator $\hat{\rho}$ is separable or not.

To solve this problem we use, in chapter 3, the geometrical representation of Hermitian operators in the Hilbert-Schmidt vector space to map the problem of separability to a problem in convex geometry [49]. By using this representation we

derive certain inequalities, the violation of which is a signature of entanglement in a quantum state in complete analogy to Bell's argument. We also show how witness operators can be recovered from our formalism. In order to solve the problem of separability we proceed in two steps: In chapter 4 we first derive a sufficient inseparability criterion based on the singular value decomposition, which in analogy to the Peres-Horodecki criterion is easy to check, because no complicated optimization problems have to be solved. This criterion can prove the entanglement of states for which the Peres-Horodecki criterion fails and thus by combining both criteria we can significantly enlarge the class of inseparable states that can be detected. In the second step, in chapter 5, we derive an optimization problem the positive solution of which is a *necessary and sufficient* signature of entanglement. We show that this optimization problem can be solved by using the methods of operations research and we develop an algorithm which accomplishes this task. The latter can be implemented on modern computers and be efficiently solved for Hilbert spaces with up to 1000 dimensions. Under a certain assumption, which is confirmed by the numerical tests, the algorithm presented in section 5.5 always converges in contrast to existing approaches in the case of entangled density operators to an optimal witness operator. Moreover, as an additional result we obtain the coefficients of convex decomposition in the case of separable density operators. To the best of our knowledge, this is the first algorithm able to efficiently treat the separability problem in a deterministic way. In section 3.3 we prove that both criteria are operational. This means that analogous to the Bell inequalities our criteria can be rewritten as a sum over expectation values of local Hermitian operators which can be observed in an experiment. Furthermore, we show in chapter 6 how our results can be extended from bipartite quantum systems to multipartite systems with only slight modifications. In chapter 7 we conclude by summarizing our results and providing an outlook.

3 Geometrical interpretation of entanglement

> Imagination is more important than knowledge.
> The knowledge is limited, whereas imagination embraces the entire world, stimulating progress, giving birth to evolution.
>
> Albert Einstein

So far we have introduced various criteria for entanglement and discussed their properties. In the present chapter we will represent the density operators in the Hilbert-Schmidt vector space of Hermitian operators. This geometrical representation enables us to find new inseparability criteria, which analogous to Bell's argument detect entanglement in a given density operator by violating certain inequalities. Furthermore, it turns out that our formalism can be mapped onto the formalism of witness operators and we will see that the physical property – *entanglement* – can be detected in an experiment. Our starting point is a proof that only pure separable states have to be taken into account for the construction of entanglement criteria.

3.1 Starting point

Entanglement is a physical property of a quantum system and therefore should be measurable in an experiment. But what kind of measurement can detect entanglement? To answer this question we recall that in quantum mechanical experiments the possible measurement outputs are described as expectation values of observables which correspond to Hermitian operators. Let us assume that we perform a measurement of the observable $\hat{O}$ and that the density operator $\hat{\rho}$ characterizes

the state that should be tested for entanglement. Both operators act on the entire Hilbert space. Due to its hermiticity the operator $\hat{O}$ can be written as

$$\hat{O} = \sum_{n=1}^{N} \lambda_n |O_n\rangle\langle O_n| \,, \quad \lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_N \tag{3.1}$$

where $|O_n\rangle$ denotes an eigenvector with the real-valued eigenvalue λ_n. Of course, $\hat{\rho}$ can be decomposed in the same manner

$$\hat{\rho} = \sum_{n=1}^{N} \rho_n |\Psi_n\rangle\langle\Psi_n|, \tag{3.2}$$

but due to its positivity the eigenvalues ρ_n are non-negative. Furthermore, the normalization of the density operator yields

$$\mathrm{Tr}\,\{\hat{\rho}\} = \sum_n \rho_n = 1. \tag{3.3}$$

The measurement output of the experiment can then be calculated as

$$\left\langle \hat{O} \right\rangle = \mathrm{Tr}\left\{\hat{O}\hat{\rho}\right\} = \sum_n \rho_n \langle\Psi_n|\hat{O}|\Psi_n\rangle. \tag{3.4}$$

Using the positivity of the eigenvalues ρ_n and the normalization of $\hat{\rho}$ we obtain the lower bound

$$\sum_{n=1}^{N} \rho_n \langle\Psi_n|\hat{O}|\Psi_n\rangle \geq \min_n \langle\Psi_n|\hat{O}|\Psi_n\rangle \geq \min_{|\Psi\rangle} \langle\Psi|\hat{O}|\Psi\rangle \tag{3.5}$$

and the upper bound

$$\sum_{n=1}^{N} \rho_n \langle\Psi_n|\hat{O}|\Psi_n\rangle \leq \max_n \langle\Psi_n|\hat{O}|\Psi_n\rangle \leq \max_{|\Psi\rangle} \langle\Psi|\hat{O}|\Psi\rangle. \tag{3.6}$$

The maximal expectation value of a Hermitian operator $\hat{O}$ with respect to pure states corresponds to the maximal eigenvalue $\lambda_{\max}$, as shown in appendix A.1, that is

$$\max_{|\Psi\rangle} \langle\Psi|\hat{O}|\Psi\rangle = \lambda_{\max} = \lambda_1. \tag{3.7}$$

Furthermore, the maximum is obtained if we use the eigenstate $|\Psi\rangle = |O_1\rangle$ of $\hat{O}$. This solution is unique only if the largest eigenvalue is not degenerate. In a degenerate case, where for example $\lambda_1 = \lambda_2$, any state of the form

$$|\Psi\rangle = \alpha|O_1\rangle + \beta|O_2\rangle, \quad |\alpha|^2 + |\beta|^2 = 1 \tag{3.8}$$

leads to the maximal value, Eq. (3.7).

In the same manner the lower bound of the expectation value, Eq. (3.4), can be calculated and we arrive at

$$\min_{|\Psi\rangle}\langle\Psi|\hat{O}|\Psi\rangle = \lambda_{\min} = \lambda_N \tag{3.9}$$

with the minimization eigenvector $|\Psi\rangle = |O_N\rangle$. Again, this solution is unique only if the smallest eigenvalue λ_N is not degenerate.

So far we have used arbitrary density operators for the computation of the bounds for the possible experimental outputs and have seen that they are confined by the largest and smallest eigenvalue of the corresponding observable. Now we will analyze whether a separable density operator, Eq. (2.14),

$$\hat{\rho}_{sep} = \sum_{n=1}^{\infty} p_n |a_n b_n\rangle\langle a_n b_n| \tag{3.10}$$

can reach these bounds. The coefficients p_n are no longer the eigenvalues of $\hat{\rho}_{sep}$, but they are still non-negative and normalized. Hence we can apply the same arguments as above and arrive at

$$c_{\max} \equiv \max_{|ab\rangle}\langle ab|\hat{O}|ab\rangle \geq \left\langle \hat{O} \right\rangle_{sep} \geq \min_{|ab\rangle}\langle ab|\hat{O}|ab\rangle \equiv c_{\min} \tag{3.11}$$

with

$$\left\langle \hat{O} \right\rangle_{sep} = \mathrm{Tr}\left\{\hat{O}\hat{\rho}_{sep}\right\} = \sum_n p_n \langle a_n b_n|\hat{O}|a_n b_n\rangle. \tag{3.12}$$

Unless the eigenvectors $|O_1\rangle$ and $|O_N\rangle$ of the observable $\hat{O}$ are product states the bounds $c_{\min}$ and $c_{\max}$ for the separable states cannot reach the extremal values. Excluding this case we can say that the possible experimental outputs for separable

states are confined by the inequalities

$$\lambda_1 > c_{\max} \geq c_{\min} > \lambda_N \tag{3.13}$$

and hence they cover a smaller interval of possible experimental outputs than arbitrary, in particular entangled states. Thus, if the expectation value of $\hat{O}$ with respect to an unknown density operator $\hat{\rho}$ is not located in the interval $[c_{\min}, c_{\max}]$, $\hat{\rho}$ must be entangled.

We are now in the position to answer the question formulated at the beginning of this subsection:

> We can detect entangled states by performing a measurement of an observable $\hat{O}$ with inseparable eigenstate $|O_1\rangle$ or $|O_N\rangle$ corresponding to the non-degenerate largest eigenvalue λ_1 or smallest eigenvalue λ_N.
>
> This statement leads to an even stronger result: All measurements which correspond to this kind of observables can detect at least one inseparable quantum state. In particular this state can be chosen to be either $|O_1\rangle$ or $|O_N\rangle$.

The following example will clarify this statement.

3.1.1 Maximally entangled states

Let us assume an experimental setup which describes a measurement of the observable[1]

$$\hat{O}_{MES} = |\Psi_{\max}\rangle\langle\Psi_{\max}| \tag{3.14}$$

where $|\Psi_{\max}\rangle$ denotes a maximally entangled state, Eq. (2.18),

$$|\Psi_{\max}\rangle \equiv \frac{1}{\sqrt{N_A}} \sum_{n=1}^{N_A} |a_n b_n\rangle. \tag{3.15}$$

Here $\{|a_n\rangle \in \mathcal{H}_A\}$ and $\{|b_n\rangle \in \mathcal{H}_B\}$ are arbitrary sets of orthonormal vectors. Due to the simple form of $\hat{O}_{MES}$ we can easily calculate the bounds of the possible

[1] This kind of measurement has been performed in the teleportation experiments presented in [35, 50] with $\dim \mathcal{H}_A = \dim \mathcal{H}_B = 2$.

experimental outputs. They are given by the largest eigenvalue $\lambda_{\max} = 1$ and the smallest eigenvalue $\lambda_{\min} = 0$ of the observable. The eigenvalue $\lambda_{\max}$ is not degenerate, therefore the maximal expectation value of $\hat{O}_{MES}$ can only be reached for the pure entangled state $|\Psi_{\max}\rangle$. However, for the degenerate eigenvalue $\lambda_{\min}$ we can find separable eigenstates

$$|\Psi\rangle = |a_n b_m\rangle\,, \quad n = 1 \ldots N_A,\, m = 1 \ldots N_B, n \neq m. \tag{3.16}$$

As a result, the lower bound $c_{\min}$ of the expectation value of the observable $\hat{O}_{MES}$ with respect to separable states, Eq. (3.13), is equal to the global bound $\lambda_{\min}$, that is

$$c_{\min} = \min_{|ab\rangle} \langle ab|\hat{O}_{MES}|ab\rangle = \lambda_{\min} = 0. \tag{3.17}$$

Hence, this bound cannot be used for entanglement detection.

Due to the non-negativity of the observable $\hat{O}_{MES}$ we can estimate $c_{\max}$, Eq. (3.11), as

$$\begin{aligned} c_{\max} &= \max_{|ab\rangle} \langle ab|\hat{O}_{MES}|ab\rangle \\ &\leq \max_{|ab\rangle} \left(\langle ab|\hat{O}_{MES}|ab\rangle + \sum_{n=2}^{N_B} \langle a\varphi_n|\hat{O}_{MES}|a\varphi_n\rangle \right) \\ &= \max_{|a\rangle} \langle a|\mathrm{Tr}_B \left\{ \hat{O}_{MES} \right\} |a\rangle \end{aligned} \tag{3.18}$$

where the orthonormal state vectors $|\varphi_n\rangle$ are orthogonal to $|b\rangle$. The partial trace over the observable $\hat{O}_{MES}$ results in the scaled identity operator $\hat{\mathbb{1}}/N_A$ and hence the upper bound for $c_{\max}$ is given by

$$c_{\max} \leq \frac{1}{N_A} \max_{|a\rangle} \langle a|\hat{\mathbb{1}}|a\rangle = \frac{1}{N_A}. \tag{3.19}$$

This inequality can be replaced by the equality

$$c_{\max} = \frac{1}{N_A} \tag{3.20}$$

because the product states

$$|ab\rangle = |a_n b_n\rangle, \;\; n \in 1 \ldots N_A \tag{3.21}$$

lead to this maximal value. Thus, if the expectation value of $\hat{O}_{MES}$ with respect to an unknown density operator $\hat{\rho}$ exceeds $1/N_A$, $\hat{\rho}$ must be entangled. In other words all quantum states which violate the inequality

$$\mathrm{Tr}\left\{\hat{O}_{MES}\hat{\rho}\right\} \leq \frac{1}{N_A} \tag{3.22}$$

are entangled. This inequality can be interpreted as a criterion for entanglement which we call the MES-criterion[2]. We emphasize that unlike the constant global bound $\lambda_{\max} = 1$ the bound for possible experimental outputs for separable states, Eq. (3.20), depends strongly on the number of dimensions of the smaller Hilbert space. Therefore this criterion becomes more sensitive for Hilbert spaces with higher dimensionality.

3.1.2 Witness operators

We have already seen that it is possible to find observables, e.g. $\hat{O}_{MES}$, which can detect entanglement by violating inequalities (3.22). In subsection 2.2.4 we have presented a separability criterion based on witness operators $\hat{W}$ which verifies entanglement by violation of certain inequalities as well. This leads to the interesting question, whether there is a connection between the observables $\hat{O}$ with inseparable eigenstate $|O_1\rangle$ or $|O_N\rangle$ corresponding to the non-degenerate largest eigenvalue λ_1 or smallest eigenvalue λ_N and the witness operators $\hat{W}$?

In order to answer this question we consider an operator $\hat{O}$ with $\lambda_{\max} > c_{\max} \geq c_{\min} > \lambda_{\min}$. In this case we can define two operators

$$\hat{W}_1 \equiv \hat{O} - c_{\min}\hat{\mathbb{1}} \tag{3.23}$$

and

$$\hat{W}_2 \equiv c_{\max}\hat{\mathbb{1}} - \hat{O} \tag{3.24}$$

which by construction fulfill condition (2.27)

$$\mathrm{Tr}\left\{\hat{W}_q\hat{\rho}_{sep}\right\} \geq 0, \quad q = 1, 2 \tag{3.25}$$

of the witness operators. Thus, the operator $\hat{O}$ and the witness operators $\hat{W}_{1,2}$ are

[2]MES denotes maximally entangled states.

connected by the simple transformations above. In other words all results which can be obtained for the witness operators can easily be transformed into the results for the operators $\hat{O}$ and vice versa. The witness operators form a subset of the $\hat{O}$ operators which have to fulfill an extra condition with

$$c_{\min} = \min_{|ab\rangle \in \mathcal{H}} \langle ab|\hat{W}|ab\rangle = 0. \tag{3.26}$$

Therefore, in the following we will use the $\hat{O}$ operators notation in order to avoid this condition, which is not necessary for our purpose.

3.2 Geometrical interpretation

In the previous section we have demonstrated that all Hermitian operators $\hat{O}$ with inseparable eigenstates corresponding to the non-degenerate largest and smallest eigenvalue can detect at least one inseparable quantum state. In this section we want to examine the question whether such an operator exists for all inseparable states $\hat{\rho}$.

It is shown in [42] that for all non-separable states at least one witness operator exists which can detect their entanglement. Since the $\hat{O}$-operators and the witness operators are connected by a simple transformation, see subsection 3.1.2, this proof answers the question of the present section positively. However, in our approach we will present an alternative proof and introduce a notation that will be useful in subsequent sections.

3.2.1 Hilbert-Schmidt vector space

As shown in appendix A.2 all Hermitian operators acting on a N dimensional complex Hilbert space $\mathcal{H}$ can be represented by a real valued Euclidian N^2-dimensional vector space $V_{HS} = \mathbb{R}^{N^2}$, which is called Hilbert-Schmidt space [51–53]. Thus a Hermitian operator $\hat{A}$ can be associated with a vector $\vec{A} \in \mathbb{R}^{N^2}$. Moreover, the trace operation over the product of two Hermitian operators defines a scalar product

$$\vec{A}_1 \cdot \vec{A}_2 \equiv \mathrm{Tr}\left\{\hat{A}_1 \hat{A}_2\right\} \tag{3.27}$$

where $\vec{A}_{\{1,2\}}$ are the associated vectors in the Hilbert-Schmidt space of the operators $\hat{A}_{\{1,2\}}$. Let us assume that the set of N quantum states $\{|\Psi_n\rangle\}$ builds an orthonormal basis of the Hilbert space $\mathcal{H}$, then the set of Hermitian operators

$$\Omega \equiv \left\{\hat{\sigma}_n,\, n = 1 \ldots N^2\right\} \equiv \left\{|\Psi_n\rangle\langle\Psi_n|, \frac{|\Psi_k\rangle\langle\Psi_m| + |\Psi_m\rangle\langle\Psi_k|}{\sqrt{2}}, i\frac{|\Psi_k\rangle\langle\Psi_m| - |\Psi_m\rangle\langle\Psi_k|}{\sqrt{2}};\, n, m \neq k \in [1, N]\right\} \tag{3.28}$$

is a possible set of basis vectors in the Hilbert-Schmidt vector space. It is easy to show that the operators $\hat{\sigma}_n$ are complete

$$\dim \Omega = \dim V_{HS} = N^2 \tag{3.29}$$

and orthonormal

$$\mathrm{Tr}\left\{\hat{\sigma}_n \hat{\sigma}_m\right\} = \delta_{nm} \tag{3.30}$$

with respect to the scalar product, Eq. (3.27). Therefore, any Hermitian operator $\hat{A} \in \mathcal{H}$ can be decomposed in a linear combination of $\hat{\sigma}_n$

$$\hat{A} = \sum_{n=1}^{N^2} a_n \hat{\sigma}_n \tag{3.31}$$

where the real coefficients a_n are determined by the relation

$$a_n \equiv \mathrm{Tr}\left\{\hat{A}\hat{\sigma}_n\right\}. \tag{3.32}$$

The associated vector $\vec{A}$ of the operator $\hat{A}$ can then be written as

$$\vec{A} = (a_1, a_2, \ldots, a_{N^2}). \tag{3.33}$$

So far we have demonstrated that an arbitrary Hermitian operator can be associated with an N^2-dimensional Hilbert-Schmidt vector. In the following we particularly want to look at the properties of the density operators, which means $\hat{A} = \hat{\rho}$.

All density operators satisfy the normalization condition

$$\mathrm{Tr}\left\{\hat{\rho}\right\} = 1. \tag{3.34}$$

By choosing an alternative basis $\tilde{\Omega} \equiv \left\{\hat{\tilde{\sigma}}_n,\, n \in 1 \ldots N^2\right\}$ of the Hilbert-Schmidt space, which contains a weighted identity operator as the first element

$$\hat{\tilde{\sigma}}_1 \equiv \frac{1}{\sqrt{N}}\hat{\mathbb{1}} \tag{3.35}$$

we obtain that due to the normalization condition, Eq. (3.34), the first coefficient r_1 of the associated vector $\vec{R}$ is constant

$$r_1 = \mathrm{Tr}\left\{\hat{\rho}\hat{\tilde{\sigma}}_1\right\} = \frac{1}{\sqrt{N}}. \tag{3.36}$$

As a result, the linear decomposition of $\hat{\rho}$ is given by

$$\hat{\rho} = \frac{1}{N}\hat{\mathbb{1}} + \sum_{n=2}^{N^2} r_n \hat{\tilde{\sigma}}_n \tag{3.37}$$

where the coefficients $r_n = \mathrm{Tr}\left\{\hat{\tilde{\sigma}}_n\hat{\rho}\right\}$ are the remaining components of $\vec{R}$. These coefficients contain the complete information about the quantum state $\hat{\rho}$ and hence, it is sufficient to represent the density operators by a vector

$$\vec{r} \equiv (r_2, r_3, \ldots, r_{N^2}) \tag{3.38}$$

in a sub vector space $V^{\perp}$ of V_{HS}, which is perpendicular to the associated Hilbert-Schmidt vector of the identity operator. The dimensionality of this vector space is

$$\dim V^{\perp} = N^2 - 1. \tag{3.39}$$

The density operators are not only normalized but also positive. Due to this positivity constraint they obey the inequality

$$\mathrm{Tr}\left\{\hat{\rho}^2\right\} \leq 1 \tag{3.40}$$

where the equality only holds for pure states. With the help of Eqs. (3.37) and (3.38) we can transfer this inequality to the Hilbert-Schmidt vector space and arrive at

$$|\vec{r}|^2 \leq \frac{N-1}{N}. \tag{3.41}$$

In other words the associated vectors of density operators are confined in a sphere

with radius $|\vec{r}| = \sqrt{1-1/N}$ in $V^{\perp}$ and only the vectors corresponding to pure states touch the surface of the sphere. However, in general not all vectors which touch the surface of this sphere correspond to a valid quantum state. This can be seen as follows: Let the set $\{|\Psi_n\rangle,\, n = 1 \ldots N\}$ be an orthonormal basis of the Hilbert space. Then all pure states can be written as a linear combination of these basis vectors

$$|\Psi\rangle = \sum_{n=1}^{N} \left(\psi_n^r + i\psi_n^i\right) |\Psi_n\rangle \tag{3.42}$$

with $2N$ real parameters $\{\psi_n^r\}$ and $\{\psi_n^i\}$. Due to the normalization condition $\langle\Psi|\Psi\rangle = 1$ and due to the invariance of the quantum states with respect to a global phase the number of needed parameters is reduced by two. Thus, all pure quantum states can be parameterized with the help of

$$2\,\dim\mathcal{H} - 2 = 2N - 2 \tag{3.43}$$

real numbers. By contrast, the surface of a sphere in $V^{\perp}$ is parameterized by

$$\dim V^{\perp} - 1 = N^2 - 2 \tag{3.44}$$

real numbers. Hence, the associated Hilbert-Schmidt vectors $\vec{P}$ of the pure quantum states $|\Psi\rangle$ only form a subset of the surface of a sphere in $V^{\perp}$ with one exception. Namely, in the case of a two dimensional Hilbert space the vectors $\vec{P}$ lie dense on the surface [54], i.e. all points of the surface of a sphere in $V^{\perp}$ with radius $|\vec{r}| = \frac{1}{\sqrt{2}}$ correspond to a valid pure quantum state $|\Psi\rangle \in \mathcal{H}$.

The following example will clarify the properties of the Hilbert-Schmidt representation of Hermitian operators.

Example

The simplest example is a two dimensional Hilbert space. Let the vectors $|0\rangle$ and $|1\rangle$ be the basis vectors of this space and let

$$\hat{A} = \sum_{m,n=0}^{1} A_{nm} |n\rangle\langle m| \tag{3.45}$$

be a Hermitian operator, for which we want to find the associated Hilbert-Schmidt vector. First of all, we define the basis of the associated Hilbert-Schmidt vector space V_{HS} as

$$\hat{\sigma}_1 = \frac{1}{\sqrt{2}}\left(|0\rangle\langle 0| + |1\rangle\langle 1|\right) = \frac{1}{\sqrt{2}}\hat{\mathbb{1}} \tag{3.46}$$

$$\hat{\sigma}_2 = \frac{1}{\sqrt{2}}\left(|0\rangle\langle 0| - |1\rangle\langle 1|\right) \tag{3.47}$$

$$\hat{\sigma}_3 = \frac{1}{\sqrt{2}}\left(|0\rangle\langle 1| + |1\rangle\langle 0|\right) \tag{3.48}$$

$$\hat{\sigma}_4 = \frac{i}{\sqrt{2}}\left(|0\rangle\langle 1| - |1\rangle\langle 0|\right) \tag{3.49}$$

where the $\hat{\sigma}$-operators fulfill the orthogonality relation, Eq. (3.30). By definition the associated Hilbert-Schmidt vector of $\hat{A}$ is given by

$$\begin{aligned}\vec{A} &= \left(\mathrm{Tr}\left\{\hat{\sigma}_1\hat{A}\right\}, \mathrm{Tr}\left\{\hat{\sigma}_2\hat{A}\right\}, \mathrm{Tr}\left\{\hat{\sigma}_3\hat{A}\right\}, \mathrm{Tr}\left\{\hat{\sigma}_4\hat{A}\right\}\right) \\ &= \frac{1}{\sqrt{2}}\left(A_{00} + A_{11}, A_{00} - A_{11}, 2\,\mathrm{Re}\left\{A_{01}\right\}, 2\,\mathrm{Im}\left\{A_{01}\right\}\right). \end{aligned} \tag{3.50}$$

If $\hat{A}$ is a density operator, i.e. $\hat{A} = \hat{\rho}$, the normalization of density operators leads to a constant first component

$$r_1 = \mathrm{Tr}\left\{\hat{\rho}\hat{\sigma}_1\right\} = \frac{1}{\sqrt{2}}\mathrm{Tr}\left\{\hat{\rho}\hat{\mathbb{1}}\right\} = \frac{1}{\sqrt{2}} \tag{3.51}$$

of the associated Hilbert-Schmidt vector $\vec{R}$. As a consequence, any qubit[3] state $\hat{\rho}$ can be represented by the linear combination

$$\hat{\rho} = \frac{1}{2}\hat{\mathbb{1}} + \sum_{n=2}^{4} r_n\hat{\sigma}_n \tag{3.52}$$

where $r_n = \mathrm{Tr}\left\{\hat{\rho}\hat{\sigma}_n\right\}$ with $n = 2, 3, 4$ are the remaining components of $\vec{R}$. The normalization condition, Eq. (3.51), makes it possible to represent density operators in a sub vector space $V^{\perp}$ of V_{HS} because the 3-dimensional vector $\vec{r} = (r_2, r_3, r_4)$ contains the complete information about the quantum state $\hat{\rho}$. Due to the non-

[3] A quantum state in a two dimensional Hilbert space is called qubit.

negativity of the density operators

$$\mathrm{Tr}\left\{\hat{\rho}^2\right\} \leq 1 \tag{3.53}$$

these associated vectors $\vec{r}$ are confined in a sphere with radius $|\vec{r}| = \frac{1}{\sqrt{2}}$. This sphere is similar to the Bloch sphere [54] except that the Bloch sphere is a unit sphere because the basis operators are defined in an alternative way, where the basis operators are the non-normalized Pauli spin operators [27]. Moreover, it is shown in [54] that every point on the surface of the Bloch sphere corresponds to a valid pure quantum state.

3.2.2 Entanglement in the Hilbert-Schmidt vector space

So far we have seen that the Hermitian operators can be represented as vectors in the Hilbert-Schmidt vector space. Now we would like to find the difference between the separable and entangled states in this representation. Due to the definition, Eq. (2.14),

$$\hat{\rho}_{sep} \equiv \sum_{n=1}^{\infty} p_n |a_n b_n\rangle\langle a_n b_n| \tag{3.54}$$

with

$$\sum_{n=1}^{\infty} p_n = 1, \;\; p_n \geq 0$$

the separable states can be decomposed in a convex sum over pure product states and therefore form a convex set $\mathcal{J}$. In the Hilbert-Schmidt vector space this means

$$\vec{R}_{sep} = \sum_{n=1}^{\infty} p_n \vec{P}_n \tag{3.55}$$

where the vectors $\vec{P}_n$ represent the associated Hilbert-Schmidt vectors of the product states $|a_n b_n\rangle\langle a_n b_n|$. Thus, the associated vectors $\vec{R}_{sep}$ of the separable density operators form a convex set $\mathcal{K}$ in V_{HS}. By definition, an entangled state $\hat{\rho}_{ent}$ cannot be decomposed in such a way and consequently the associated Hilbert-Schmidt vector $\vec{R}_{ent}$ of $\hat{\rho}_{ent}$ cannot be contained in $\mathcal{K}$

$$\vec{R}_{ent} \notin \mathcal{K}. \tag{3.56}$$

Since $\vec{R}_{ent}$ and $\mathcal{K}$ are two disjunct convex sets[4], there exists, see for example [49] *definition 9.1*, a hyperplane $\mathcal{E}$ which divides the vector space V_{HS} in two half spaces so that $\vec{R}_{ent}$ and $\mathcal{K}$ are in different half spaces. We denote this hyperplane by

$$\mathcal{E} = \left\{ \vec{x} : \vec{O}_{\mathcal{E}} \cdot \vec{x} = \vec{O}_{\mathcal{E}} \cdot \vec{x}_0 \right\} \tag{3.57}$$

where $\vec{O}_{\mathcal{E}}$ is the normal vector and $\vec{x}_0$ represents a point on the hyperplane. The two half spaces are thus

$$V_+ \equiv \left\{ \vec{x} : \vec{O}_{\mathcal{E}} \cdot \vec{x} > \vec{O}_{\mathcal{E}} \cdot \vec{x}_0 \right\} \tag{3.58}$$

$$V_- \equiv \left\{ \vec{x} : \vec{O}_{\mathcal{E}} \cdot \vec{x} < \vec{O}_{\mathcal{E}} \cdot \vec{x}_0 \right\}. \tag{3.59}$$

Let the associated vector $\vec{R}_{ent}$ be an element of V_+ and the convex set $\mathcal{K}$ be contained in V_- respectively, then the inequality

$$\vec{O}_{\mathcal{E}} \cdot \vec{R}_{ent} > \vec{O}_{\mathcal{E}} \cdot \vec{R}_{sep} \tag{3.60}$$

is valid for all $\vec{R}_{sep} \in \mathcal{K}$. Figure 3.1 gives a pictorial clarification of this statement in a two dimensional vector space. In the original Hilbert space $\mathcal{H}$ inequality (3.60) translates into the relation

$$\mathrm{Tr}\left\{ \hat{O}_{\mathcal{E}} \hat{\rho}_{ent} \right\} > \mathrm{Tr}\left\{ \hat{O}_{\mathcal{E}} \hat{\rho}_{sep} \right\}, \quad \forall \hat{\rho}_{sep} \in \mathcal{J} \tag{3.61}$$

where $\hat{O}_{\mathcal{E}}$, $\hat{\rho}_{ent}$ and $\hat{\rho}_{sep}$ are the associated Hermitian operators to $\vec{O}_{\mathcal{E}}$, $\vec{R}_{ent}$ and $\vec{R}_{sep}$. With this result we are now in the position to derive a necessary and sufficient inseparability criterion:

> An unknown density operator $\hat{\rho}$ is inseparable if and only if there exists at least one Hermitian operator $\hat{O}_{\mathcal{E}}$ such that the inequality
>
> $$\mathrm{Tr}\left\{ \hat{O}_{\mathcal{E}} \hat{\rho} \right\} > \mathrm{Tr}\left\{ \hat{O}_{\mathcal{E}} \hat{\rho}_{sep} \right\} \tag{3.62}$$
>
> is valid for all separable density operators $\hat{\rho}_{sep} \in \mathcal{J}$.

From a theoretical point of view this criterion is quite powerful. However, it is not useful for constructing operators $\hat{O}_{\mathcal{E}}$ that detect a given inseparable state because

[4] A point forms a convex set with only one element.

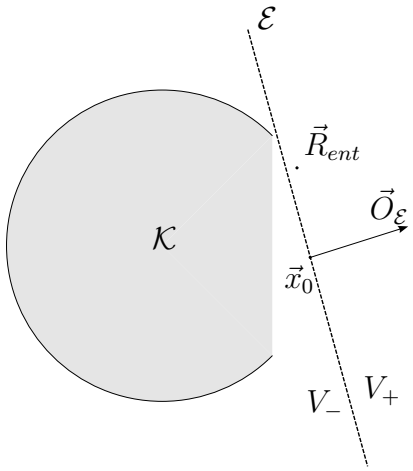


Figure 3.1:
One can always find a line $\mathcal{E}$, which divides the vector space in two half spaces V_- and V_+ such that two disjunct convex sets $\mathcal{K}$ (grey arc) and $\vec{R}_{ent}$ are in different half spaces. Here $\mathcal{K}$ is formed by all possible convex superpositions of vectors $\vec{P}$ (dark border of the arc) and the line $\mathcal{E}$ is determined by the vector $\vec{x}_0 \in \mathcal{E}$ and its normal vector $\vec{O}_{\mathcal{E}}$. The direction of $\vec{O}_{\mathcal{E}}$ is chosen such that $\vec{R}_{ent}$ lies in half space V_+.

the knowledge about the unknown set $\mathcal{J}$ consisting of *all* separable states is needed. However, in subsection 3.1 we have demonstrated that the expectation value of a Hermitian operator $\hat{O}$ with respect to the separable density operators $\hat{\rho}_{sep} \in \mathcal{J}$ is located in the interval $[c_{\min}, c_{\max}]$ where the bounds $c_{\min}$ and $c_{\max}$ are given by pure product states, Eq. (3.11). Hence, we can reduce the set $\mathcal{J}$ over all separable density operators to the set over pure product states and the necessary and sufficient inseparability criterion from above becomes (this has already been proven in a different form for witness operators [42]):

> An unknown density operator $\hat{\rho}$ is inseparable if and only if there exists at least one Hermitian operator $\hat{O}_{\mathcal{E}}$ such that the inequality
>
> $$\mathrm{Tr}\left\{\hat{O}_{\mathcal{E}}\hat{\rho}\right\} > \langle ab|\hat{O}_{\mathcal{E}}|ab\rangle \tag{3.63}$$
>
> is valid for all pure product states with $|a\rangle \in \mathcal{H}_A$ and $|b\rangle \in \mathcal{H}_B$. By using the definition of $c_{\max}$, Eq. (3.11), this inequality becomes
>
> $$\mathrm{Tr}\left\{\hat{O}_{\mathcal{E}}\hat{\rho}\right\} > c_{\max}. \tag{3.64}$$

Since the pure product states can be parameterized, Eq. (3.42), they are in principle known. We will show in chapter 5 that with the help of the inequality above it is possible to find a Hermitian operator $\hat{O}_{\mathcal{E}}$ that detects a given entangled state. We call this Hermitian operator the entanglement indicator.

3.3 Non-locality

In the previous section we have demonstrated that for all entangled states there exists an entanglement indicator $\hat{O}_{\mathcal{E}}$ which can detect its entanglement. Furthermore we have assumed $\hat{O}_{\mathcal{E}}$ to be a global operator which acts on both subsystems of Alice and Bob simultaneously. This contradicts however a very important property of entanglement namely non-locality. Usually entangled states are shared by two spatially separated subsystems. It is in general not possible to measure the expectation value of $\hat{O}_{\mathcal{E}}$ in such a situation. A prominent example which describes spatially separated entangled states is the paradox of A. Einstein, B. Podolsky and N. Rosen presented in [1], where the two subsystems can be arbitrarily far from each other. Therefore the task of the present section is to clarify the question: Is it possible to detect entanglement only by local observations and classical communication? In other words is it possible to find a set of local Hermitian operators which act on $\mathcal{H}_A$ and a set of local Hermitian operators which act on $\mathcal{H}_B$ such that the sum of their expectation values has different bounds for entangled and separable states? An example of this kind of operators are the Bell-CHSH observables, Eq. (2.22).

To answer the question above we use the fact that the Hilbert space $\mathcal{H}$ is a direct product of two Hilbert spaces $\mathcal{H}_A$ and $\mathcal{H}_B$. This property maps to the associated Hilbert-Schmidt vector space. Let the sets

$$\Omega_A = \left\{\hat{\sigma}_n^A,\, n \in 1 \ldots N_A^2\right\} \quad \text{and} \quad \Omega_B = \left\{\hat{\sigma}_m^B,\, m \in 1 \ldots N_B^2\right\} \tag{3.65}$$

be the orthonormal bases of the associated Hilbert-Schmidt vector spaces of Alice and Bob respectively. Then due to their completeness the direct product of Ω_A and Ω_B with

$$\Omega = \Omega_A \otimes \Omega_B = \left\{\hat{\sigma}_n^A \otimes \hat{\sigma}_m^B,\, n \in 1 \ldots N_A^2,\, m \in 1 \ldots N_B^2\right\} \tag{3.66}$$

builds a basis of the entire Hilbert-Schmidt vector space. Therefore all Hermitian

operators $\hat{O}$ which act on $\mathcal{H}$ can be written as

$$\hat{O} = \sum_{n=1}^{N_A^2} \sum_{m=1}^{N_B^2} o_{nm} \hat{\sigma}_n^A \otimes \hat{\sigma}_m^B \tag{3.67}$$

where the real coefficients o_{nm} are given by

$$o_{nm} = \mathrm{Tr}\left\{ \hat{O} \hat{\sigma}_n^A \otimes \hat{\sigma}_m^B \right\}. \tag{3.68}$$

By using this relation we can calculate the expectation value of an arbitrary global Hermitian operator $\hat{O}$ as a sum

$$\left\langle \hat{O} \right\rangle = \sum_{n=1}^{N_A^2} \sum_{m=1}^{N_B^2} o_{nm} \left\langle \hat{\sigma}_n^A \otimes \hat{\sigma}_m^B \right\rangle \tag{3.69}$$

over expectation values of local $\hat{\sigma}$-operators. Hence, it is always possible to determine expectation values of any global Hermitian operator by local observations and classical communication only. Let us assume that the density operator $\hat{\rho}$ is entangled. Then as discussed in subsection 3.2.2 there exists at least one entanglement indicator $\hat{O}_{\mathcal{E}}$ which fulfills the inequality, Eq. (3.64),

$$\mathrm{Tr}\left\{ \hat{O}_{\mathcal{E}} \hat{\rho} \right\} > \max_{|ab\rangle} \langle ab | \hat{O}_{\mathcal{E}} | ab \rangle = c_{\max} \tag{3.70}$$

and therefore detects the entanglement of $\hat{\rho}$. By rewriting $\hat{O}_{\mathcal{E}}$ in the form of Eq. (3.67) this inequality is equivalent to the sum over expectation values of local $\hat{\sigma}$-operators and makes it possible to detect the entanglement of $\hat{\rho}$ by local observations and classical communication only.

In the next step we would like to find a decomposition of an entanglement indicator $\hat{O}_{\mathcal{E}}$ which requires a smaller number of summands. In appendix A.4.2 we show that with the help of the singular value decomposition we can construct bases, Eq. (A.42),

$$\tilde{\Omega}_A = \left\{ \hat{\tilde{\sigma}}_n^A,\, n \in 1 \ldots N_A^2 \right\} \quad \text{and} \quad \tilde{\Omega}_B = \left\{ \hat{\tilde{\sigma}}_m^B,\, m \in 1 \ldots N_B^2 \right\} \tag{3.71}$$

such that the operator $\hat{O}_{\mathcal{E}}$ has the diagonal representation

$$\hat{O}_{\mathcal{E}} = \sum_{k=1}^{K} o_k \hat{\tilde{\sigma}}_k^A \otimes \hat{\tilde{\sigma}}_k^B \tag{3.72}$$

where $\{o_k\}$ are the uniquely determined and positive singular values of the matrix (o_{nm}) and $K \leq \min\{N_A^2, N_B^2\}$ denotes the rank of (o_{nm}). Hence all global Hermitian operators and in particular all entanglement indicators can be decomposed in a sum over local Hermitian operators with at most $N_A^2 \leq N_B^2$ summands.

So far we have considered arbitrary local Hermitian operators as basis sets of the associated Hilbert-Schmidt vector spaces of Alice and Bob. However, not every Hermitian operator corresponds to an experimental setup. Hence, the question appears, whether it is always possible to detect entanglement in an experiment. In other words, is it possible to determine the expectation value of an entanglement indicator by performing local measurements and by classical communication? In order to answer this question we again use the geometrical representation of Hermitian operators. Let us assume that Alice has an experimental setup which corresponds to a set of observables

$$\mathcal{M}_A = \left\{ \hat{A}_n,\, n \in 1 \ldots N_A^2 \right\}. \tag{3.73}$$

In the associated Hilbert-Schmidt vector space V_{HS}^A they correspond to a set of vectors $\left\{ \vec{A}_n,\, n \in 1 \ldots N_A^2 \right\}$. If these vectors are linearly independent, they form a complete but possibly not orthonormal basis of V_{HS}^A. Hence, all vectors $\vec{X} \in V_{HS}^A$ can be written as a linear superposition

$$\vec{X} = \sum_{n=1}^{N_A^2} x_n \vec{A}_n, \tag{3.74}$$

where the uniquely determined real coefficients x_n can be calculated by solving a linear system of equations. As a consequence, in the original Hilbert space $\mathcal{H}_A$ all Hermitian operators $\hat{X}$ which act on Alice's Hilbert space can be decomposed as

$$\hat{X} = \sum_{n=1}^{N_A^2} x_n \hat{A}_n. \tag{3.75}$$

Furthermore let us assume that Bob also has the possibility to perform experiments

which correspond to a set of observables

$$\mathcal{M}_B = \left\{ \hat{B}_m,\, m \in 1 \dots N_B^2 \right\} \tag{3.76}$$

and form a complete but possibly not orthonormal basis in an associated Hilbert-Schmidt vector space. Then the direct product of both sets

$$\mathcal{M} \equiv \mathcal{M}_A \otimes \mathcal{M}_B = \left\{ \hat{A}_n \otimes \hat{B}_m,\, n \in 1 \dots N_A^2,\, m \in 1 \dots N_B^2 \right\} \tag{3.77}$$

is a valid complete basis of the entire Hilbert-Schmidt vector space. As a consequence, all Hermitian operators and in particular all entanglement indicators which act an $\mathcal{H}$ can be decomposed in this basis. Therefore, we can determine the expectation value of an arbitrary entanglement indicator by performing local measurements and by classical communication.

> Hence, under the assumption that Alice and Bob respectively have experimental setups which correspond to a complete set of linearly independent observables, it is possible to detect entanglement in a measurement. This assumption can be made because due to tomographical methods, that are for example described in [25, 27, 28, 55], we can always find a set of observables, the expectation values of which completely describe an arbitrary quantum state. Thus these observables are complete and build a valid basis in the associated Hilbert-Schmidt vector space.

Example

In the present example we consider two quantum systems Alice and Bob which are embedded in two dimensional Hilbert spaces $\mathcal{H}_A$ and $\mathcal{H}_B$ with the orthonormal basis vectors $\{|a_0\rangle, |a_1\rangle\}$ and $\{|b_0\rangle, |b_1\rangle\}$ respectively. The Hilbert space of the entire system is therefore $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$. We assume that Alice and Bob share a quantum state described by the density operator

$$\hat{\rho}_W = \alpha |\Psi_{\max}\rangle\langle\Psi_{\max}| + \frac{1-\alpha}{4}\,\hat{\mathbb{1}}\,, \quad 0 \le \alpha \le 1 \tag{3.78}$$

where $\hat{\mathbb{1}}$ is the identity operator and $|\Psi_{\max}\rangle$ denotes a maximally entangled state

$$|\Psi_{\max}\rangle = \frac{1}{\sqrt{2}}\left(|a_0 b_0\rangle + |a_1 b_1\rangle\right). \tag{3.79}$$

Quantum states of this form are called Werner states. It is shown in [11] that Werner states are entangled if and only if $\alpha > \frac{1}{3}$.

As discussed in subsection 3.1.1 the MES-observable

$$\hat{O}_{MES} = |\Psi_{\max}\rangle\langle\Psi_{\max}| \tag{3.80}$$

can detect entanglement by violating the inequality (3.22)

$$\mathrm{Tr}\left\{\hat{O}_{MES}\hat{\rho}\right\} = \frac{3\alpha+1}{4} \leq \frac{1}{2}. \tag{3.81}$$

It is remarkable that for the Werner states the MES-criterion is necessary and sufficient[5]. If the systems of Alice and Bob are spatially separated, it is impossible to measure the expectation value of the global observable $\hat{O}_{MES}$ in an experiment. Therefore we are now looking for a decomposition of this observable in local operators in order to have a possibility to perform the measurement.

As discussed in the previous subsection we represent $\hat{O}_{MES}$ in the associated Hilbert-Schmidt vector space V_{HS}. The sets, Eq. (3.28),

$$\Omega_A = \left\{\hat{\sigma}_n^A\right\} = \left\{|a_0\rangle\langle a_0|, |a_1\rangle\langle a_1|, \frac{|a_0\rangle\langle a_1| + |a_1\rangle\langle a_0|}{\sqrt{2}}, i\frac{|a_0\rangle\langle a_1| - |a_1\rangle\langle a_0|}{\sqrt{2}}\right\} \tag{3.82}$$

and

$$\Omega_B = \left\{\hat{\sigma}_n^B\right\} = \left\{|b_0\rangle\langle b_0|, |b_1\rangle\langle b_1|, \frac{|b_0\rangle\langle b_1| + |b_1\rangle\langle b_0|}{\sqrt{2}}, i\frac{|b_1\rangle\langle b_0| - |b_0\rangle\langle b_1|}{\sqrt{2}}\right\} \tag{3.83}$$

can be chosen to be the bases of the associated Hilbert-Schmidt vector spaces of Alice and Bob. By using the completeness of $\Omega_{A,B}$ the operator $\hat{O}_{MES}$ can be linearly decomposed as

$$\hat{O}_{MES} = \sum_{n,m=1}^{4} o_{nm}\hat{\sigma}_n^A \otimes \hat{\sigma}_m^B \tag{3.84}$$

where due to the special choice of the bases the matrix (o_{nm}) only has positive

[5] In [47] this statement has already been proven for the witness operator $\hat{W} = \hat{\mathbb{1}} - \frac{1}{2}|\Psi_{\max}\rangle\langle\Psi_{\max}|$.

diagonal entries which are given by

$$(o_{nm}) = \begin{pmatrix} \frac{1}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & \frac{1}{2} \end{pmatrix}. \tag{3.85}$$

Hence, the diagonal representation of $\hat{O}_{MES}$ is given by

$$\hat{O}_{MES} = \sum_{n=1}^{4} o_n \hat{\sigma}_n^A \otimes \hat{\sigma}_n^B = \sum_{n=1}^{4} \frac{1}{2} \hat{\sigma}_n^A \otimes \hat{\sigma}_n^B. \tag{3.86}$$

Moreover, as described in [27, 28], it is possible to perform experiments, which correspond to the $\hat{\sigma}$-operators. Hence we have a prescription how to detect the entanglement of Werner states in an experiment by only using local observations and classical communication.

3.4 Summary

By using the geometrical representation of Hermitian operators in the associated Hilbert-Schmidt vector space we can map the separability problem to a problem in convex geometry, i.e. detection of entanglement is equivalent to the search for a hyperplane which separates two convex sets. As a consequence, we have demonstrated that for any entangled state there exists at least one entanglement indicator which detects its entanglement by violating inequality (3.64), and hence defines a necessary and sufficient inseparability criterion. The bound of this inequality is given by the pure product states and therefore is in principle known. With the simple transformation in Eq. (3.24) we can show that each entanglement indicators defines a witness operator. Hence, all results which can be obtained for the witness operators can easily be transformed into the results for the entanglement indicators and vice versa. Furthermore, the geometrical representation allows us to show that global Hermitian operators can always be decomposed in local Hermitian operators. As a result, the physical property – *entanglement* – can be observed in an experiment consisting of local measurements and classical communication.

4 SVD-criterion

> Everything should be made as simple as possible, but not one bit simpler.
>
> Albert Einstein

So far we have demonstrated that for any entangled state there exists at least one entanglement indicator $\hat{O}_{\mathcal{E}}$, which can detect its entanglement by violating inequality (3.64). Based on these results we will now derive a sufficient inseparability criterion, which like the Peres-Horodecki criterion is easy to check. Moreover, in contrast to the Peres-Horodecki criterion the new criterion can find the entanglement of states with positive partial transpose. Thus by combining both criteria we can significantly enlarge the class of inseparable states that can be detected.

4.1 Experiment

The following calculations are motivated by quantum tomography experiments [27, 28] for the reconstruction of the density matrix of two qubits. These experiments consist of two steps. In the first step an entangled state $\hat{\rho}$ is prepared and in the second step the state is completely characterized by means of tomographic reconstruction. The tomography method is based on coincidence measurements of the expectation values of the Pauli spin operators

$$\tilde{r}_{nm} = \left\langle \hat{\tilde{\sigma}}_n^A \otimes \hat{\tilde{\sigma}}_m^B \right\rangle = \mathrm{Tr}\left\{ \hat{\rho}\, \hat{\tilde{\sigma}}_n^A \otimes \hat{\tilde{\sigma}}_m^B \right\}, \quad n,m = 1\ldots 4 \tag{4.1}$$

with respect to the quantum state $\hat{\rho}$. As discussed in subsection 3.2.1 the Pauli spin operators build a *complete,* orthogonal but not a normalized basis in the associated Hilbert-Schmidt vector space and therefore the tomographical matrix $(\tilde{r}_{nm})$ contains the full information about $\hat{\rho}$. The question arises whether it is possible to

verify entanglement[1] of a quantum state from the knowledge of its tomographical matrix. In order to answer this question we introduce two orthonormal sets

$$\overline{\Omega}^{A,B} = \left\{ \hat{\overline{\sigma}}_n^{A,B} = \frac{1}{\sqrt{2}} \hat{\tilde{\sigma}}_n^{A,B} \right\} \tag{4.2}$$

of basis vectors in the associated Hilbert-Schmidt vector spaces of Alice and Bob. The density operator can then be written as

$$\hat{\rho} = \sum_{nm=1}^{4} r_{nm} \hat{\overline{\sigma}}_n^A \otimes \hat{\overline{\sigma}}_m^B \tag{4.3}$$

with

$$r_{nm} = \tilde{r}_{nm}/2. \tag{4.4}$$

In subsection 3.3 we have shown that for any Hermitian operator $\hat{O}$ and therefore especially for the density operator $\hat{\rho}$ there exist bases $\Omega^{A,B} = \left\{ \hat{\sigma}_n^{A,B},\, n = 1 \ldots 4 \right\}$ such that $\hat{\rho}$ has a diagonal representation, Eq. (3.72),

$$\hat{\rho} = \sum_{n=1}^{4} r_n \hat{\sigma}_n^A \otimes \hat{\sigma}_n^B \tag{4.5}$$

where r_n are the singular values of the matrix (r_{nm}). Based on this representation we introduce the observable

$$\hat{O}_{SVD} = \sum_{n=1}^{4} \hat{\sigma}_n^A \otimes \hat{\sigma}_n^B \tag{4.6}$$

which we call the SVD-operator[2].

For the detection of entanglement in a quantum state $\hat{\rho}$ it is sufficient, as discussed in subsection 3.2.2, to fulfill the inequality (3.64)

$$\mathrm{Tr}\left\{ \hat{O}_{SVD} \hat{\rho} \right\} > \max_{|a\rangle,|b\rangle} \langle a, b | \hat{O}_{SVD} | a, b \rangle \tag{4.7}$$

with $|a\rangle \in \mathcal{H}_A$ and $|b\rangle \in \mathcal{H}_B$. By using the orthonormality of the $\hat{\sigma}$-operators the left hand side of this inequality can easily be calculated and is equal to the sum

[1] In the experiment described in [27] the density matrix was reconstructed first. Then the Peres-Horodecki criterion was used for the verification of entanglement.

[2] SVD denotes singular value decomposition.

over the singular values of the matrix (ρ_{nm})

$$\mathrm{Tr}\left\{\hat{O}_{SVD}\hat{\rho}\right\} = \sum_{n,m=1}^{4} r_n \mathrm{Tr}\left\{\left(\hat{\sigma}_n^A \otimes \hat{\sigma}_n^B\right)\left(\hat{\sigma}_m^A \otimes \hat{\sigma}_m^B\right)\right\} = \sum_{n=1}^{4} r_n. \tag{4.8}$$

In section 3.3 we have seen in the example that for maximally entangled states this sum is equal to two. By contrast, the right hand side of inequality (4.7) is bounded by one. This is due to the fact that the sets $\left\{\hat{\sigma}_n^A\right\}$ and $\left\{\hat{\sigma}_n^B\right\}$ define complete bases for Hermitian operators in the associated Hilbert-Schmidt vector spaces of Alice and Bob. Therefore all projectors $|a\rangle\langle a|$ and $|b\rangle\langle b|$ can be represented by linear combinations

$$|a\rangle\langle a| = \sum_{n=1}^{4} a_n \hat{\sigma}_n^A \quad \text{and} \quad |b\rangle\langle b| = \sum_{n=1}^{4} b_n \hat{\sigma}_n^B. \tag{4.9}$$

The scalar product between the SVD-operator and these projectors yields

$$\mathrm{Tr}\left\{\hat{O}_{SVD}|ab\rangle\langle ab|\right\} = \sum_{n=1}^{4} a_n b_n \tag{4.10}$$

where again the orthonormality of the $\hat{\sigma}$-operators was used. Applying the Schwarz inequality we see that this expression is bounded by

$$\sum_{n=1}^{4} a_n b_n \leq \sqrt{\sum_{n=1}^{4} a_n^2 \sum_{m=1}^{4} b_m^2}\,. \tag{4.11}$$

But the sum over the squares of the coefficients a_n and b_n is equal to the trace over the squared projectors

$$\sum_{n=1}^{4} a_n^2 = \mathrm{Tr}\left\{\left(\sum_{n=1}^{4} a_n \hat{\sigma}_n^A\right)^2\right\} = \mathrm{Tr}\left\{\left(|a\rangle\langle a|\right)^2\right\} = 1 \tag{4.12}$$

and

$$\sum_{n=1}^{4} b_n^2 = \mathrm{Tr}\left\{\left(|b\rangle\langle b|\right)^2\right\} = 1 \tag{4.13}$$

and therefore the right hand side of inequality (4.7) is bounded by one.

Hence, the answer to the question at the beginning of this section is:

> The sum over the singular values of the tomographical matrix, Eq. (4.1), can be used to verify entanglement in a given quantum state. For this purpose it is sufficient to show that this sum exceeds 2, because due to the renormalization of the Pauli spin operators, Eq. (4.4), the singular values of the tomographical matrix are twice as large as the singular values of the matrix (r_{nm}).

4.2 General case

The results of the previous section can be generalized to Hilbert spaces with higher dimensions. Let us assume that the dimensionality N_A of Alice's Hilbert space $\mathcal{H}_A$ is smaller than the dimensionality N_B of Bob's Hilbert space $\mathcal{H}_B$ and that the density operator of the quantum state is given by

$$\hat{\rho} = \sum_{n=1}^{N_A^2} \sum_{m=1}^{N_B^2} r_{nm} \hat{\overline{\sigma}}_n^A \otimes \hat{\overline{\sigma}}_m^B. \tag{4.14}$$

As discussed in subsection 3.3, $\hat{\rho}$ can be written in diagonal form, Eq. (3.72), as

$$\hat{\rho} = \sum_{n=1}^{N_A^2} r_n \hat{\sigma}_n^A \otimes \hat{\sigma}_n^B \tag{4.15}$$

where the values r_n denote the non-negative singular values of the matrix (r_{nm}). Based on this diagonal representation we can define the SVD-operator

$$\hat{O}_{SVD} \equiv \sum_{n=1}^{N_A^2} \hat{\sigma}_n^A \otimes \hat{\sigma}_n^B. \tag{4.16}$$

There are two reasons why we use this definition of $\hat{O}_{SVD}$. First, because its expectation value with respect to pure product states is bounded by one. The proof of this statement is similar to the previous section, we only have to replace the upper bound of the sums in Eqs. (4.9), (4.10), (4.11), (4.12) and (4.13) by N_A^2.

This proof is valid for all operators of the form

$$\hat{\overline{O}} = \sum_{n=1}^{N_A^2} \hat{\overline{\sigma}}_n^A \otimes \hat{\overline{\sigma}}_n^B \tag{4.17}$$

with arbitrary $\hat{\overline{\sigma}}$-operators which are orthonormal with respect to the trace scalar product, Eq. (3.27). However, if the $\hat{\overline{\sigma}}$-operators correspond to the diagonal form of the density operator $\hat{\rho}$, Eq. (4.15), the expectation value of $\hat{\overline{O}}$ with respect to $\hat{\rho}$ is maximal as shown in appendix A.4.3. This is the second reason for our choice of the definition of $\hat{O}_{SVD}$. Hence, if the sum over the singular values r_n

$$S_{SVD} \equiv \sum_{n=1}^{N_A^2} r_n = \mathrm{Tr}\left\{\hat{O}_{SVD}\hat{\rho}\right\} \tag{4.18}$$

exceeds one inequality (3.64)

$$\mathrm{Tr}\left\{\hat{O}_{SVD}\hat{\rho}\right\} > 1 \geq \max_{|ab\rangle} \langle ab|\hat{O}_{SVD}|ab\rangle \tag{4.19}$$

is valid and we have a sufficient criterion for $\hat{\rho}$ being entangled. We will call this criterion the SVD-criterion.

In the next step we want to analyze the question: How large can the sum over the singular values of (r_{nm}), Eq. (4.14), be? In other words our goal is to maximize the sum S_{SVD} under the constraints that density operators are non-negative and normalized. These constraints lead to the necessary condition that the trace over the squared density operator

$$\mathrm{Tr}\left\{\hat{\rho}^2\right\} \leq 1 \tag{4.20}$$

is less or equal to one. By using the diagonal representation, Eq. (4.15), this inequality can be rewritten as

$$\mathrm{Tr}\left\{\hat{\rho}^2\right\} = \mathrm{Tr}\left\{\left(\sum_{n=1}^{N_A^2} r_n \hat{\sigma}_n^A \otimes \hat{\sigma}_n^B\right)^2\right\} = \sum_{n=1}^{N_A^2} r_n^2 \leq 1 \tag{4.21}$$

where the orthogonality of the $\hat{\sigma}$-operators was used. The maximization problem is thus

$$S_{SVD} = \max_{r_n} \sum_{n=1}^{N_A^2} r_n \tag{4.22}$$

under the constraint

$$\sum_{n=1}^{N_A^2} r_n^2 \leq 1. \tag{4.23}$$

This maximization problem can be solved with the help of Lagrange multipliers and it turns out that the optimal value is equal to N_A which is the minimum over the dimensions of the Hilbert spaces of Alice and Bob. The maximal value is reached if the singular values

$$r_n = 1/N_A, \quad n = 1 \ldots N_A^2 \tag{4.24}$$

are equally distributed. The bound $\mathcal{S}_{SVD} = N_A$ is sharp, because it can be reached by all maximally entangled states

$$|\Psi_{\max}\rangle = \frac{1}{\sqrt{N_A}} \sum_{n=1}^{N_A} |a_n b_n\rangle \tag{4.25}$$

where $\{|a_n\rangle\}$ and $\{|b_n\rangle\}$ denote arbitrary orthonormal states. This can easily be shown by using the sets , Eq. (3.28),

$$\begin{aligned} &\overline{\Omega}_A = \left\{\hat{\overline{\sigma}}_n^A,\, n = 1 \ldots N_A^2\right\} \equiv \\ &\left\{|a_n\rangle\langle a_n|, \frac{|a_k\rangle\langle a_m| + |a_m\rangle\langle a_k|}{\sqrt{2}}, i\frac{|a_k\rangle\langle a_m| - |a_m\rangle\langle a_k|}{\sqrt{2}},\ n, k \neq m \in [1, N_A]\right\} \end{aligned} \tag{4.26}$$

and

$$\begin{aligned} &\overline{\Omega}_B = \left\{\hat{\overline{\sigma}}_n^B,\, n = 1 \ldots N_B^2\right\} \equiv \\ &\left\{|b_n\rangle\langle b_n|, \frac{|b_k\rangle\langle b_m| + |b_m\rangle\langle b_k|}{\sqrt{2}}, i\frac{|b_m\rangle\langle b_k| - |b_k\rangle\langle b_m|}{\sqrt{2}},\ n, k \neq m \in [1, N_A]\right\} \end{aligned} \tag{4.27}$$

which represent bases of the associated Hilbert-Schmidt vector spaces. For these bases the projector $|\Psi_{\max}\rangle\langle\Psi_{\max}|$ has the equally distributed diagonal representation with

$$\langle\Psi_{\max}|\hat{\overline{\sigma}}_n^A \otimes \hat{\overline{\sigma}}_m^B|\Psi_{\max}\rangle = \frac{1}{N_A}\delta_{nm}, \quad n, m \leq N_A^2 \tag{4.28}$$

where the set $\overline{\Omega}_B$ was re-sorted in such a way that all elements $\hat{\overline{\sigma}}_m^B$ which consist of Hilbert vectors $|b_n\rangle$ with $n > N_A^2$ were moved to the end of the set. Hence, in contrast to the constant value $S_{SVD} = 1$ of the expectation value of the SVD-operator with respect to separable states, Eq. (4.19), the expectation value of the SVD-

operator with respect to arbitrary density operators is bounded by the minimum over the dimensions of the Hilbert spaces of Alice and Bob. Consequently the SVD-criterion becomes more sensitive for larger Hilbert spaces.

4.3 PPT entangled states

As discussed in subsection 2.2.3 the Peres-Horodecki-criterion is necessary and sufficient for 2×2 and 2×3 systems. However, already in the case of 3×3 systems this criterion is only sufficient. An example of an entangled state which has positive partial transpose (PPT), is presented in [56, 57]. Based on this example we will show that the SVD-criterion can detect the entanglement of these states. We consider two 3-dimensional Hilbert spaces $\mathcal{H}_A$ and $\mathcal{H}_B$ with orthonormal bases $\{|a_n\rangle\}$ and $\{|b_n\rangle\}$. The basis of the entire Hilbert space can be described by the set

$$\{|\Psi_n\rangle,\, n = 1 \ldots 9\} = \{|a_n b_m\rangle,\, n, m = 1 \ldots 3\}\,. \tag{4.29}$$

Furthermore let the density operator of the entire quantum system be given by

$$\hat{\rho}\,(\alpha) = \sum_{n,m=1}^{9} \rho_{nm}^{\alpha} |\Psi_n\rangle\langle\Psi_m| \tag{4.30}$$

where the density matrix (ρ_{nm}^{α}) has the special form

$$(\rho_{nm}^{\alpha}) = \frac{1}{8\alpha+1} \begin{pmatrix} \alpha & 0 & 0 & 0 & \alpha & 0 & 0 & 0 & \alpha \\ 0 & \alpha & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \alpha & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \alpha & 0 & 0 & 0 & 0 & 0 \\ \alpha & 0 & 0 & 0 & \alpha & 0 & 0 & 0 & \alpha \\ 0 & 0 & 0 & 0 & 0 & \alpha & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{1+\alpha}{2} & 0 & \frac{\sqrt{1-\alpha^2}}{2} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \alpha & 0 \\ \alpha & 0 & 0 & 0 & \alpha & 0 & \frac{\sqrt{1-\alpha^2}}{2} & 0 & \frac{1+\alpha}{2} \end{pmatrix} \tag{4.31}$$

with $0 < \alpha < 1$. It is shown in [56, 57] that this quantum state is entangled despite the fact that it has a positive partial transpose.

With the help of Eq. (3.28) we can construct the sets $\overline{\Omega}_A = \left\{\hat{\overline{\sigma}}_n^A\right\}$ and $\overline{\Omega}_B = \left\{\hat{\overline{\sigma}}_m^B\right\}$

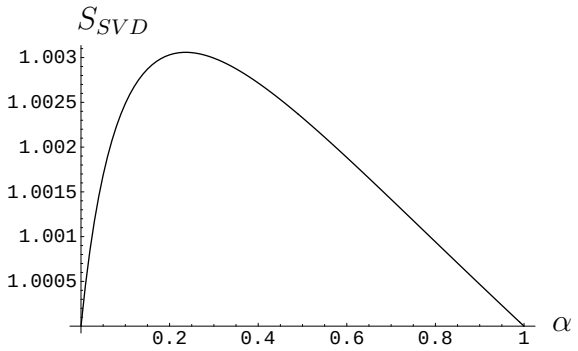


Figure 4.1:
This plot shows the sum S_{SVD} over the singular values of the density matrix, Eq. (4.31), as a function of the parameter α. It is evident that S_{SVD} exceeds unity for all valid values of α and hence, the SVD-criterion can detect the entanglement of this PPT entangled state.

by using the bases $\{|a_n\rangle\}$ and $\{|b_n\rangle\}$. Then as discussed in the previous section, the density operator, Eq. (4.30), can be written as

$$\hat{\rho}(\alpha) = \sum_{n,m=1}^{9} r_{nm}^{\alpha} \hat{\sigma}_n^A \otimes \hat{\sigma}_m^B. \tag{4.32}$$

By calculating the singular value decomposition of (r_{nm}^{α}) one can show that the sum S_{SVD}, Eq. (4.18), exceeds unity for all valid values of the parameter α and therefore detects the entanglement of $\hat{\rho}(\alpha)$. We illustrate the dependence between S_{SVD} and the parameter α in Fig. (4.1). Hence by using the density operator above, Eq. (4.30), it is shown that the SVD-criterion can detect entanglement of PPT entangled states and therefore extends the Peres-Horodecki criterion. This can also be seen with the help of the following general argument.

Let $\hat{\rho}$ be a density operator of the Hilbert space $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$ with $N_A = \dim \mathcal{H}_A$ and $N_B = \dim \mathcal{H}_B$. As discussed in section 4.2, it can be written as

$$\hat{\rho} = \sum_{n=1}^{N_A^2} \sum_{m=1}^{N_B^2} r_{nm} \hat{\sigma}_n^A \otimes \hat{\sigma}_n^B. \tag{4.33}$$

Due to fact that r_{nm} are real coefficients the partial transpose of $\hat{\rho}$ is

$$\hat{\rho}^{\mathrm{PTA}} = \sum_{n=1}^{N_A^2} \sum_{m=1}^{N_B^2} r_{nm} \left(\hat{\sigma}_n^A\right)^T \otimes \hat{\sigma}_n^B. \tag{4.34}$$

Hence, the matrices (r_{nm}) of the density operator and of its partial transpose are equal and the sum over the singular values or equivalently the SVD-criterion does not depend on the partial transpose operation. As a result we can say that the SVD-criterion and the Peres-Horodecki criterion detect two different sets of entangled states. Hence by combining both criteria we can significantly enlarge the set of inseparable states that can be detected in a straightforward way.

4.4 Transformation

This section is motivated by the following example for which the notation and definitions of the previous section are used. Let the density operator be

$$\hat{\rho} = \sum_{n,m=1}^{9} \rho_{nm} |\Psi_n\rangle\langle\Psi_m| \tag{4.35}$$

with the density matrix

$$(\rho_{nm}) = \frac{1}{9} \begin{pmatrix} 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & \sqrt{\frac{3}{7}} \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & \sqrt{\frac{3}{7}} \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{9}{7} & 0 & \frac{3\sqrt{6}}{7} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{3}{7} & 0 \\ \sqrt{\frac{3}{7}} & 0 & 0 & 0 & \sqrt{\frac{3}{7}} & 0 & \frac{3\sqrt{6}}{7} & 0 & \frac{9}{7} \end{pmatrix}. \tag{4.36}$$

By applying the sufficient but not necessary Peres-Horodecki and the SVD criteria it can be shown that the partial transpose of this operator is positive and that the sum S_{SVD} over the singular values, Eq. (4.18), is smaller than one. Thus, it is

unclear whether $\hat{\rho}$ is separable or not.

Nevertheless with the help of the results in appendix A.6 it can be proven that $\hat{\rho}$ is inseparable. It is shown there, that the transformation with *non singular* operators $\hat{A} \in \mathcal{H}_A$ and $\hat{B} \in \mathcal{H}_B$ according to Eq. (A.81)

$$\hat{\tilde{\rho}} = \mathrm{Tr}\left\{\hat{A}^\dagger \otimes \hat{B}^\dagger\, \hat{\rho}\, \hat{A} \otimes \hat{B}\right\}^{-1} \hat{A}^\dagger \otimes \hat{B}^\dagger\, \hat{\rho}\, \hat{A} \otimes \hat{B} \tag{4.37}$$

conserves the entanglement of a quantum state. This means that $\hat{\tilde{\rho}}$ is entangled *if and only if* $\hat{\rho}$ is entangled.

Let the operators $\hat{A}$ and $\hat{B}$ be given by

$$\hat{A} = \sum_{n,m=1}^{3} a_{nm} |a_n\rangle\langle a_m| \quad \text{and} \quad \hat{B} = \hat{\mathbb{1}} \tag{4.38}$$

with

$$(a_{nm}) = \begin{pmatrix} \sqrt{\frac{3}{13}} & 0 & 0 \\ 0 & \sqrt{\frac{3}{13}} & 0 \\ 0 & 0 & \sqrt{\frac{7}{13}} \end{pmatrix}. \tag{4.39}$$

By applying the transformation, Eq. (4.37), the density matrix of the new density operator $\hat{\tilde{\rho}}$ can be calculated to be

$$(\tilde{\rho}_{nm}) = \frac{1}{13} \begin{pmatrix} 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 3 & 0 & \sqrt{6} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 1 & 0 & \sqrt{6} & 0 & 3 \end{pmatrix} \tag{4.40}$$

and thus is equal to the density matrix of the PPT entangled state $\hat{\rho}(\alpha)$, Eq. (4.31), with $\alpha = \frac{1}{5}$. It was demonstrated in the previous section that the SVD-criterion can detect the entanglement of this state. Hence, the transformations presented in Eq. (4.37) can improve the SVD-criterion. In contrast to this result it is shown in

[56] that the positivity of eigenvalues of the partial transpose is invariant under this kind of transformations and therefore the Peres-Horodecki criterion cannot detect entanglement of $\hat{\rho}$ for any pair of operators $\hat{A}$ and $\hat{B}$.

4.5 Connection to MES-criterion

We have seen that the maximal value of the SVD-criterion can be reached by maximally entangled states $|\Psi_{\max}\rangle$. Furthermore, due to Eq. (4.28) it is shown that there exist sets of operators, Eqs. (4.26) and (4.27), for which the projector $|\Psi_{\max}\rangle\langle\Psi_{\max}|$ has the diagonal representation

$$|\Psi_{\max}\rangle\langle\Psi_{\max}| = \sum_{n=1}^{N_A^2} r_n \hat{\sigma}_n^A \otimes \hat{\sigma}_n^B = \frac{1}{N_A} \sum_{n=1}^{N_A^2} \hat{\sigma}_n^A \otimes \hat{\sigma}_n^B \tag{4.41}$$

with equally distributed coefficients $r_n = 1/N_A$. The sum on the right hand side of Eq. (4.41)

$$\hat{O}_{SVD} = \sum_{n=1}^{N_A^2} \hat{\sigma}_n^A \otimes \hat{\sigma}_n^B \tag{4.42}$$

is proportional to the SVD-operators defined by Eq. (4.16). As a consequence, the maximally entangled states build a *subset* of the SVD-operators.

On the other hand, as shown in subsection 3.1.1, the violation of the inequality

$$\mathrm{Tr}\left\{\hat{O}_{MES}\hat{\rho}\right\} \leq \frac{1}{N_A} \tag{4.43}$$

with

$$\hat{O}_{MES} = |\Psi_{\max}\rangle\langle\Psi_{\max}| \tag{4.44}$$

defines the MES-criterion. The combination of both results yields the new statement:

> The MES-criterion can indicate the entanglement of a quantum state only if the SVD-criterion does.

4.6 Summary

- The sufficient but not necessary SVD-criterion is based on data that can be obtained in experiments. Furthermore, it uses expectation values of local observables and can therefore detect the inseparability of spatially separated, non-local quantum systems. Hence, in contrast to the Peres-Horodecki criterion the SVD-criterion is an *operational* criterion for the detection of entanglement.

- Similar to the Peres-Horodecki-criterion, the SVD-criterion allows us to verify entanglement without solving complicated optimization problems. It suffices to calculate the singular value decomposition of the matrix (r_{nm}), Eq. (4.14), and consequently this criterion is *easy* to check.

- Perhaps the most important property is described in section 4.3. By combining the Peres-Horodecki criterion and the SVD-criterion the set of inseparable states which can be detected by applying an easy test is increased.

5 Max-Min criterion

> Truth is much too complicated to allow anything but approximations.
>
> John von Neumann

In chapter 3 we have demonstrated that a density operator $\hat{\rho}$ is inseparable if and only if an entanglement indicator $\hat{O}_{\mathcal{E}}$ exists which satisfies the following inequality (3.64)

$$\mathrm{Tr}\left\{\hat{O}_{\mathcal{E}}\hat{\rho}\right\} > \max_{|ab\rangle}\langle ab|\hat{O}_{\mathcal{E}}|ab\rangle = c_{\max}, \quad |a\rangle \in \mathcal{H}_A,\, |b\rangle \in \mathcal{H}_B. \tag{5.1}$$

Otherwise the density operator is separable. In contrast to the SVD-criterion this inseparability criterion is *necessary and sufficient*. Therefore the task of the present section is the question whether it is possible to find an entanglement indicator for a given inseparable quantum state. Our starting point is a derivation of an optimization problem which is based on inequality (5.1). We need this optimization problem to develop an iterative procedure which is mainly based on the methods of operations research[1]. Under a certain assumption this procedure results for inseparable density operators in an optimal entanglement indicator and hence answers the question above. Furthermore, in the case of separable states we obtain the convex decomposition, Eq. (2.14), as an additional result. This is by definition the proof for the separability.

[1] In [58] operations research is described as: "Operations research is a vast branch of mathematics which encompasses many diverse areas of minimization and optimization. Thousands of books have been written worldwide on the subject of operations research. The central objective of operations research is optimization, i.e., "to do things best under the given circumstances." This general concept has great many applications, for instance, in agricultural planning, biotechnology, data analysis ...."

5.1 Optimization problem

Let us consider an inseparable quantum state $\hat{\rho}_{ent}$. Then as discussed before there exists an entanglement indicator $\hat{O}_{\mathcal{E}}$ which satisfies inequality (5.1). By using the relations

$$\langle ab|\hat{O}_{\mathcal{E}}|ab\rangle = \mathrm{Tr}\left\{\hat{O}_{\mathcal{E}}|a,b\rangle\langle a,b|\right\} \tag{5.2}$$

and

$$\min_x\left(-f\left(x\right)\right) = \max_x\left(f\left(x\right)\right) \tag{5.3}$$

we can write

$$\eta \equiv \min_{|ab\rangle}\left(\mathrm{Tr}\left\{\hat{O}_{\mathcal{E}}\left(\hat{\rho}_{ent} - |ab\rangle\langle ab|\right)\right\}\right) > 0 \tag{5.4}$$

where a positive parameter η was introduced, which is determined by the difference between the expectation value of $\hat{O}_{\mathcal{E}}$ with respect to $\hat{\rho}_{ent}$ and the maximal expectation value of $\hat{O}_{\mathcal{E}}$ with respect to pure product states. This means that η represents the "quality" of the entanglement indicator $\hat{O}_{\mathcal{E}}$. In order to find the optimal entanglement indicator we consider the optimization problem

$$\eta_{\max} = \sup_{\left\{\hat{O}_{\mathcal{E}}\right\}}\left(\min_{|ab\rangle}\left(\mathrm{Tr}\left\{\hat{O}_{\mathcal{E}}\left(\hat{\rho}_{ent} - |ab\rangle\langle ab|\right)\right\}\right)\right) > 0, \tag{5.5}$$

where $\left\{\hat{O}_{\mathcal{E}}\right\}$ denotes the set of all entanglement indicators for a given inseparable state $\hat{\rho}_{ent}$. However, in the present form this optimization problem is not well defined, since by rescaling a given $\hat{O}_{\mathcal{E}}$ we can always find another entanglement indicator

$$\hat{\tilde{O}}_{\mathcal{E}} = \alpha\hat{O}_{\mathcal{E}}, \;\; \alpha > 1 \tag{5.6}$$

which yields a larger $\eta_{\max}$ and leads a divergence for $\alpha \to \infty$. To avoid this problem, only bounded $\hat{O}_{\mathcal{E}}$ shall be taken into account. This can be achieved by introducing the normalization condition[2]

$$\left\|\hat{O}_{\mathcal{E}}\right\| \leq 1. \tag{5.7}$$

It is remarkable that due to the finite dimensionality of the Hilbert space any valid operator norm, see [51] theorem 5.4.4, guarantees that $\hat{O}_{\mathcal{E}}$ is bounded.

[2] We postpone the special choice of the norm to section 5.3.

Equation (5.5) now reads

$$\eta_{\max} = \sup_{\{\hat{O}_{\mathcal{E}}, \|\hat{O}_{\mathcal{E}}\| \leq 1\}} \left(\min_{|ab\rangle} \left(\mathrm{Tr} \left\{ \hat{O}_{\mathcal{E}} \left(\hat{\rho}_{ent} - |ab\rangle\langle ab| \right) \right\} \right) \right) > 0. \tag{5.8}$$

In the next step we expand the set of possible input operators of the optimization problem to all Hermitian operators, which by definition only adds non-positive values

$$\eta = \min_{|ab\rangle} \left(\mathrm{Tr} \left\{ \hat{O} \left(\hat{\rho}_{ent} - |ab\rangle\langle ab| \right) \right\} \right) \leq 0, \;\; \hat{O} \notin \left\{ \hat{O}_{\mathcal{E}} \right\} \tag{5.9}$$

of the "quality" parameter η to the problem and does not change the optimal result $\eta_{\max}$. The final optimization problem is therefore given by

$$\eta_{\max} = \sup_{\{\hat{O}, \|\hat{O}\| \leq 1\}} \left(\min_{|a.b\rangle} \left(\mathrm{Tr} \left\{ \hat{O} \left(\hat{\rho}_{ent} - |ab\rangle\langle ab| \right) \right\} \right) \right) > 0 \tag{5.10}$$

where $\left\{ \hat{O}, \left\| \hat{O} \right\| \leq 1 \right\}$ denotes the set of all bounded Hermitian operators.

So far we have assumed inseparable density operators and have seen that the optimization problem yields a positive $\eta_{\max}$. By contrast, the solution of the optimization problem with respect to separable density operators $\hat{\rho}_{sep}$ is equal to zero. This can be seen in the following way. In section 3.1 we have shown that for all Hermitian operators $\hat{O}$ and all separable $\hat{\rho}_{sep}$ inequality (3.11)

$$\mathrm{Tr} \left\{ \hat{O} \hat{\rho}_{sep} \right\} \leq \max_{|ab\rangle} \langle ab|\hat{O}|ab\rangle, \quad |a\rangle \in \mathcal{H}_A, \, |b\rangle \in \mathcal{H}_B \tag{5.11}$$

is valid. This means that the "quality" parameter η, Eq. (5.4), is non-positive and hence the solution of the optimization problem, Eq. (5.10), in the case of separable density operators

$$\eta_{\max} = \sup_{\{\hat{O}, \|\hat{O}\| \leq 1\}} \left(\min_{|a.b\rangle} \left(\mathrm{Tr} \left\{ \hat{O} \left(\hat{\rho}_{sep} - |a, b\rangle\langle a, b| \right) \right\} \right) \right) \leq 0 \tag{5.12}$$

is bounded by zero. This bound is sharp because the result $\eta_{\max} = 0$ can always be reached by the observables which are proportional to the identity operator, i.e. $\hat{O} = \alpha \hat{\mathbb{1}}$ with $\alpha \in \mathbb{R}$.

By combining the results of Eq. (5.10) and Eq. (5.12) we can formulate a new necessary and sufficient inseparability criterion, which we call the Max-Min criterion:

> An unknown density operator $\hat{\rho}$ is inseparable if and only if the solution of the optimization problem with respect to all bounded Hermitian operators
>
> $$\eta_{\max} = \sup_{\{\hat{O}, \|\hat{O}\| \leq 1\}} \left(\min_{|a.b\rangle} \left(\mathrm{Tr} \left\{ \hat{O} \left(\hat{\rho} - |ab\rangle\langle ab| \right) \right\} \right) \right) \tag{5.13}$$
>
> is positive. In the case of a separable density operator this problem yields
>
> $$\eta_{\max} = 0. \tag{5.14}$$

In the following sections we will analyze the question whether it is possible to solve the Max-Min criterion. In fact, the problem requires minimization over *all* pure product states and maximization over *all* bounded Hermitian operators. The corresponding parameter space is huge, and at first sight the optimization problem seems to be unsolvable. However, by rewriting the Max-Min criterion, Eq. (5.13), in the form of a linear program and adopting the methods of operations research we can develop an iterative method that successfully finds the optimal entanglement indicator in every case.

5.2 Operations research

For our purpose we will only use a part of operations research, namely the linear programming or linear optimization. The goal of linear programming is the maximization of linear functions, which are often called cost functions, under linear constraints. This kind of optimization problem defines linear programs and can always be written [59] in the following canonical form.

Find a vector $\vec{x} = (x_1, x_2, \ldots, x_N)$ which maximizes the cost function

$$z(\vec{x}) = \sum_{n=1}^{N} c_n x_n \tag{5.15}$$

subject to M linear constraints formulated as inequalities

$$\sum_{n=1}^{N} d_{mn} x_n \leq b_m, \quad m \in 1, 2, \ldots, M \tag{5.16}$$

$$x_n \geq 0. \tag{5.17}$$

The matrix form for this problem consists of finding the vector $\vec{x}$, such that

$$z_{\max} = \max_{\vec{x}} \vec{c} \cdot \vec{x} \tag{5.18}$$

subject to

$$\mathbf{D}\vec{x} \preccurlyeq \vec{b} \tag{5.19}$$

$$\vec{x} \succcurlyeq \vec{0} \tag{5.20}$$

where $\mathbf{D}$ is a $N \times M$ matrix and the relation $\succcurlyeq$ is defined by equations (5.16) and (5.17).

The big advantage of linear programming is the fact, that the optimization problem, Eqs. (5.18), (5.19) and (5.20), either has no solution or the global maximum $z_{\max}$ can be found. Hence, if an optimization problem can be written in the form of a linear program, it is possible to solve this problem.

In order to solve linear programs the simplex method[3] is usually used. This method results in a vector $\vec{x}_{\max}$ that maximizes the cost function, Eq. (5.18). Furthermore the simplex method eliminates the redundant constraints in the matrix $\mathbf{D}$ and yields as an additional information extant rows of $\mathbf{D}$. Thus, by solving the linear program, Eq. (5.18), (5.19) and (5.20), we get the optimal vector $\vec{x}_{\max}$ and a matrix $\mathbf{D}_{new}$ of the type $N \times M_{new}$ with $M_{new} \leq M$, which is free from redundant information. It is shown in [60] that the maximal number of rows of $\mathbf{D}_{new}$ cannot exceed the number of coefficients in the vector $\vec{x}$ which means

$$M_{new} \leq N \tag{5.21}$$

and that the substitution of the original matrix $\mathbf{D}$ by $\mathbf{D}_{new}$ does not change the result of the linear program.

[3] An introduction to the simplex method can be found in [60].

5.3 Max-Min criterion in the form of a linear program

In this section we will show that the Max-Min criterion, Eq. (5.13), can be written in the form of a linear program. In the Hilbert-Schmidt vector space the Max-Min criterion, Eq. (5.13), without the normalization condition, Eq. (5.7), has the form

$$\eta_{\max} = \sup_{\vec{O}} \left(\min_{\vec{P}} \left(\vec{O} \cdot \left(\vec{R} - \vec{P} \right) \right) \right) \text{ with } \vec{P}, \vec{R}, \vec{O} \in V^{\perp} \tag{5.22}$$

where $\vec{O}$, $\vec{P}$ and $\vec{R}$ are the associated Hilbert-Schmidt vectors of the observable $\hat{O}$, the product state $|ab\rangle\langle ab|$ and the density operator $\hat{\rho}$ respectively. Furthermore, as discussed in subsection 3.2.1, we can restrict our calculation to the sub-vector space $V^{\perp}$ which is perpendicular to the associated Hilbert-Schmidt vector of the identity operator. The dimensionality of the problem is therefore

$$\dim V^{\perp} = N^2 - 1 \tag{5.23}$$

where $N = \dim \mathcal{H}$ is the dimension of the original Hilbert space $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$. By introducing a new variable c the Max-Min criterion, Eq. (5.22), can be written as

$$\eta_{\max} = \sup_{\vec{O},c} \left(\vec{O} \cdot \vec{R} - c \right) \text{ under the constraints } \left(\vec{O} \cdot \vec{P} - c \right) \leq 0 \quad \forall \vec{P}. \tag{5.24}$$

In the expressions above we can introduce the scalar products

$$\vec{O} \cdot \vec{R} - c = \begin{pmatrix} \vec{O} \\ c \end{pmatrix} \cdot \begin{pmatrix} \vec{R} \\ -1 \end{pmatrix} \quad \text{and} \quad \vec{O} \cdot \vec{P} - c = \begin{pmatrix} \vec{O} \\ c \end{pmatrix} \cdot \begin{pmatrix} \vec{P} \\ -1 \end{pmatrix}. \tag{5.25}$$

Hence by adding an extra dimension to $V^{\perp}$ and by introducing three new vectors $\vec{\tilde{O}} \equiv \left(\vec{O}, c \right)$, $\vec{\tilde{P}} \equiv \left(\vec{P}, -1 \right)$ and $\vec{\tilde{R}} \equiv \left(\vec{R}, -1 \right)$ the Max-Min criterion can be reduced to the maximization problem

$$\eta_{\max} = \sup_{\vec{\tilde{O}}} \vec{\tilde{O}} \cdot \vec{\tilde{R}} \tag{5.26}$$

under the linear constraints

$$\vec{\tilde{O}} \cdot \vec{\tilde{P}} \leq 0 \quad \forall \vec{\tilde{P}}. \tag{5.27}$$

The number of constraints is infinite, because the set of vectors $\left\{\vec{\tilde{P}}\right\}$ is continuous. In order to construct a linear program which consists of a finite number of constraints, we have to introduce a discrete subset of M pure product states

$$\mathcal{S} = \{|a_n b_n\rangle\langle a_n b_n|,\, n = 1 \ldots M\} \tag{5.28}$$

that translates into a discrete set of associated Hilbert-Schmidt vectors

$$\mathcal{A} = \left\{\vec{P}_n,\, n = 1 \ldots M\right\}. \tag{5.29}$$

The resulting optimization problem is then given by[4]

$$\eta_{\max} = \max_{\vec{O}} \vec{\tilde{O}} \cdot \vec{\tilde{R}} \tag{5.30}$$

subject to the constraints

$$\vec{\tilde{O}} \cdot \vec{\tilde{P}}_n \leq 0 \quad \forall \vec{P}_n \in \mathcal{A} \tag{5.31}$$

and is only a discrete version of the Max-Min criterion. The constraints can be written in matrix form

$$\tilde{\mathbf{D}} \cdot \vec{\tilde{O}} \preccurlyeq \vec{0} \tag{5.32}$$

where $\tilde{\mathbf{D}} \equiv \left(\vec{\tilde{P}}_1, \vec{\tilde{P}}_2, \ldots, \vec{\tilde{P}}_M\right)$ is an $N^2 \times M$ matrix with $\vec{P}_n \in \mathcal{A}$.

The optimization problem now looks very similar to the linear program presented in section 5.2. However according to Eq. (5.20) the components $\tilde{o}_n$ of the vector $\vec{\tilde{O}}$ should be non-negative. This can be achieved by introducing [59] positive slack variables x_n with $\tilde{o}_n \equiv x_{2n-1} - x_{2n}$. Then the optimization problem can be written in the canonical form of a linear program

$$\eta_{\max} = \max_{\vec{x}} \vec{x} \cdot \vec{\overline{R}} \equiv \max_{\vec{x}} \left[\begin{pmatrix} \vec{x}_{\text{odd}} \\ \vec{x}_{\text{even}} \end{pmatrix} \cdot \begin{pmatrix} \vec{\tilde{R}} \\ -\vec{\tilde{R}} \end{pmatrix} \right] \tag{5.33}$$

[4] The supremum was replaced by the maximum because the optimization problem now has a finite number of constraints.

subject to the conditions

$$\overline{\mathbf{D}} \cdot \vec{x} \equiv \left(\tilde{\mathbf{D}}, -\tilde{\mathbf{D}}\right) \cdot \begin{pmatrix} \vec{x}_{\text{odd}} \\ \vec{x}_{\text{even}} \end{pmatrix} \preccurlyeq \vec{0} \tag{5.34}$$

$$\vec{x} \equiv \begin{pmatrix} \vec{x}_{\text{odd}} \\ \vec{x}_{\text{even}} \end{pmatrix} \succcurlyeq \vec{0} \tag{5.35}$$

where $\vec{x}_{\text{odd}}$ contains the odd coefficients x_{2n-1} and $\vec{x}_{\text{even}}$ contains the even coefficients x_{2n}, respectively. This linear program is unbounded and as discussed in section 5.1 an additional normalization condition, Eq. (5.7), for the operator $\hat{O}$ should be introduced. In the Hilbert-Schmidt vector space this can be realized by using the l_1 norm [51]

$$\left\|\vec{O}\right\|_1 = \sum_{n=1}^{N^2-1} |o_n| \leq 1. \tag{5.36}$$

Due to the non-negativity of the slack variables it can be rewritten in the linear form

$$\left\|\vec{O}\right\|_1 \leq \sum_{n=1}^{N^2-1} x_{2n} + x_{2n-1} \leq 1 \tag{5.37}$$

and the final linear program is given by

$$\eta_{\max} = \max_{\vec{x}} \vec{x} \cdot \overrightarrow{R} \tag{5.38}$$

under the constraints

$$\mathbf{D} \cdot \vec{x} \equiv \begin{pmatrix} \vec{P}_1 & -1 & -\vec{P}_1 & 1 \\ \vec{P}_2 & -1 & -\vec{P}_2 & 1 \\ \vdots & \vdots & \vdots & \vdots \\ 1, \ 1, \ \ldots, \ 1, & 0, & 1, \ 1, \ \ldots, \ 1, & 0 \end{pmatrix} \cdot \vec{x} \preccurlyeq \begin{pmatrix} \vec{0} \\ 1 \end{pmatrix} \tag{5.39}$$

$$\vec{x} \succcurlyeq \vec{0}. \tag{5.40}$$

Hence, by considering a discrete subset of product states, Eq. (5.28), the Max-Min criterion can be formulated as a linear program with $2N^2 = \dim \vec{x}$ variables and $M + 1$ linear constraints.

The simplex method can be used to solve this linear program and determine the optimal vector $\vec{x}_{\max}$ and the new $2N^2 \times M_{new}$ matrix $\mathbf{D}_{new}$. Due to the definitions

of $\vec{x}$, Eq. (5.33), and of $\mathbf{D}$, Eq. (5.39), these results yield the wanted vector

$$\vec{O}_{\max} = (o_1, o_2, \ldots, o_{N^2-1}) \text{ with } o_n = x_{2n-1} - x_{2n} \tag{5.41}$$

that maximizes the optimization problem, Eq. (5.22), and a new discrete set

$$\mathcal{A}_{new} = \left\{ \vec{P}_n,\, n = 1 \ldots M_{new} \right\} \tag{5.42}$$

where the vectors $\vec{P}_n$ correspond to the rows of $\mathbf{D}_{new}$. Moreover, the variable $c = x_{2N^2-1} - x_{2N^2}$ introduced in Eq. (5.24) is equal to the maximal overlap

$$c_{\max} = \max_{\vec{P}_n \in \mathcal{A}_{new}} \vec{P}_n \cdot \vec{O}_{\max} \tag{5.43}$$

between the vectors $\vec{P}_n$ and the resulting vector $\vec{O}_{\max}$.

In the original Hilbert space this solution yields a subset of pure product states

$$\mathcal{S}_{new} = \{ |a_n b_n\rangle\langle a_n b_n|,\, n = 1 \ldots M_{new} \} \tag{5.44}$$

and the observable $\hat{O}_{\max}$ which optimizes the discrete version of the Max-Min criterion

$$\eta_{\max} = \max_{\left\{\hat{O}, \left\|\hat{O}\right\|_1 \leq 1\right\}} \left(\min_{|a_n b_n\rangle} \left(\mathrm{Tr} \left\{ \hat{O} \left(\hat{\rho} - |a_n b_n\rangle\langle a_n b_n| \right) \right\} \right) \right) \tag{5.45}$$

with $|a_n b_n\rangle\langle a_n b_n| \in \mathcal{S}_{new}$.

Hence, by introducing a discrete subset, Eq. (5.28), we can rewrite the Max-Min criterion in the form of a linear program which provides a discrete solution to the continuous optimization problem. By using the simplex method we can solve this linear program in a very efficient way. In addition to the optimal observable $\hat{O}_{\max}$, which maximizes the cost function, it also filters out the redundant constraints of the problem. Moreover due to Eq. (5.21) the number of remaining constraints M_{new} does not exceed the number of coefficients in the vector $\vec{O}_{\max}$. This means that

$$M_{new} \leq N^2 = (\dim \mathcal{H})^2 . \tag{5.46}$$

The following example is meant to clarify the concepts of linear programs on the basis of a two dimensional vector space.

Example

Let

$$\mathcal{A} = \left\{ \vec{P}_1, \vec{P}_2, \vec{P}_3 \right\} = \left\{ \left(\frac{7}{8}, \frac{7}{16} \right), \left(-\frac{7}{8}, 0 \right), \left(0, \frac{7}{16} \right) \right\} \tag{5.47}$$

be a discrete set of $M = 3$ vectors $\vec{P}_n$ which define a convex body $\mathcal{K}$ as a linear combination of all possible convex superpositions. Furthermore let

$$\vec{R} = \left(1, \frac{3}{10} \right) \tag{5.48}$$

be a point lying outside of $\mathcal{K}$. The goal of the present example is to find the vector $\vec{O} = (o_1, o_2)$ that maximizes the expression

$$\eta_{\max} = \max_{\vec{O}} \left(\min_{\vec{P}_n \in \mathcal{A}} \left(\vec{O} \cdot \left(\vec{R} - \vec{P}_n \right) \right) \right) \tag{5.49}$$

under the constraint

$$\left\| \vec{O} \right\|_1 \leq 1. \tag{5.50}$$

According to the arguments of the previous section this optimization problem can be rewritten in the form of the linear program

$$\eta_{\max} = \max_{\vec{x}} \left\{ (x_1 - x_2) + \frac{3}{10} (x_3 - x_4) - (x_5 - x_6) \right\} \tag{5.51}$$

subject to

$$\mathbf{D} \cdot \vec{x} \equiv \begin{pmatrix} \frac{7}{8} & \frac{7}{16} & -1 & -\frac{7}{8} & -\frac{7}{16} & 1 \\ -\frac{7}{8} & 0 & -1 & \frac{7}{8} & 0 & 1 \\ 0 & \frac{7}{16} & -1 & 0 & -\frac{7}{16} & 1 \\ 1 & 1 & 0 & 1 & 1 & 0 \end{pmatrix} \cdot \begin{pmatrix} x_1 \\ x_3 \\ x_5 \\ x_2 \\ x_4 \\ x_6 \end{pmatrix} \preccurlyeq \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} \tag{5.52}$$

$$(x_1, x_2, x_3, x_4, x_5, x_6) \succcurlyeq (0, 0, 0, 0, 0, 0) \tag{5.53}$$

and can be solved by using the simplex method. We obtain the optimal vector

$$\vec{x}_{\max} = \left(\frac{1}{5}, 0, 0, 0, \frac{4}{5}, \frac{7}{40} \right) \tag{5.54}$$

and the new matrix

$$\mathbf{D}_{new} = \begin{pmatrix} \frac{7}{8} & \frac{7}{16} & -1 & -\frac{7}{8} & -\frac{7}{16} & 1 \\ -\frac{7}{8} & 0 & -1 & \frac{7}{8} & 0 & 1 \\ 1 & 1 & 0 & 1 & 1 & 0 \end{pmatrix}. \tag{5.55}$$

The knowledge about $\vec{x}_{\max}$ makes it possible to find the vector that maximizes the function defined in Eq. (5.49)

$$\vec{O}_{\max} = (x_1 - x_2, x_3 - x_4) = \left(\frac{1}{5}, -\frac{4}{5}\right), \tag{5.56}$$

the maximal overlap between $\vec{O}_{\max}$ and $\vec{P}_n$

$$c_{\max} = x_5 - x_6 = -\frac{7}{40} \tag{5.57}$$

and the maximal value of the cost function

$$\eta_{\max} = \frac{27}{200}. \tag{5.58}$$

Furthermore, with the help of the matrix $\mathbf{D}_{new}$ a new discrete set of points can be constructed. The constraints originating from the points $\vec{P}_1$ and $\vec{P}_2$ survive and therefore the new set is

$$\mathcal{A}_{new} = \left\{\vec{P}_1, \vec{P}_2\right\}. \tag{5.59}$$

Fig. 5.1 (a) visualizes this optimization problem.

In the next step we will show that the solution of the problem, Eq. (5.49), strongly depends on the choice of the basis of the vector space as can be seen in the following calculations. We now consider the same optimization problem but in a different coordinate system, which is connected to the previous one by a unitary transformation

$$\begin{pmatrix} x' \\ y' \end{pmatrix} = \mathbf{U} \cdot \begin{pmatrix} x \\ y \end{pmatrix} \tag{5.60}$$

where $\mathbf{U}$ denotes the unitary matrix

$$\mathbf{U} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}. \tag{5.61}$$

The distances between the points in this new coordinate system do not change and one would expect that the solution of the optimization problem does not change either. However, by setting up the new linear program and solving it we obtain the new resulting optimization vector

$$\vec{O}'_{\max} = (0, -1) \tag{5.62}$$

which does not correspond to the previous one. Furthermore, due to the transformation of the coordinate system the maximal value of the cost function

$$\eta'_{\max} = \frac{1}{\sqrt{2}}\frac{21}{80} \tag{5.63}$$

increases and the new set

$$\mathcal{A}'_{new} = \left\{\vec{P}_1\right\} \tag{5.64}$$

only contains the vector $\vec{P}_1$. This behavior appears because the l_1-norm, which is used for the normalization condition, Eq. (5.50), is not invariant under unitary transformations. Hence, the solution of the problem, Eq. (5.49), strongly depends on the choice of the basis of the vector space and it is not meaningful to compare the results of the Max-Min criterion in different coordinate systems. In Fig. 5.1 (a) and (b) we give a pictorial interpretation of the difference between the solutions of the linear program in different coordinate systems.

5.4 Subset update

In section 5.3 we have demonstrated, that we can solve the Max-Min criterion by considering a discrete set $\mathcal{S}$ of pure product states. As a result we obtain the optimal observable $\hat{O}_{\max}$, the maximal expectation value $c_{\max}$ of $\hat{O}_{\max}$ with respect to the elements of $\mathcal{S}$, a new set of product states $\mathcal{S}_{new}$ which is free from redundant information and the optimal value $\eta_{\max}$ of the Max-Min criterion. In the Hilbert-Schmidt vector space we can give the geometrical interpretation of this solution. The vector $\vec{O}_{\max}$ corresponding to $\hat{O}_{\max}$ and the maximal expectation value $c_{\max}$ define a hyperplane

$$\mathcal{E} = \left\{\vec{x} : \vec{O}_{\mathcal{E}} \cdot \vec{x} = c_{\max}\right\} \tag{5.65}$$

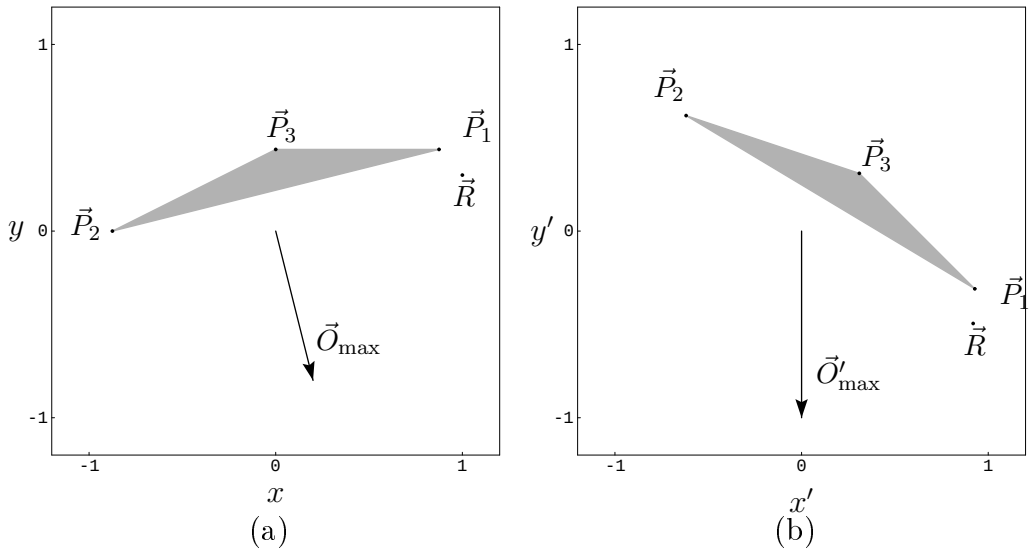


Figure 5.1:
The grey triangle, which is formed by all possible convex combinations of the vectors $\left\{\vec{P}_1, \vec{P}_2, \vec{P}_3\right\}$, and the vector $\vec{R}$ represent two disjunct convex sets in two different coordinate systems (a) and (b), which are linked to each other by a rotation of 45°. The vectors $\vec{O}_{\max}$ and $\vec{O}'_{\max}$ maximize the optimization problem (5.49). Both are not connected by the same rotation, because the l_1-norm, which is used in the optimization problem, is not invariant under unitary transformations.

which divides the vector space V_{HS} in two half spaces so that the vector $\vec{R}$ and the set $\mathcal{A}$, which correspond to the density operator $\hat{\rho}$ and the set $\mathcal{S}$, are in different half spaces. But the set $\mathcal{A}$ is only a subset of the convex set $\mathcal{K}$ over all separable states and hence the solution of the linear program is only a discrete *approximation* of the full optimization problem. Therefore the task of the present section is to determine its accuracy. In other words, is it possible to violate the approximative solution of the linear program and to find vectors, which correspond to pure product states and have larger overlap with $\vec{O}_{\max}$ than the elements of the set $\mathcal{A}_{new}$?

This question can be answered in the original Hilbert space where we are looking for pure product states with

$$\langle \psi\varphi|\hat{O}_{\max}|\psi\varphi\rangle \geq c_{\max}. \tag{5.66}$$

For a given input state $|\alpha_0\beta_0\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$ and a given Hermitian operator $\hat{O}_{\max}$ which acts on $\mathcal{H}$ we can define a new operator

$$\hat{B} \equiv \langle \alpha_0|\hat{O}_{\max}|\alpha_0\rangle \tag{5.67}$$

acting on $\mathcal{H}_B$. In appendix A.1 we show, Eq. (A.1), that the eigenvector $|\beta_1\rangle \in \mathcal{H}_B$ corresponding to the maximal eigenvalue of $\hat{B}$ maximizes the expectation value

$$\langle \beta_1|\hat{B}|\beta_1\rangle = \max_{|\beta\rangle\in\mathcal{H}_B} \langle \beta|\hat{B}|\beta\rangle. \tag{5.68}$$

By using the definition of $\hat{B}$, Eq. (5.67), we obtain

$$\langle \alpha_0\beta_0|\hat{O}_{\max}|\alpha_0\beta_0\rangle \leq \langle \alpha_0\beta_1|\hat{O}_{\max}|\alpha_0\beta_1\rangle. \tag{5.69}$$

Analogously, the resulting state $|\beta_1\rangle$ can again be used to define an operator

$$\hat{A} \equiv \langle \beta_1|\hat{O}_{\max}|\beta_1\rangle \tag{5.70}$$

which acts on $\mathcal{H}_A$ and whose eigenstate $|\alpha_1\rangle \in \mathcal{H}_A$ corresponding to the maximal eigenvalue satisfies the inequality

$$\langle \alpha_0\beta_1|\hat{O}_{\max}|\alpha_0\beta_1\rangle \leq \langle \alpha_1\beta_1|\hat{O}_{\max}|\alpha_1\beta_1\rangle. \tag{5.71}$$

Furthermore, in appendix A.5.2 we show that for a given input product state $|\alpha_1\beta_1\rangle$

and a non-negative observable $\hat{O}_{pos}$ an unnormalized state

$$|\Psi\rangle \equiv \hat{O}_{pos}|\alpha_1\beta_1\rangle \tag{5.72}$$

can be defined with the Schmidt decomposition

$$|\Psi\rangle = \sum_{n=1}^{N} s_n|\psi_n\varphi_n\rangle,\ s_1 \geq s_2 \geq \ldots \geq s_N, \tag{5.73}$$

where the product state $|\psi_1\varphi_1\rangle$ corresponding to the largest Schmidt factor s_1 obeys the inequality

$$\langle\alpha_1\beta_1|\hat{O}_{pos}|\alpha_1\beta_1\rangle \leq \langle\psi_1\varphi_1|\hat{O}_{pos}|\psi_1\varphi_1\rangle. \tag{5.74}$$

To use this relation for the purpose of the present section, we introduce a new non-negative observable

$$\hat{O}_{pos} \equiv \hat{\mathbb{1}} + \hat{O}_{\max}, \tag{5.75}$$

where the normalization condition, Eq. (5.36), guarantees[5] its positivity. Thus, by using $|\alpha_1\beta_1\rangle$ as an input state, a new product state $|\alpha_2\beta_2\rangle \equiv |\psi_1\varphi_1\rangle$ can be found which satisfies the inequality

$$\langle\alpha_1\beta_1|\hat{O}_{pos}|\alpha_1\beta_1\rangle \leq \langle\alpha_2\beta_2|\hat{O}_{pos}|\alpha_2\beta_2\rangle. \tag{5.76}$$

In view of the definition of $\hat{O}_{pos}$ the new state also satisfies the inequality

$$\langle\alpha_1\beta_1|\hat{O}_{\max}|\alpha_1\beta_1\rangle \leq \langle\alpha_2\beta_2|\hat{O}_{\max}|\alpha_2\beta_2\rangle. \tag{5.77}$$

Hence, starting with the input state $|\alpha_0\beta_0\rangle$ and the operator $\hat{O}_{\max}$ it is possible to calculate two output states $|\alpha_1\beta_1\rangle$ and $|\alpha_2\beta_2\rangle$ such that the expectation values

$$\begin{array}{ccccc} \langle\alpha_0\beta_0|\hat{O}_{\max}|\alpha_0\beta_0\rangle & \leq & \langle\alpha_1\beta_1|\hat{O}_{\max}|\alpha_1\beta_1\rangle & \leq & \langle\alpha_2\beta_2|\hat{O}_{\max}|\alpha_2\beta_2\rangle \\ \left\langle\hat{O}_{\max}\right\rangle_0 & \leq & \left\langle\hat{O}_{\max}\right\rangle_1 & \leq & \left\langle\hat{O}_{\max}\right\rangle_2 \end{array} \tag{5.78}$$

increase. The obtained result can again be improved by using the output state

[5] The l_1 norm of the associated Hilbert-Schmidt vector $\vec{O}_{\max}$, Eq. (5.36), and its absolute value $\sqrt{\vec{O}_{\max}\cdot\vec{O}_{\max}}$ is bounded by unity. In the original Hilbert space this means that the trace over the squared operator $\mathrm{Tr}\left\{\hat{O}^2_{\max}\right\}$ is less than one and that the minimal eigenvalue of $\hat{O}_{\max}$ is bounded by -1. Therefore, the operator $\hat{O}_{pos} \equiv \hat{\mathbb{1}} + \hat{O}_{\max}$ is a non-negative operator.

$|\alpha_2\beta_2\rangle$ as the new input state and by iterating this procedure. These iterations yield a monotonically increasing series of expectation values

$$\left\langle \hat{O}_{\max} \right\rangle_0 \leq \ldots \leq \left\langle \hat{O}_{\max} \right\rangle_n \leq \ldots \leq \left\langle \hat{O}_{\max} \right\rangle_{\text{fin}}, \tag{5.79}$$

which is bounded, Eq. (3.13), and therefore convergent. The sequence of the states $|\alpha_n\beta_n\rangle$ converges[6], too. The final state $|\alpha_{fin}\beta_{fin}\rangle$ has to fulfill the relation, Eq. (5.73),

$$\hat{O}_{\max}|\alpha_{\text{fin}}\beta_{\text{fin}}\rangle = s_1|\alpha_{\text{fin}}\beta_{\text{fin}}\rangle + \sum_{n=2}^{N} s_n|\psi_n\varphi_n\rangle, \quad s_1 \geq s_2 \geq \ldots \geq s_N \tag{5.80}$$

where the right hand side of the equation denotes the Schmidt decomposition of the state $|\Psi\rangle = \hat{O}_{\max}|\alpha_{\text{fin}}\beta_{\text{fin}}\rangle$. This relation is a necessary condition, as shown in appendix A.5.2, so that the expectation value of the observable $\hat{O}_{\max}$ with respect to *all* pure product states

$$\left\langle \hat{O}_{\max} \right\rangle_{\text{fin}} = \langle\alpha_{\text{fin}}\beta_{\text{fin}}|\hat{O}_{\max}|\alpha_{\text{fin}}\beta_{\text{fin}}\rangle \tag{5.81}$$

is the global maximum. We can now answer the question of the present section.

By identifying the input state $|\alpha_0\beta_0\rangle$ with the elements $|a_nb_n\rangle$ of the set $\mathcal{S}_{new}$ the above iterative procedure yields the product states $|\alpha^n_{\text{fin}}\beta^n_{\text{fin}}\rangle$ which have larger or equal overlap with $\hat{O}_{\max}$ than $|\alpha_0\beta_0\rangle$.

Moreover, by adding these states to the subset $\mathcal{S}_{new}$ a new updated subset $\mathcal{S}$ can be defined and allows to proceed with the methods described in section 5.3, i.e. to define a new linear program and to solve it. Due to the fact that the updated subset $\mathcal{S}$ includes $\mathcal{S}_{new}$, the new optimal value $\eta^{new}_{\max}$ of this new linear program has to be smaller than the old $\eta_{\max}$ and therefore constitutes a better approximation of the Max-Min criterion. Hence, iterative steps consist of the subset update and the solution of the linear program yields a monotonically decreasing series

$$\eta^1_{\max} \geq \eta^2_{\max} \geq \ldots \geq \eta^{\text{final}}_{\max} \tag{5.82}$$

[6]It was assumed here that the largest Schmidt factor s_1 is not degenerate. If for example $s_1 = s_2$ there are two final states which reach the maximal expectation value $\left\langle \hat{O}_{\max} \right\rangle_{\text{fin}}$. For our purpose it is sufficient to use only one of them.

which, as discussed in subsection 5.1, is bounded by zero and therefore converges. Thus, by combining the methods of linear programming, as described in section 5.3, and the subset update described in this section we can formulate a convergent iterative procedure. In the subsequent sections we will rewrite this iterative procedure in the form of an algorithm which can be implemented on modern computers and show that this algorithm results in an optimal entanglement indicator.

5.5 Algorithm based on the Max-Min criterion

Step 1: Initialization

Let $\hat{\rho}$ be a density operator of the entire Hilbert space $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$ of Alice and Bob with $N_A = \dim \mathcal{H}_A$ and $N_B = \dim \mathcal{H}_B$. As discussed in chapter 4 the sufficient SVD-criterion can be used to verify the entanglement of $\hat{\rho}$. It is based on the diagonal representation of the density operator

$$\hat{\rho} = \sum_{n=1}^{K} r_n \hat{\sigma}_n^A \otimes \hat{\sigma}_n^B \tag{5.83}$$

where $K \leq \min\{N_A^2, N_B^2\}$ denotes the rank of $\hat{\rho}$ and r_n are the singular values of $\hat{\rho}$. If the sum over r_n exceeds unity, the algorithm exits with the answer that $\hat{\rho}$ is an entangled state. If this is not the case the SVD-operator, Eq. (4.6),

$$\hat{O}_{SVD} = \sum_{n=1}^{K} \hat{\sigma}_n^A \otimes \hat{\sigma}_n^B \tag{5.84}$$

will be the initial operator $\hat{O}_{\max}$. Furthermore, the eigenvectors

$$\hat{\sigma}_n^A = \sum_{m=1}^{N_A} \lambda_m^n |\psi_m^n\rangle\langle\psi_m^n| \text{ and } \hat{\sigma}_n^B = \sum_{m=1}^{N_B} \gamma_m^n |\varphi_m^n\rangle\langle\varphi_m^n| \tag{5.85}$$

of the $\hat{\sigma}$-operators define the initial discrete subset $\mathcal{S}_{new}$ of product states by

$$\begin{aligned} \mathcal{S}_{new} \equiv \{&|a_n b_n\rangle\langle a_n b_n|,\ n = 1 \ldots M_{new}\} \equiv \\ &\{|\psi_m^n\rangle\langle\psi_m^n| \otimes |\varphi_k^n\rangle\langle\varphi_k^n|,\ n = 1 \ldots K,\ m = 1 \ldots N_A,\ k = 1 \ldots N_B\}\,. \end{aligned} \tag{5.86}$$

Hence, the initialization step of the algorithm yields an initial operator $\hat{O}_{\max}$ and an initial subset $\mathcal{S}_{new}$.

Step 2: Subset update

The inputs of the second step are the observable $\hat{O}_{\max}$ and the subset $\mathcal{S}_{new}$ consisting of M_{new} product states. By using the results of section 5.4 for each product state $|a_n b_n\rangle \in \mathcal{S}_{new}$ a new product state $|\alpha_{\text{fin}}^n \beta_{\text{fin}}^n\rangle$ can be calculated which has larger or equal overlap with $\hat{O}_{\max}$ than $|a_n b_n\rangle$. The union of these new states with $\mathcal{S}_{new}$ yields the updated subset

$$\mathcal{S} \equiv \mathcal{S}_{new} \cup \{|\alpha_{\text{fin}}^n \beta_{\text{fin}}^n\rangle\langle\alpha_{\text{fin}}^n \beta_{\text{fin}}^n|,\, n = 1 \ldots M_{new}\} \tag{5.87}$$

which defines the output of the second step.

Step 3: Linear program

The input of the third step is a discrete set $\mathcal{S}$ of pure product states and the density operator. As discussed in section 5.3 by using this input the Max-Min criterion can be rewritten in the form of a linear program which can be solved with the help of the simplex algorithm. The results are the optimal observable $\hat{O}_{\max}$, a new set $\mathcal{S}_{new}$ of product states which is free from redundant information and the optimal value $\eta_{\max}$ of the Max-Min criterion. These results build the output of the third step.

Step 4: Exit conditions

There are two exit conditions for the algorithm.

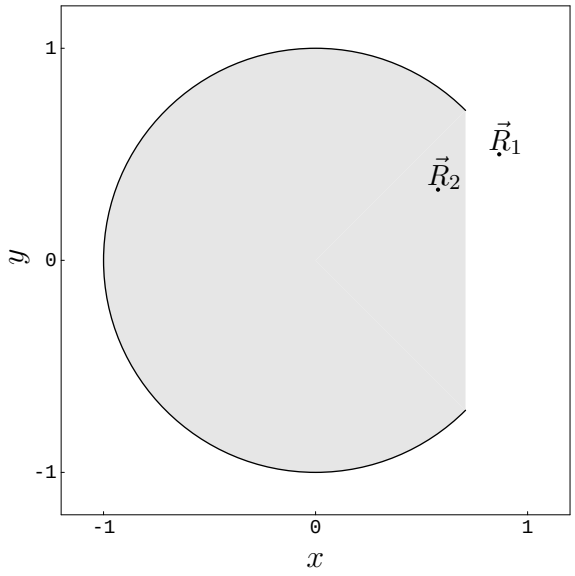
1. As discussed in subsection 5.1 the cost function $\eta_{\max}$ of the approximate Max-Min criterion can only be zero, Eq. (5.14), if the density operator is separable. Thus, in the case of vanishing $\eta_{\max}$ the algorithm exits with the answer that $\hat{\rho}$ is a separable state.

2. During the update of the discrete subset $\mathcal{S}_{new}$, in the second step of the algorithm, a new state has been calculated for each element of $\mathcal{S}_{new}$. If all of these new states are equal to the corresponding input states, the updated subset $\mathcal{S}$ is identical to the original subset $\mathcal{S}_{new}$ and the algorithm runs into an infinite loop. Therefore, if this is the case the algorithm exits.

If neither exit condition is fulfilled the algorithm proceeds with step two.

5.6 Graphical illustration of the algorithm

Before we discuss the properties of the algorithm described in the previous section we explain its concepts by studying an example for the case of a two dimensional vector space.



Setup

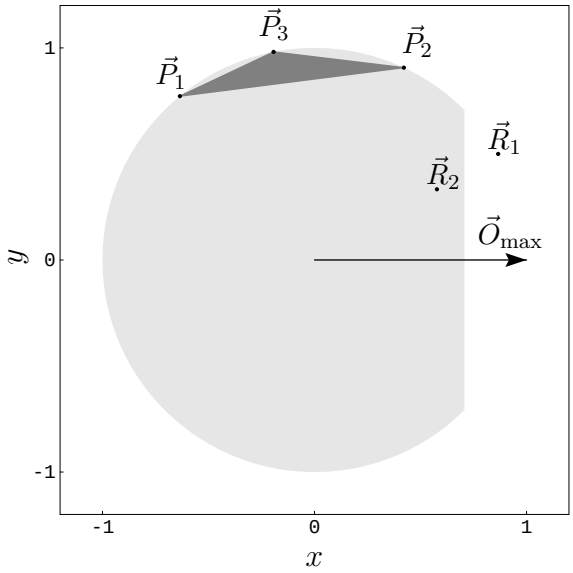
The gray region in this picture denotes the convex body $\mathcal{K}$ whose border (black line) is formed by the continuous set of vectors

$$\vec{P}(\varphi) \equiv (\cos\varphi, \sin\varphi), \quad \frac{1}{4}\pi \leq \varphi \leq \frac{7}{4}\pi. \tag{5.88}$$

The vector $\vec{R}_1 = \left(\frac{\sqrt{3}}{3}, \frac{1}{2}\right)$ describes a point that does not belong to $\mathcal{K}$ and the vector $\vec{R}_2 = \frac{2}{3}\vec{R}_1$ denotes a point that belongs to $\mathcal{K}$.
The problem is to find a vector $\vec{O}_{\max}$ which solves the optimization problem

$$\eta_{\max} = \max_{\vec{o}, \|\vec{o}\|_1 \leq 1} \left\{ \min_{\frac{1}{4}\pi \leq \varphi \leq \frac{7}{4}\pi} \left\{ \vec{O} \cdot \left(\vec{R}_1 - P\,\vec{(}\varphi) \right) \right\} \right\}$$

and to prove that $\vec{R}_2 \in \mathcal{K}$. One can solve this simple problem intuitively and would expect $\vec{O}_{\max} = (1, 0)$ to be the solution.



Initialization

In the two dimensional case it is impossible to use the SVD-criterion to construct the initialization vector $\vec{O}_{\max}$ and the initialization subset $\mathcal{A}_{new}$. Therefore we use a randomly chosen subset

$$\mathcal{A} = \{(-0.635, 0.773), (0.421, 0.907), (-0.193, 0.981)\}.$$

of three points to set up a linear program. In the picture the dark grey triangle represents the convex body formed by the elements of $\mathcal{A}$.
By using the simplex algorithm we can solve the linear program[a]. The results are the maximal value of the cost function

$$\eta_{\max} = 0.449$$

and the vector

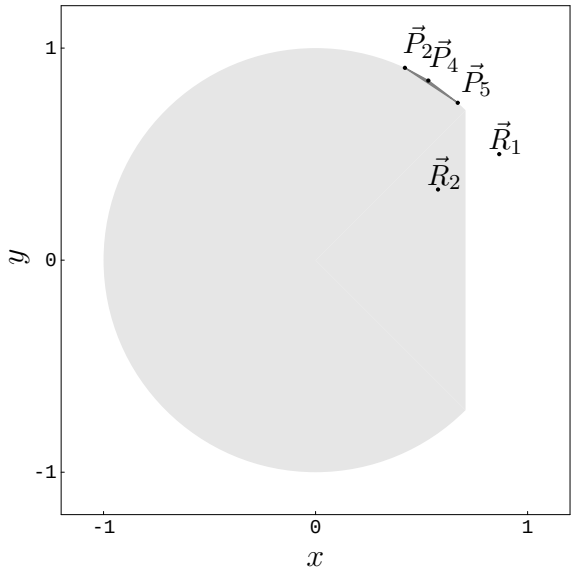
$$\vec{O}_{\max} = (1.000, 0.000).$$

Moreover, the simplex algorithm yields the new subset

$$\mathcal{A}_{new} = \left\{\vec{P}_2\right\} = \{(0.421, 0.907)\}$$

as an additional result and this subset is now free from redundant information. We use these results as output of the initialization step of the algorithm.

[a] Here and in the following examples we use the GNU Linear Programming Kit (GLPK) implementation of the simplex algorithm [61] for the numerical calculation. All numerical values are calculated with the precision 10^{-8}.



Subset update

In this step two new vectors

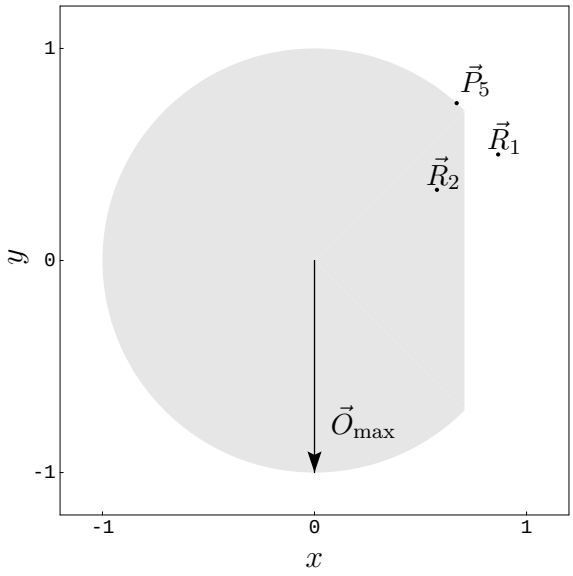
$$\vec{P}_4 = (0.532, 0.850) \text{ and } \vec{P}_5 = (0.670, 0.742)$$

have been found[a], which violate the inequality

$$\vec{O}_{\max} \cdot \vec{R} > \vec{O}_{\max} \cdot \vec{P}_n \tag{5.89}$$

where $\vec{O}_{\max}$ corresponds to the solution of the previous step of the algorithm. By adding these points to the subset $\mathcal{A}_{new}$ a new subset $\mathcal{A}$ is defined. In the picture the dark grey triangle represents the new subset.

[a] In a two dimensional example Eqs. (5.69), (5.71) and (5.77) cannot be used to find vectors, which violate the initial solution of the discrete version of optimization problem. Therefore, for this example a random search was used.



Linear program

By using the vectors $\vec{P}_n \in \mathcal{A}$ a new linear program was constructed and solved. In the picture above the vector

$$\vec{O}_{\max} = (0.000, -1.000)$$

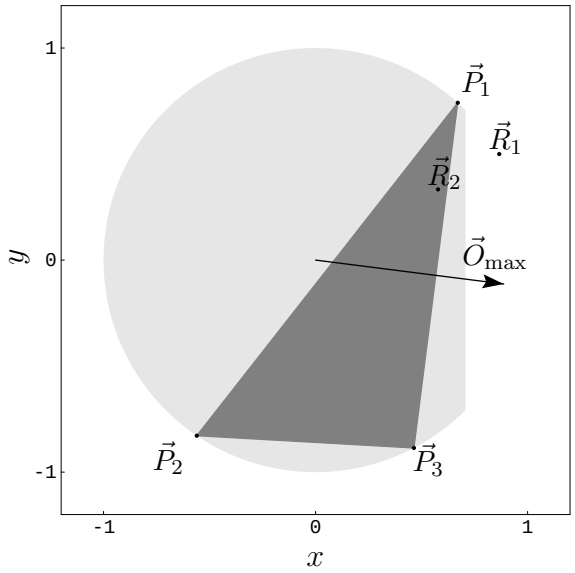
and the set

$$\mathcal{A}_{new} = \left\{\vec{P}_5\right\} = \{(0.670, 0.742)\}$$

correspond to this solution. At first sight it seems that this solution is worse than the one calculated in the initialization step. However, the central parameter of the algorithm is the value of the cost function

$$\eta_{\max} = 0.242.$$

Comparing this parameter with the previous one, we see that the approximation of the full optimization problem has been improved.
By using $\vec{O}_{\max}$ and $\mathcal{A}_{new}$ as input the algorithm proceeds with step two.



First exit condition

In the case of the vector $\vec{R}_2$ the algorithm exits after 5 iterations because the cost function $\eta_{\max}$ vanishes. This happens because $\vec{R}_2$ is an element of the convex body built by all possible convex superpositions of the elements of the subset

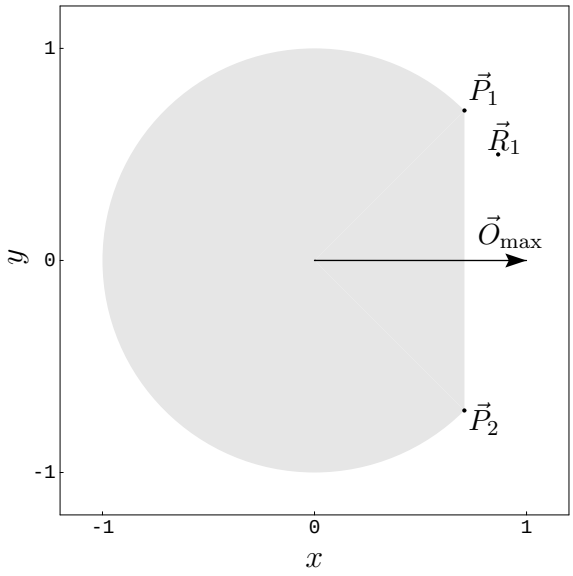
$$\mathcal{A}_{new} = \left\{\vec{P}_1, \vec{P}_2, \vec{P}_3\right\} = \{(0.670, 0.742), (-0.560, -0.828), (0.464, -0.886)\}$$

which is represented as the dark grey triangle in the picture above. Hence, $\vec{R}_2$ can be written as a convex sum of the elements of $\mathcal{A}_{new}$, which yields the wanted proof that $\vec{R}_2 \in \mathcal{K}$.
In the case of the vector $\vec{R}_1$ the cost function does not vanish and the results of the linear program are the vector

$$\vec{O}_{\max} = (0.887, -0.112)$$

and the new subset

$$\mathcal{A}_{new} = \left\{\vec{P}_1, \vec{P}_3\right\} = \{(0.670, 0.742), (0.464, -0.886)\}.$$



Second exit condition

After 15 iterations of steps two and three the algorithm exits because no additional vectors can be found which violate inequality (5.89). As intuitively expected the final vector

$$\vec{O}_{\max} = (1.000, 0.000)$$

is the result of the algorithm. The picture above visualizes this situation. The final set $\mathcal{A}_{new}$ consists of the two vectors

$$\vec{P}_1 = (0.707, 0.707) \approx \vec{P}\left(\frac{1}{4}\pi\right) \text{ and } \vec{P}_2 = (0.707, -0.708) \approx \vec{P}\left(\frac{7}{4}\pi\right),$$

which correspond to the borders of the interval, Eq. (5.88), that defines the continuous set $\vec{P}(\varphi)$.

5.7 Separable states

Now we investigate the meaning of the first exit condition of the algorithm presented in section 5.5, which occurs if the cost function $\eta_{\max}$ vanishes. This is only the case, Eq. (5.14), if the density operator $\hat{\rho}$ is separable. But due to the fact that the algorithm always acts on a discrete subset, Eq. (5.44),

$$\mathcal{S}_{new} = \{|a_n b_n\rangle\langle a_n b_n|,\, n = 1 \ldots M_{new}\} \tag{5.90}$$

of pure product states we have an additional information. Namely, the density operator is separable in elements of $\mathcal{S}_{new}$. In other words M_{new} non-negative numbers p_n exist such that

$$\hat{\rho} = \sum_{n=1}^{M_{new}} p_n |a_n b_n\rangle\langle a_n b_n|, \quad |a_n b_n\rangle \in \mathcal{S}_{new} \tag{5.91}$$

or in matrix form

$$\rho_{kl}^{uv} = \sum_{n=1}^{M_{new}} p_n \, a_{nk}^* \, a_{nl} \, b_{nu}^* \, b_{nv} \tag{5.92}$$

where a_{nl}, b_{nv} and ρ_{kl}^{uv} are the expansion coefficients of $|a_n\rangle$, $|b_n\rangle$ and $\hat{\rho}$ in arbitrary bases of Alice and Bob. The last relation defines a linear system of equations, which can be solved using the standard methods of linear algebra. Moreover, due to Eq. (5.46) the number M_{new} of elements of the discrete subset $\mathcal{S}_{new}$ is bounded by the square of the number of dimensions of the Hilbert space. Hence, all separable states can be decomposed[7] in a *finite* sum

$$\hat{\rho} = \sum_{n=1}^{(\dim \mathcal{H})^2} p_n |a_n b_n\rangle\langle a_n b_n| \tag{5.93}$$

over product states. The next example clarifies these results.

Example

Let $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$ be the entire Hilbert space of Alice and Bob with

$$\dim \mathcal{H}_A = \dim \mathcal{H}_B = 2 \tag{5.94}$$

[7] A different proof for this statement can be found in [57, 62]

n	p_n	α_n	γ_n	β_n	δ_n
1	$\frac{1}{16}$	0	1	1	0
2	$\frac{3}{16}$	0	1	0	1
3	$\frac{1}{16}$	1	0	0	1
4	$\frac{1}{8}$	$-\frac{1}{\sqrt{2}}$	$i\frac{1}{\sqrt{2}}$	$\frac{1}{\sqrt{2}}$	$i\frac{1}{\sqrt{2}}$
5	$\frac{1}{8}$	$\frac{1}{\sqrt{2}}$	$i\frac{1}{\sqrt{2}}$	$\frac{1}{\sqrt{2}}$	$-i\frac{1}{\sqrt{2}}$
6	$\frac{1}{8}$	$-\frac{1}{\sqrt{2}}$	$\frac{1}{\sqrt{2}}$	$-\frac{1}{\sqrt{2}}$	$\frac{1}{\sqrt{2}}$
7	$\frac{1}{8}$	$\frac{1}{\sqrt{2}}$	$\frac{1}{\sqrt{2}}$	$\frac{1}{\sqrt{2}}$	$\frac{1}{\sqrt{2}}$
8	$\frac{3}{16}$	1	0	1	0

Table 5.1:
By solving the linear system of equations, Eq. (5.92), we can find the explicit decomposition of the separable Werner state, Eq. (5.95), as a convex sum $\sum_{n=1}^{8} p_n|a_nb_n\rangle\langle a_nb_n|$, with $|a_n\rangle = \alpha_n|0\rangle + \gamma_n|1\rangle$ and $|b_n\rangle = \beta_n|0\rangle + \delta_n|1\rangle$. This table contains the values of p_n and the coefficients of the states $|a_nb_n\rangle$.

and let the density operator be

$$\hat{\rho}_W = \frac{1}{4}|\Psi_{\max}\rangle\langle\Psi_{\max}| + \frac{3}{16}\hat{\mathbb{1}} \tag{5.95}$$

where $|\Psi_{\max}\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$ denotes a maximally entangled state. As discussed in subsection 3.3, $\hat{\rho}_W$ is a separable Werner state and can be decomposed as a convex sum, Eq. (5.91). The task of this example is to find this decomposition.

To do this we apply the algorithm, described in section 5.5, with $\hat{\rho}$ as input. After one loop the algorithm exits with the answer that $\hat{\rho}$ is separable. Furthermore, we get the set $\mathcal{S}_{new}$ as an additional result. By setting up the linear system of equations, Eq. (5.92), and solving it we can find the explicit decomposition of the density operator

$$\hat{\rho} = \sum_{n=1}^{8} p_n|a_nb_n\rangle\langle a_nb_n|, \quad |a_nb_n\rangle \in \mathcal{S}_{new} \tag{5.96}$$

as a convex sum over pure product states. The numerical values of p_n and the coefficients of the states $|a_nb_n\rangle$ are listed in Table 5.1.

Hence the first exit condition $\eta_{\max} = 0$ of the algorithm does not only give the possibility to prove that the input density operator $\hat{\rho}$ is separable but allows one to calculate the components of the convex sum, Eq. (5.91), too.

5.8 Entangled states

If no additional product states can be found which violate the current discrete solution of the Max-Min criterion during the subset update the algorithm exits in order to avoid an infinite loop. This is equivalent, Eq. (5.81), to the *necessary* condition on $\langle a_n b_n|\hat{O}_{\max}|a_n b_n\rangle$ with $|a_n b_n\rangle \in \mathcal{S}_{new}$ to be the global maximum of the expectation value of the observable $\hat{O}_{\max}$ with respect to *all* pure product states. Moreover, according to numerical tests, which have been performed by using the optimization package of Mathematica 5.1, it seems that this condition is *sufficient*. Thus the second exit condition of the algorithm yields

$$\mathrm{Tr}\left\{\hat{O}_{\max}\hat{\rho}\right\} > \max_{|ab\rangle}\langle ab|\hat{O}_{\max}|ab\rangle = c_{\max} \tag{5.97}$$

with $|a\rangle \in \mathcal{H}_A$ and $|b\rangle \in \mathcal{H}_B$. This is the case, Eq. (3.64), if and only if $\hat{\rho}$ is an entangled state.

Hence, under the assumption that inequality (5.97) is valid, the second exit condition of the algorithm presented in section 5.5 is *necessary* and *sufficient* to detect entanglement of $\hat{\rho}$. As a consequence, the resulting operator $\hat{O}_{\max}$ is the optimal entanglement indicator.

This statement is strongly correlated to the quality of the numerical tests. In order to avoid this numerical uncertainty we will now discuss the question whether it is possible to estimate the upper bound for the maximal expectation value

$$c_{\max} = \max_{|ab\rangle}\langle ab|\hat{O}_{\max}|ab\rangle. \tag{5.98}$$

Let $\hat{O}$ be an arbitrary Hermitian operator with diagonal representation

$$\hat{O} = \sum_{n=1}^{K} o_n \hat{\sigma}_n^A \otimes \hat{\sigma}_n^B, \quad o_1 \geq o_2 \geq \ldots \geq o_K \tag{5.99}$$

where the set $\{o_n\}$ denotes the singular values of $\hat{O}$. It is shown in appendix A.4.4 that the operator $\hat{P}_{\max} \equiv \hat{\sigma}_1^A \otimes \hat{\sigma}_1^B$ maximizes the scalar product

$$\max_{\hat{P}} \mathrm{Tr}\left\{\hat{O}\hat{P}\right\} = o_1 \tag{5.100}$$

under the constraint that $\hat{P}$ is a Kronecker product of two Hermitian operators $\hat{A} \in \mathcal{H}_A$ and $\hat{B} \in \mathcal{H}_B$ with

$$\mathrm{Tr}\left\{\hat{A}^2\right\} = \mathrm{Tr}\left\{\hat{B}^2\right\} = 1. \tag{5.101}$$

The pure product states $|a\rangle\langle a| \otimes |b\rangle\langle b|$ satisfy this condition and therefore the maximal expectation value $c_{\max}$, Eq. (5.97), is bounded by the largest singular value of $\hat{O}$.

In the special case of inequality (5.97) this bound can be improved due to the fact, that adding the scaled identity operator to $\hat{O}_{\max}$

$$\mathrm{Tr}\left\{\left(\hat{O}_{\max} + \alpha\hat{\mathbb{1}}\right)\hat{\rho}\right\} > \max_{|ab\rangle}\langle ab|\left(\hat{O}_{\max} + \alpha\hat{\mathbb{1}}\right)|ab\rangle \tag{5.102}$$

with $|a\rangle \in \mathcal{H}_A$, $|b\rangle \in \mathcal{H}_B$ and $\alpha \in \mathbb{R}$ does not change the validity of the inequality. We use this fact to introduce the new operator

$$\hat{O}(\alpha) \equiv \hat{O}_{\max} + \alpha\hat{\mathbb{1}} = \sum_{k=1}^{K} o_n(\alpha)\,\hat{\sigma}_n^A(\alpha) \otimes \hat{\sigma}_n^B(\alpha) \tag{5.103}$$

and define the real-valued function

$$f(\alpha) \equiv o_1(\alpha) - \alpha. \tag{5.104}$$

where $o_1(\alpha)$ denotes the largest singular value of $\hat{O}(\alpha)$. Within this approach the best upper bound for $c_{\max}$ is given by the minimum of $f(\alpha)$

$$\min_{\alpha} f(\alpha) \geq c_{\max}. \tag{5.105}$$

If $\hat{\rho}$ satisfies the inequality

$$\mathrm{Tr}\left\{\hat{\rho}\hat{O}_{\max}\right\} > \min_{\alpha} f(\alpha) \tag{5.106}$$

the state is guaranteed to be entangled, because the combination of the last two inequalities

$$\mathrm{Tr}\left\{\hat{\rho}\hat{O}_{\max}\right\} > \min_{\alpha} f(\alpha) \geq c_{\max} \tag{5.107}$$

leads to the sufficient condition, Eq. (5.97). However, in the next example we show that there are inseparable density operators which violate this inequality, and hence no rigorous statement about the entanglement of these operators can be made. As a consequence we can say that the bound determined by the minimum of the function $f(\alpha)$ is not sharp.

Example

This example is based on a PPT entangled state, which is presented in [57]. Let $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$ be the entire Hilbert space of Alice and Bob with

$$\dim \mathcal{H}_A = 2 \quad \text{and} \quad \dim \mathcal{H}_B = 4 \tag{5.108}$$

and let the decomposition of the density operator in the bases $\{|a_n\rangle\}$ and $\{|b_n\rangle\}$ of $\mathcal{H}_A$ and $\mathcal{H}_B$ be

$$\hat{\rho} = \sum_{n,m=1}^{2} \sum_{k,l=1}^{4} \rho_{nm}^{kl} |a_n\rangle\langle a_m| \otimes |b_k\rangle\langle b_l| = \sum_{n,m=1}^{8} \rho_{nm} |\Psi_n\rangle\langle\Psi_m| \tag{5.109}$$

where the set

$$\{|\Psi_n\rangle,\, n = 1 \ldots 8\} = \{|a_n\rangle \otimes |b_m\rangle,\, n = 1, 2\,, m = 1, 2, 3\}\,. \tag{5.110}$$

denotes the basis of the entire Hilbert space and the density matrix is given by

$$(\rho_{nm}) = \frac{1}{18} \begin{pmatrix} 2 & 0 & 0 & 0 & 0 & 2 & 0 & 0 \\ 0 & 2 & 0 & 0 & 0 & 0 & 2 & 0 \\ 0 & 0 & 2 & 0 & 0 & 0 & 0 & 2 \\ 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 3 & 0 & 0 & \sqrt{3} \\ 2 & 0 & 0 & 0 & 0 & 2 & 0 & 0 \\ 0 & 2 & 0 & 0 & 0 & 0 & 2 & 0 \\ 0 & 0 & 2 & 0 & \sqrt{3} & 0 & 0 & 3 \end{pmatrix}. \tag{5.111}$$

The partial transpose of this state is positive. Moreover, the sum over the singular values of $\hat{\rho}$ is smaller than one with

$$\sum_{n=1}^{4} r_n = 0.8493 < 1. \tag{5.112}$$

Hence, the sufficient Peres-Horodecki and SVD criteria don't give a clear answer whether $\hat{\rho}$ is inseparable or not. Therefore we use the algorithm described in section 5.5 with $\hat{\rho}$ as input. It exits after 159 iterations because of the second exit condition. The final value of the cost function

$$\eta_{\max} = 1.779 \times 10^{-3} > 0 \tag{5.113}$$

is larger than zero. Additional results of the algorithm are the optimal entanglement indicator $\hat{O}_{\max}$ and the maximal overlap

$$c_{\max} = 78.630 \times 10^{-3} = \langle a_n b_n | \hat{O}_{\max} | a_n b_n \rangle, \ |a_n b_n\rangle \in \mathcal{S}_{new} \tag{5.114}$$

between this observable and elements of the final discrete subset $\mathcal{S}_{new}$. By using the optimization package of Mathematica 5.1 we can confirm that $c_{\max}$ is the *absolute* maximum of the expectation value of $\hat{O}_{\max}$ with respect to all pure product states.

Hence, under the assumption that $c_{\max}$ is this absolute maximum

$$c_{\max} = \max_{|ab\rangle} \langle ab | \hat{O}_{\max} | ab \rangle, \quad |a\rangle \in \mathcal{H}_A, \, |b\rangle \in \mathcal{H}_B \tag{5.115}$$

the density operator $\hat{\rho}$, Eq. (5.109), is inseparable.

This statement is strongly correlated to the quality of the numerical methods, which have been used. Therefore, in the next step we discuss the possibility to avoid the numerical uncertainty and estimate the upper bound of the maximal expectation value $c_{\max}$ by using the relation (5.105). This bound is given by the minimal value of the function

$$f(\alpha) = o_1(\alpha) - \alpha \tag{5.116}$$

where $o_1(\alpha)$ denotes the maximal singular value of the operator

$$\hat{O}(\alpha) = \hat{O}_{\max} + \alpha \hat{\mathbb{1}}. \tag{5.117}$$

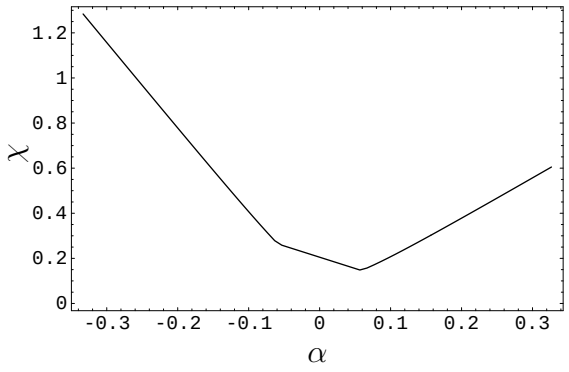


Figure 5.2:
This plot shows the behavior of the function $f(\alpha)$, Eq. (5.104), which corresponds to the PPT entangled state $\hat{\rho}$, Eq. (5.109), close to its minimum. This function does not go below $\mathrm{Tr}\left\{\hat{\rho}\hat{O}_{\max}\right\} = 80.409 \times 10^{-3}$ and therefore does not provide a strict proof for $\hat{\rho}$ to be inseparable.

Fig. 5.2 shows the behavior of $f(\alpha)$ close to its minimum

$$\min_{\alpha} f(\alpha) = 148.40 \times 10^{-3}. \tag{5.118}$$

By comparing this bound to the expectation value of $\hat{O}_{\max}$ with respect to the density operator

$$80.409 \times 10^{-3} = \mathrm{Tr}\left\{\hat{\rho}\hat{O}_{\max}\right\} < \min_{\alpha} f(\alpha) \tag{5.119}$$

we see that the estimated upper bound of $c_{\max}$ does not allow a rigorous statement about the entanglement of $\hat{\rho}$. On the other hand we know that $\hat{\rho}$ is inseparable, as shown in [57]. Hence, by using the PPT entangled state, Eq. (5.111), we have shown that the bound which is determined by the minimum of the function $f(\alpha)$ is not sharp.

5.9 How large can the dimension of the Hilbert space be?

In section 5.5 we presented an algorithm which converges to an optimal entanglement indicator $\hat{O}_{\max}$ under the assumption that the maximal expectation value of $\hat{O}_{\max}$ with respect to pure product states can be found. But, what is the maximal dimension of the Hilbert space in which this algorithm can reasonably be implemented with the capacity of modern computers?

The main part of the algorithm consists of two iterative steps: the subset update and the linear program. The subset update is based on the diagonalization of the observables $\hat{A} \in \mathcal{H}_A$, Eq. (5.70), and $\hat{B} \in \mathcal{H}_B$, Eq. (5.67), and on the Schmidt decomposition of a state $|\Psi\rangle \in \mathcal{H}$, Eq. (5.73). These calculations only depend linearly on the number of dimensions of the Hilbert spaces of Alice and Bob. By contrast, the linear program step consists of $2N^2 = 2\left(\dim \mathcal{H}\right)^2$ variables, Eq. (5.39), and $M = 2N^2$ constraints, Eq. (5.21) and depends quadratically on N. It is the most time-consuming part of the algorithm and therefore we concentrate our analysis on this part.

In [63] it is demonstrated that linear programs consisting of a constraint matrix $\mathbf{D}$, Eq. (5.39), with 5034171 rows and 7365337 columns are reasonably solvable with modern computers. By using these numbers we can estimate the maximal number of the dimensions of the entire Hilbert space as

$$2N^2 \approx 2 \times 10^6 \Rightarrow N = \dim \mathcal{H} \approx 1000. \tag{5.120}$$

Hence, the algorithm, described in section 5.5, is an interesting tool for the analysis of entanglement of the density operators in Hilbert spaces with up to $N = 1000$ dimensions.

5.10 Summary

- Under the assumption, which is confirmed by numerical tests, that the global maximum of the expectation value of a Hermitian operator with respect to pure product states can be found, the algorithm presented in section 5.5 converges, in the case of entangled density operators, to an optimal entanglement indicator $\hat{O}_{\max}$. In the case of separable states, it exits because the cost function $\eta_{\max}$ vanishes. Moreover, by using the final discrete subset $\mathcal{S}_{new} = \{|a_n b_n\rangle\}$ the coefficients p_n of the convex sum

$$\hat{\rho} = \sum_{n=1}^{(\dim \mathcal{H})^2} p_n |a_n b_n\rangle\langle a_n b_n| \tag{5.121}$$

  can be found. Hence, this algorithm results in a *necessary* and *sufficient* inseparability criterion and solves the problem of the present work, namely the problem of separability [42].

- Without the assumption above a non sharp bound determined by the minimum of the function $f(\alpha)$, Eq. (5.104), for the maximal expectation value

$$c_{\max} = \max_{|ab\rangle} \langle ab|\hat{O}_{\max}|ab\rangle, \quad |a\rangle \in \mathcal{H}_A,\ |b\rangle \in \mathcal{H}_B \tag{5.122}$$

  can be estimated. By using this bound three cases can be distinguished:

  1. The final cost function $\eta_{\max}$ is zero. This result indicates a separable state $\hat{\rho}$.
  2. The expectation value $\mathrm{Tr}\left\{\hat{\rho}\hat{O}_{\max}\right\}$ is larger than the bound $\min_\alpha f(\alpha)$. This yields an inseparable density operator $\hat{\rho}$.
  3. For other outputs of the algorithm no predictions about the entanglement can be made.

- The algorithm , described in section 5.5, can reasonably be implemented on modern computers and can solve the separability problem in Hilbert spaces with up to $\dim(\mathcal{H}_A \otimes \mathcal{H}_B) = 1000$ dimensions.

- By using the results described in subsection 2.2.4 we can easily transform an entanglement indicator in a witness operator. Thus, the algorithm presented

in section 5.5 also solves the problem of finding the optimal witness operator for a given inseparable density operator.

- The current limitation of the algorithm based on the Max-Min criterion is the fact, that we could not find a rigorous proof that the iterative method used in the subset update, section 5.4, converges to the *absolute* maximum of the expectation value of $\hat{O}_{\max}$ with respect to pure product states. Hence, if in addition to the numerical tests, which have converged to the same results in all cases that we have studied, one could also work out the optimization problem

$$c_{\max} = \max_{|ab\rangle} \langle ab|\hat{O}_{\max}|ab\rangle, \quad |a\rangle \in \mathcal{H}_A,\, |b\rangle \in \mathcal{H}_B \tag{5.123}$$

analytically the separability problem would strictly be solved.

6 Multipartite entanglement

> We don't receive wisdom, we must discover it for ourselves after a journey that no one can take for us or spare us.
>
> Marcel Proust

So far we have demonstrated that the geometrical interpretation of entanglement is a powerful tool for the characterization of entanglement in bipartite quantum system. In the present chapter we will analyze whether it is possible to utilize the existing statements in multipartite quantum systems. It turns out that apart from only few exceptions, on which we will in particular focus our attention, all proofs in the previous chapters have a one-to-one correspondence in the multipartite case.

6.1 Definitions and notation

In the following we consider a finite number of quantum systems which are labeled by capital letters $A, B, C, \ldots$. Each system has a finite Hilbert space $\mathcal{H}_A, \mathcal{H}_B, \mathcal{H}_B \ldots$ which are arranged such that

$$N_A \leq N_B \leq N_C \leq \ldots \tag{6.1}$$

where $N_n = \dim \mathcal{H}_n$ denotes the dimensionality of the corresponding Hilbert space $\mathcal{H}_n$. The direct product of these Hilbert spaces

$$\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_C \otimes \ldots, \quad N = \dim \mathcal{H} = N_A N_B N_C \ldots. \tag{6.2}$$

forms the entire Hilbert space. We use normal letters to denote the pure quantum states in the local systems and capital letters to represent the quantum states of

the entire Hilbert space. The bases of the Hilbert spaces are arbitrary but fixed and all bases changes will explicitly be noted. In the product state representation

$$|\Psi\rangle = |abc\ldots\rangle \tag{6.3}$$

we again omit the tensor product sign. The operators which act on the Hilbert space are denoted by the hat symbol. In order to describe mixed quantum states we introduce the density operators which can be spectrally decomposed as

$$\hat{\rho} = \sum_{n=1}^{N} \rho_n |\Psi_n\rangle\langle\Psi_n| \tag{6.4}$$

where $|\Psi_n\rangle$ denotes an eigenvector with the non-negative eigenvalue ρ_n. Furthermore, the trace over $\hat{\rho}$ is normalized to one.

According to the definition of bipartite separable states, Eq. (2.14), we say that all multipartite density operators which can be written as a convex sum

$$\hat{\rho}_{sep} \equiv \sum_{n=1}^{\infty} p_n |a_n b_n c_n \ldots\rangle\langle a_n b_n c_n \ldots| \tag{6.5}$$

with non-negative coefficients p_n and arbitrary but normalized product states $|a_n b_n c_n \ldots\rangle \in \mathcal{H}$ are separable. Conversely, the entangled density operators cannot be decomposed in this form. The physical interpretation, that separable states can be prepared by using local operations and classical communication, is also valid in the multipartite case. Our aim is again to find an applicable criterion to determine whether a given density operator $\hat{\rho}$ is separable or not.

6.2 Geometrical interpretation of entanglement

In this section we demonstrate that in multipartite systems the bounds of the expectation values of Hermitian operators with respect to separable density operators differ from the inseparable ones. Furthermore, we show that it is possible to construct a necessary and sufficient inseparability criterion by using the geometrical Hilbert-Schmidt representation of Hermitian operators.

6.2.1 Bounds of expectation values

We have seen in section 3.1 that in bipartite systems the expectation values $\left\langle \hat{O} \right\rangle_{\hat{\rho}_{sep}}$ of a Hermitian operator

$$\hat{O} = \sum_{n=1}^{N} \lambda_n |O_n\rangle\langle O_n| \,, \quad \lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_N \tag{6.6}$$

with respect to separable density operators $\hat{\rho}_{sep}$ are located in the interval $[c_{\min}, c_{\max}]$, where the bounds $c_{\min}$ and $c_{\max}$ are given by the minimal and maximal expectation value of $\hat{O}$ with respect to pure product states. To prove this we mainly used the positivity of the coefficients p_n in the definition of the separable density operators, Eq. (2.14). In the case of multipartite systems the separable states are also defined as a convex sum, Eq. (6.5), over pure product states with non-negative coefficients p_n and therefore this result is valid in these systems, too. That is the upper bound of $\left\langle \hat{O} \right\rangle_{\hat{\rho}_{sep}}$ is given by

$$\left\langle \hat{O} \right\rangle_{\hat{\rho}_{sep}} \leq c_{\max} \equiv \max_{|abc\ldots\rangle} \langle abc\ldots|\hat{O}|abc\ldots\rangle \;\; |a\rangle \in \mathcal{H}_A,\, |b\rangle \in \mathcal{H}_B, \ldots . \tag{6.7}$$

Similarly, the lower bound is given by

$$\left\langle \hat{O} \right\rangle_{\hat{\rho}_{sep}} \geq c_{\min} \equiv \min_{|abc\ldots\rangle} \langle abc\ldots|\hat{O}|abc\ldots\rangle \;\; |a\rangle \in \mathcal{H}_A,\, |b\rangle \in \mathcal{H}_B, \ldots . \tag{6.8}$$

The expectation values of $\hat{O}$ with respect to arbitrary density operators are bounded by its largest eigenvalue λ_1 and smallest eigenvalue λ_N, as shown in appendix A.1. This result does not depend on the number of composed systems and hence we can generalize the statement given in section 3.1 to the multipartite situation:

> If the eigenstates $|O_1\rangle$ and $|O_N\rangle$ of a Hermitian operator $\hat{O}$ are inseparable and the corresponding largest and smallest eigenvalue λ_1 and λ_N are not degenerate, the expectation values of a Hermitian operator $\hat{O}$ with respect to separable states are confined by the inequalities
>
> $$\lambda_1 > c_{\max} \geq c_{\min} > \lambda_N \tag{6.9}$$
>
> and cover a smaller interval than arbitrary, in particular entangled

states. Thus, if the expectation value of $\hat{O}$ with respect to an unknown density operator $\hat{\rho}$ is not located in the interval $[c_{\min}, c_{\max}]$, $\hat{\rho}$ must be entangled.

6.2.2 Geometrical interpretation of entanglement

In subsection 3.2.2 we have demonstrated that in bipartite systems there exists at least one entanglement indicator $\hat{O}_{\mathcal{E}}$ which can detect the entanglement of a given inseparable density operator $\hat{\rho}$. To prove this result we mainly used the following four properties:

1. Hermitian operators acting on a N dimensional Hilbert space $\mathcal{H}$ constitute an Euclidian N^2-dimensional real Hilbert-Schmidt vector space $V_{HS} = \mathbb{R}^{N^2}$.
2. The dimensionality of V_{HS} is finite.
3. All separable states can be decomposed in a convex sum over pure product states and therefore form a convex set $\mathcal{J}$. In the Hilbert-Schmidt vector space this means that the associated vectors $\vec{R}_{sep}$ of the separable density operators form a convex set $\mathcal{K}$ in V_{HS}.
4. An entangled state $\hat{\rho}_{ent}$ cannot be decomposed in a convex sum over pure product states and consequently the associated Hilbert-Schmidt vector $\vec{R}_{ent}$ of $\hat{\rho}_{ent}$ cannot be contained in $\mathcal{K}$. Since $\vec{R}_{ent}$ and $\mathcal{K}$ are two disjunct convex sets, a hyperplane $\mathcal{E}$ exists which divides the vector space V_{HS} in two half spaces so that $\vec{R}_{ent}$ and $\mathcal{K}$ are in different half spaces.

One can easily see that all these properties are valid in multipartite systems. Hence the central statement of subsection 3.2.2 – the necessary and sufficient inseparability criterion – is valid, too. That is:

An unknown density operator $\hat{\rho}$ is inseparable if and only if at least one entanglement indicator $\hat{O}_{\mathcal{E}}$ exists such that

$$\mathrm{Tr}\left\{\hat{O}_{\mathcal{E}}\hat{\rho}\right\} > c_{\max}, \tag{6.10}$$

where the constant $c_{\max}$ is defined by equation (6.7).

6.2.3 Non-locality

In section 3.3 we have seen that in the case of bipartite systems it is always possible to decompose any Hermitian operator $\hat{O}$ which acts on the entire Hilbert space $\mathcal{H}$ as a sum over local Hermitian operators which act on the individual Hilbert subspaces. By using this decomposition we have demonstrated that all entangled states can be detected by local observations and classical communication only. To prove this result we mainly used the fact that the basis of the entire Hilbert-Schmidt vector space is a direct product of the bases of the associated Hilbert Schmidt vector spaces of Alice and Bob. This statement can be extended to the multipartite systems by considering the sets

$$\Omega_A = \left\{\hat{\sigma}_n^A,\, n \in 1 \ldots N_A^2\right\} \tag{6.11}$$
$$\Omega_B = \left\{\hat{\sigma}_m^B,\, m \in 1 \ldots N_B^2\right\} \tag{6.12}$$
$$\Omega_C = \left\{\hat{\sigma}_p^C,\, p \in 1 \ldots N_C^2\right\} \tag{6.13}$$
$$\vdots$$

to be the orthonormal bases of the associated Hilbert-Schmidt vector spaces of the systems $A, B, C \ldots$. Then due to their completeness the direct product

$$\Omega = \Omega_A \otimes \Omega_B \otimes \Omega_C \otimes \ldots \tag{6.14}$$

builds an orthonormal basis of the entire Hilbert-Schmidt vector space. Therefore all Hermitian operators and in particular all entanglement indicators $\hat{O}_\mathcal{E}$ which act on the entire Hilbert space $\mathcal{H}$ can be written as

$$\hat{O}_\mathcal{E} = \sum_{n=1}^{N_A^2} \sum_{m=1}^{N_B^2} \sum_{p=1}^{N_C^2} \sum_{\ldots} o_{nmp\ldots} \hat{\sigma}_n^A \otimes \hat{\sigma}_m^B \otimes \hat{\sigma}_p^C \otimes \ldots . \tag{6.15}$$

Due to the fact that $\hat{\sigma}$-operators act locally on the individual Hilbert spaces, this decomposition yields a prescription how to observe expectation values of entanglement indicators and hence how to detect entanglement by local observations and classical communication only.

Furthermore, we have seen in section 3.3 that with the help of the singular value decomposition in the case of the bipartite systems all Hermitian operators have a

diagonal representation of the form

$$\hat{O} = \sum_{n=1}^{N_A^2} o_n \hat{\tilde{\sigma}}_n^A \otimes \hat{\tilde{\sigma}}_n^B, \tag{6.16}$$

where $\{o_n\}$ denote the uniquely determined singular values of $\hat{O}$ and the $\hat{\tilde{\sigma}}$-operators are orthonormal. Unfortunately, the singular value decomposition cannot be generalized to multipartite systems, as shown in [54]. Hence, there is no one-to-one correspondence of the diagonal representation in multipartite systems. However, we can still use the singular value decomposition to reduce the number of summands in the sum, Eq. (6.15).

In order to show how this works, we study the example of a quantum system which consists of three subsystems A, B and C. Let $\hat{O}$ denote a Hermitian operator which acts on the entire Hilbert space

$$\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_C. \tag{6.17}$$

In order to find the diagonal representation we combine the subsystems B and C and introduce a new system B' which has the Hilbert space

$$\mathcal{H}_{B'} \equiv \mathcal{H}_B \otimes \mathcal{H}_C. \tag{6.18}$$

As a consequence, $\hat{O}$ now acts on a bipartite Hilbert space of A and B' and as discussed in subsection 3.3 we can find an orthonormal set

$$\tilde{\Omega}_A = \left\{ \hat{\tilde{\sigma}}_n^A,\, n \in 1 \ldots N_A^2 \right\} \tag{6.19}$$

of operators which act on $\mathcal{H}_A$ and an orthonormal set

$$\tilde{\Omega}_{B'} = \left\{ \hat{\tilde{\sigma}}_n^{B'},\, n \in 1 \ldots N_{B'}^2 \right\}$$

of operators which act on $\mathcal{H}_{B'}$ such that the Hermitian operator has diagonal representation

$$\hat{O} = \sum_{n=1}^{N_A^2} o_n \hat{\tilde{\sigma}}_n^A \otimes \hat{\tilde{\sigma}}_n^{B'} \tag{6.20}$$

with non-negative coefficients $\{o_n\}$. In the next step we use the fact that each of

the $\left\{\hat{\tilde{\sigma}}_n^{B'}\right\}$ operators acts on a bipartite Hilbert space as well and therefore can also be written in a diagonal form. This leads to the final decomposition of $\hat{O}$, which is given by

$$\hat{O} = \sum_{n=1}^{N_A^2} o_n \hat{\tilde{\sigma}}_n^A \otimes \left(\sum_{m=1}^{N_B^2} s_{nm} \hat{\overline{\sigma}}_{nm}^B \otimes \hat{\overline{\sigma}}_{nm}^C \right) = \sum_{n=1}^{N_A^2} \sum_{m=1}^{N_B^2} o_n s_{nm} \hat{\tilde{\sigma}}_n^A \otimes \hat{\overline{\sigma}}_{nm}^B \otimes \hat{\overline{\sigma}}_{nm}^C, \quad (6.21)$$

where $\{s_{nm}\}$ are the non-negative singular values of the $\left\{\hat{\tilde{\sigma}}_n^{B'}\right\}$ operators. Thus, this decomposition has not more than $N_A^2 N_B^2$ summands. By contrast, the representation of $\hat{O}$ in arbitrary bases, Eq. (6.15) , can have $N_A^2 N_B^2 N_C^2$ summands. Hence, in the tripartite case all global Hermitian operators can be decomposed as a sum over local Hermitian operators with not more than $N_A^2 N_B^2$ summands.

Finally we discuss the question whether it is always possible to detect entanglement in an experiment. In the case of bipartite systems we could positively answer this question under the assumption that Alice and Bob have experimental setups which correspond to complete sets

$$\mathcal{M}_A = \left\{\hat{A}_n,\, n \in 1 \ldots N_A^2\right\} \quad \text{and} \quad \mathcal{M}_B = \left\{\hat{B}_m,\, m \in 1 \ldots N_B^2\right\} \quad (6.22)$$

of observables, as shown in section 3.3. The completeness of $\mathcal{M}_A$ and $\mathcal{M}_B$ is defined in the associated Hilbert-Schmidt vector spaces, that is, the sets of the associated Hilbert-Schmidt vectors $\left\{\vec{A}_n\right\}$ and $\left\{\vec{B}_m\right\}$ of $\left\{\hat{A}_n\right\}$ and $\left\{\hat{B}_m\right\}$ have to be linearly independent. In this case the direct product of both sets

$$\mathcal{M} \equiv \mathcal{M}_A \otimes \mathcal{M}_B = \left\{\hat{A}_n \otimes \hat{B}_m,\, n \in 1 \ldots N_A^2,\, m \in 1 \ldots N_B^2\right\} \quad (6.23)$$

forms a valid complete but probably not orthonormal basis of the Hilbert-Schmidt vector space corresponding to the entire Hilbert space $\mathcal{H}$. As a consequence, all Hermitian operators and in particular all entanglement indicators which act on $\mathcal{H}$ can be decomposed in this basis. One can easily see that this result can be expanded to multipartite systems under the assumption that it is possible to perform measurements in each of the individual subsystems, which corresponds to a complete set of linear independent observables. Hence, we can perform an experiment, which detects entanglement of a given quantum state only by performing local measurements and by using classical communication.

6.3 SVD-criterion

In chapter 4 we have demonstrated that with the help of the diagonal representation of a density operator, Eq. (4.15), we can construct the SVD-operator, Eq. (4.16), for which the expectation value with respect to separable states is bounded by one. By contrast, its expectation value with respect to arbitrary and in particular entangled density operators is bounded by N_A, which is the minimum over the dimensions of the Hilbert spaces of Alice and Bob. On the other hand we have seen in the previous section that the diagonal representation of an operator, which is mainly based on singular value decomposition, cannot be generalized to multipartite systems. As a consequence, there is no one-to-one correspondence of the SVD-operator in these systems. However we can still use the singular value decomposition to construct Hermitian operators for which the expectation value for separable states is smaller than for entangled states.

As an example we show this for a quantum system which consists of three subsystems A, B and C. Let $\hat{\rho}$ denote a density operator which acts on the entire Hilbert space

$$\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_C. \tag{6.24}$$

Following the arguments in subsection 6.2.3 we can find bases of the associated Hilbert-Schmidt vector spaces of A, B and C such that

$$\hat{\rho} = \sum_{n=1}^{N_A^2} \sum_{m=1}^{N_B^2} r_n s_{nm} \hat{\sigma}_n^A \otimes \hat{\sigma}_{nm}^B \otimes \hat{\sigma}_{nm}^C, \tag{6.25}$$

where r_n and s_{nm} are positive and the $\hat{\sigma}$-operators fulfill the orthonormality relations

$$\mathrm{Tr}\left\{\hat{\sigma}_n^A \hat{\sigma}_m^A\right\} = \delta_{nm} \quad \text{and} \quad \mathrm{Tr}\left\{\hat{\sigma}_{np}^{B,C} \hat{\sigma}_{nq}^{B,C}\right\} = \delta_{qp} \ \ \forall n. \tag{6.26}$$

By using this representation we define the generalized SVD-operator as

$$\hat{O}_{SVD} \equiv \sum_{n=1}^{N_A^2} \hat{\sigma}_n^A \otimes \hat{\sigma}_{nm_{\max}}^B \otimes \hat{\sigma}_{nm_{\max}}^C. \tag{6.27}$$

In order to maximize the overlap between $\hat{\rho}$ and $\hat{O}_{SVD}$ we use the $\hat{\sigma}$-operators in systems B and C in this definition which correspond to the maximal value of the

coefficients s_{nm} with

$$s_{nm_{\max}} = \max_m s_{nm} \,. \tag{6.28}$$

We introduce $\hat{O}_{SVD}$ because its expectation value with respect to separable states is bounded by one and because its expectation value with respect to arbitrary states can exceed one. The proof of this statement is similar to the proof presented in chapter 4. We can again use the fact, that all projectors $|a\rangle\langle a|$, $|b\rangle\langle b|$ and $|c\rangle\langle c|$ can be represented by linear combinations

$$|a\rangle\langle a| = \sum_{n=1}^{N_A^2} a_n \hat{\sigma}_n^A, \;\; |b\rangle\langle b| = \sum_{n=1}^{N_B^2} b_{nm_{\max}} \hat{\sigma}_n^B \quad \text{and} \quad |c\rangle\langle c| = \sum_{n=1}^{N_C^2} c_n \hat{\sigma}^C_{nm_{\max}}. \tag{6.29}$$

The scalar product between the SVD-operator and these projectors yields

$$\begin{aligned} \mathrm{Tr}\left\{\hat{O}_D |abc\rangle\langle abc|\right\} &= \sum_{k=1}^{K} a_k b_{kp_{\max}} c_{kp_{\max}} \\ &\leq \sqrt{\sum_{n=1}^{N_A^2} a_n^2 \sum_{p=1}^{N_A^2} b^2_{pm_{\max}} c^2_{pm_{\max}}} \leq \sqrt{\sum_{n=1}^{N_A^2} a_n^2 \sum_{p=1}^{N_B^2} b^2_{pm_{\max}} \sum_{q=1}^{N_C^2} c^2_{qm_{\max}}} = 1 \end{aligned} \tag{6.30}$$

where the orthonormality of the $\hat{\sigma}$-operators and the Schwarz inequality was used. Furthermore, in the last step we used the fact that the sum over the squares of the coefficients $\{a_n\}$, $\{b_n\}$ and $\{c_n\}$ is equal to the trace over the squared projectors. Hence the expectation value of $\hat{O}_{SVD}$ with respect to separable states is bounded by one.

By contrast, in the case of arbitrary density operators $\hat{\rho}$, which have to fulfill the necessary condition

$$\mathrm{Tr}\left\{\hat{\rho}^2\right\} \leq 1 \tag{6.31}$$

or by using Eq. (6.25) the necessary condition

$$\mathrm{Tr}\left\{\hat{\rho}^2\right\} = \sum_{n=1}^{N_A^2} \sum_{m=1}^{N_B^2} r_n^2 s_{nm}^2 \leq 1, \tag{6.32}$$

the expectation value

$$\mathrm{Tr}\left\{\hat{\rho}\hat{O}_{SVD}\right\} = \sum_{n=1}^{N_A^2} r_n s_{nm_{\max}} \tag{6.33}$$

is bounded by N_A, i.e. the minimum over the dimensions of the individual Hilbert spaces. This bound can be reached by equally distributed coefficients with

$$r_n s_{nm_{\max}} = \frac{1}{N_A} \tag{6.34}$$

and

$$s_{nm} = 0 \quad \text{for } m \neq m_{\max}. \tag{6.35}$$

Using these results we are now in the position to formulate a sufficient inseparability criterion in the case of multipartite systems which is a generalization of the SVD-criterion for bipartite systems:

> If the sum over the coefficients $r_n s_{nm_{\max}}$, which are defined in Eqs. (6.25) and (6.28), of a density operator $\hat{\rho}$ exceeds one, the inequality (6.10) is valid and yields a sufficient criterion for $\hat{\rho}$ being entangled.

6.4 Max-Min criterion

In chapter 5 we have demonstrated that in the case of bipartite systems a density operator $\hat{\rho}$ is inseparable if and only if the solution of the optimization problem, which we call the Max-Min criterion, is positive. For the derivation of this statement we mainly used the necessary and sufficient inseparability criterion based on the existence of an entanglement indicator, as described in subsection 3.2.2. In subsection 6.2.2 we have seen that this criterion can be generalized to the multipartite case and hence we can generalize the Max-Min criterion.

> A density operator $\hat{\rho}$ is inseparable if and only if the solution of the Max-Min criterion
>
> $$\eta_{\max} = \sup_{\{\hat{O}, \|\hat{O}\| \leq 1\}} \left(\min_{|abc\ldots\rangle} \left(\mathrm{Tr} \left\{ \hat{O} \left(\hat{\rho} - |abc\ldots\rangle\langle abc\ldots| \right) \right\} \right) \right) \tag{6.36}$$
>
> is positive, with $|a\rangle \in \mathcal{H}_A$, $|b\rangle \in \mathcal{H}_B \ldots$. In the case of a separable density operator this problem yields
>
> $$\eta_{\max} = 0. \tag{6.37}$$

In order to solve the Max-Min criterion we have shown in section 5.3 that by introducing a discrete subset of pure product states it is possible to rewrite the optimization problem in the form of a linear program which can be solved by adopting the methods of operations research. In all proofs of this statement we did not use the fact that the entire Hilbert space is only composed of two Hilbert spaces. Thus, all results in section 5.3 which we obtained for the bipartite case are valid in the multipartite case, too. As a result, we can say that:

By introducing a discrete subset of M pure product states

$$\mathcal{S} = \{|a_n b_n c_n \ldots\rangle\langle a_n b_n c_n \ldots|,\, n = 1 \ldots M\} \tag{6.38}$$

we can rewrite the Max-Min criterion in the form of a linear program which provides a discrete solution to the continuous optimization problem. By using the simplex method we can solve this linear program in a very efficient way and obtain the optimal observable $\hat{O}_{\max}$, which maximizes the cost function

$$\eta_{\max} = \max_{\left\{\hat{O}, \left\|\hat{O}\right\|_1 \leq 1\right\}} \left(\min_{|a_n b_n c_n \ldots\rangle \in \mathcal{S}} \left(\mathrm{Tr}\left\{ \hat{O} \left(\hat{\rho} - |a_n b_n c_n \ldots\rangle\langle a_n b_n c_n \ldots| \right) \right\} \right) \right). \tag{6.39}$$

Here $\left\|\hat{O}\right\|_1$ denotes the l_1-norm of the associated Hilbert-Schmidt vector of the operator $\hat{O}$. Moreover, the simplex method filters out the redundant constraints of the problem which yields a new subset of pure product states

$$\mathcal{S}_{new} = \{|a_n b_n c_n \ldots\rangle\langle a_n b_n c_n \ldots|,\, n = 1 \ldots M_{new}\} \tag{6.40}$$

with

$$M_{new} \leq \min\left\{M, (\dim \mathcal{H})^2\right\}. \tag{6.41}$$

Due to the discreteness of the set $\mathcal{S}$ the solution provided by the linear program is only an *approximation* of the full optimization problem. Therefore, in order to determine the accuracy of this discrete solution we presented, in section 5.4, two methods how to find pure product states which have larger overlap with $\hat{O}_{\max}$ than the elements of the set $\mathcal{S}$. The first method is mainly based on the Schmidt decomposition of an inseparable state, Eq. (5.73), which is determined by the singular

value decomposition, as shown in appendix A.5.2. Due to the fact, that the singular value decomposition does not exist in the multipartite case, we cannot use this method. By contrast, the second method presented in section 5.4 is based on the fact that the eigenstate $|\alpha_1\rangle$ of an Hermitian operator $\hat{A}$ which corresponds to the largest eigenvalue maximizes the expression

$$\langle\alpha_1|\hat{A}|\alpha_1\rangle = \max_{|\alpha\rangle}\langle\alpha|\hat{A}|\alpha\rangle \tag{6.42}$$

and does not depend on the structure of the Hilbert space. Hence this method can be generalized to the multipartite case. That is, for a given input state $|\alpha_0\beta_0\gamma_0\ldots\rangle \in \mathcal{H}$ and a given observable $\hat{O}_{\max}$ we can define a new operator

$$\hat{A} \equiv \langle\beta_0\gamma_0\ldots|\hat{O}_{\max}|\beta_0\gamma_0\ldots\rangle. \tag{6.43}$$

By calculating the largest eigenvalue and the corresponding eigenvector $|\alpha_1\rangle \in \mathcal{H}_A$ of $\hat{A}$ we can find a new product state which enlarges the expectation value of $\hat{O}_{\max}$

$$\langle\alpha_1\beta_0\gamma_0\ldots|\hat{O}_{\max}|\alpha_1\beta_0\gamma_0\ldots\rangle \geq \langle\alpha_0\beta_0\gamma_0\ldots|\hat{O}_{\max}|\alpha_0\beta_0\gamma_0\ldots\rangle. \tag{6.44}$$

In analogy to the calculations above the resulting state $|\alpha_1\rangle$ can again be used to define an operator

$$\hat{B} \equiv \langle\alpha_1\gamma_0\ldots|\hat{O}_{\max}|\alpha_1\gamma_0\ldots\rangle \tag{6.45}$$

for which the eigenstate $|\beta_1\rangle \in \mathcal{H}_B$ corresponding to the maximal eigenvalue satisfies the inequality

$$\langle\alpha_1\beta_1\gamma_0\ldots|\hat{O}_{\max}|\alpha_1\beta_1\gamma_0\ldots\rangle \geq \langle\alpha_1\beta_0\gamma_0\ldots|\hat{O}_{\max}|\alpha_1\beta_0\gamma_0\ldots\rangle. \tag{6.46}$$

By repeating this procedure for all individual Hilbert subspaces we can calculate an output state $|\alpha_1\beta_1\gamma_1\ldots\rangle \in \mathcal{H}$ which yields a larger or equal expectation value of $\hat{O}_{\max}$ than the original input state $|\alpha_0\beta_0\gamma_0\ldots\rangle \in \mathcal{H}$. The obtained result can again be improved by using the output state as the new input state and by iterating the whole procedure. These iterations yield a monotonically increasing series of expectation values which is bounded, Eq. (6.7), and therefore converges. Due to this convergence the final state $|\alpha_{\text{fin}}\beta_{\text{fin}}\gamma_{\text{fin}}\ldots\rangle$ of the sequence of the states $|\alpha_n\beta_n\gamma_n\ldots\rangle$

has to fulfill the necessary condition, so that

$$c_{\max} = \langle \alpha_{\text{fin}} \beta_{\text{fin}} \gamma_{\text{fin}} \ldots | \hat{O}_{\max} | \alpha_{\text{fin}} \beta_{\text{fin}} \gamma_{\text{fin}} \ldots \rangle \tag{6.47}$$

is the global maximum of expectation values of $\hat{O}_{\max}$ with respect to *all* pure product states. By using these results we are now in the position to reproduce the central statement of section 5.4 for the multipartite case:

> By identifying the input state $|\alpha_0 \beta_0 \gamma_0 \ldots\rangle$ with the elements of the set $\mathcal{S}_{new}$ the iterative procedure above yields product states which have larger or equal overlap with $\hat{O}_{\max}$ than $|\alpha_0 \beta_0 \gamma_0 \ldots\rangle$. Moreover, by adding these states to the subset $\mathcal{S}_{new}$ a new updated subset $\mathcal{S}$ can be constructed and allows one to define a new linear program and to solve it. Due to the fact that the updated subset $\mathcal{S}$ includes $\mathcal{S}_{new}$, the new optimal value $\eta_{\max}^{new}$ of this new linear program has to be smaller than the previous $\eta_{\max}$ and therefore constitutes a better approximation of the Max-Min criterion. Moreover, iterative steps consist of the subset update and the solution of the linear program yields a monotonically decreasing series which is bounded by zero and therefore converges. Hence, by using these two steps and the generalized SVD-operator, Eq. (6.27), as initial $\hat{O}_{\max}$ we can extend the convergent algorithm, developed in section 5.5, to the multipartite case. All properties of this algorithm which we have discussed in the last four sections of chapter 5 are valid in the multipartite case as well.

6.5 Summary

In the present chapter we have demonstrated that the geometrical representation of Hermitian operators in the associated Hilbert-Schmidt vector space can also be used to characterize entanglement in multipartite quantum system. Furthermore, we have seen that most of the proofs which have been obtained for the bipartite case have a one-to-one correspondence in the multipartite case. The exceptions are the statements which are based on the singular value decomposition, which cannot be generalized to the multipartite systems. In conclusion we repeat the most important results.

- We have demonstrated that for any entangled state there exists at least one entanglement indicator, which detects its entanglement by violating inequality (6.10), and hence defines a necessary and sufficient inseparability criterion. The bound of this inequality is given by the pure product states. Furthermore, the geometrical representation allowed us to show that global Hermitian operators can always be decomposed in local Hermitian operators. As a result, the physical property – *entanglement* – can be observed in an experiment consisting of local observations and classical communication.

- We can generalize the sufficient SVD-criterion to the multipartite case. This criterion allows us to verify entanglement of a density operator without solving complicated optimization problems and consequently is *easy* to check.

- We can generalize the Max-Min criterion to the multipartite case, too. It is formulated as an optimization problem, which can be solved by using a convergent, iterative algorithm consisting of two steps, a linear program and a subset update. The properties of this algorithm are:

  - In the case of entangled density operators the algorithm converges to an entanglement indicator $\hat{O}_{\max}$, which is optimal if the assumption is fulfilled that the global maximum of the expectation of a Hermitian operator with respect to pure product states can be found. All numerical tests have confirmed this assumption. Moreover, in the case of separable density operators we obtain the coefficients of the convex decomposition, Eq. (6.5), as an additional result. Hence, this algorithm solves the problem of separability.
  - The algorithm can be implemented on modern computers and efficiently be solved for Hilbert spaces with up to $\dim(\mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_C \otimes \ldots) = 1000$ dimensions.

7 Conclusion and outlook

> Problems cannot be solved by thinking within the framework in which the problems were created.
>
> Albert Einstein

7.1 Conclusion

The question – ***What is entanglement?*** – was the starting point of this thesis and motivated us to have a closer look for applicable inseparability criteria which can solve the separability problem. We have shown that by using the geometrical representation of the Hermitian operators in the Hilbert-Schmidt vector space it is possible to derive inequalities, the violation of which, in analogy to Bell's inequalities, is a signature of entanglement in a quantum state. These inequalities lead to two different inseparability criteria, the sufficient SVD-criterion and the necessary and sufficient Max-Min criterion. The first of them is based on the singular value decomposition of the density operator in the Hilbert-Schmidt vector space and can detect entanglement, similar to the Peres-Horodecki criterion, by a simple calculation. Moreover, we have shown that the SVD-criterion can prove the entanglement of states for which the Peres-Horodecki criterion fails and thus by combining both criteria the class of inseparable states that can be detected is enlarged. The Max-Min criterion is defined as a continuous optimization problem the positive solution of which is a necessary and sufficient signature of entanglement. We have seen that the discrete version of this optimization problem can be solved with the help of the methods of operations research. By using this observation we have developed a powerful algorithm which in the case of inseparable states always converges to an optimal entanglement indicator. In the case of separable states this algorithm results in their convex decomposition, which by definition is the proof for separability. Moreover, we have shown that the Max-Min criterion can be implemented on

modern computers and be efficiently solved for Hilbert spaces with up to 1000 dimensions. We could not find an analytical confirmation of the numerical result that the iterative method used by the algorithm converges to the *absolute* maximum of the expectation value of the entanglement indicator with respect to pure product states. This is the current limitation of our approach. To avoid this numerical uncertainty we have found a non-sharp bound for the desired expectation value. Finally, we have shown that both criteria are valid in bipartite quantum systems as well as in multipartite systems.

7.2 Outlook

Most of the previous chapters were motivated by a question for which we have successfully found an answer. However, according to the proverb that *each answer leads to new questions* a lot of new questions appear. In the outlook we give a collection of questions which we find most interesting.

7.2.1 Maximization problem

In chapter 5 we have derived the necessary and sufficient Max-Min criterion for the detection of entanglement. This criterion can be solved by using the iterative algorithm presented in section 5.5 under the assumption that the maximal expectation value of a Hermitian operator with respect to pure product states can be found. Due to numerical tests we have a clear indication that the iterative method described in section 5.4 converges to this expectation value. However we have not yet found a rigorous mathematical proof for this result. Hence the question appears:

Is it possible to find the maximum of the expectation value

$$c = \langle \Psi | \hat{O} | \Psi \rangle \tag{7.1}$$

under the constraint that $|\Psi\rangle = |abc\ldots\rangle$ is a normalized product state.

A positive answer to this question would lead to a strict mathematical solution of the separability problem.

7.2.2 Non-classical correlations

In chapter 2 we have defined the difference between a separable and an entangled state via the possibility to write the corresponding density operator as a convex sum, Eq. (2.14)

$$\hat{\rho}_{sep} \equiv \sum_{n=1}^{\infty} p_n |a_n b_n\rangle\langle a_n b_n| \tag{7.2}$$

where $|a_n\rangle \in \mathcal{H}_A$ and $|b_n\rangle \in \mathcal{H}_B$ are arbitrary but normalized and $p_n \geq 0$. Hence, the physical interpretation of entanglement is a preparation rule, in other words a state described by a separable density operator can always be prepared locally. Furthermore, we have shown in section 3.3 that inseparable states can be detected by performing local measurements and by classical communication. On the other hand, we have seen in subsection 2.2.2, that entanglement is a necessary condition for a quantum system to violate the Bell inequalities. The violation of these inequalities is a proof of the statement that quantum correlations can be stronger than correlations allowed by the so-called local realistic theories (LRT). Thus, the question arises whether all entangled states lead to non-classical correlations? In order to answer this question we have to invert Bell's argument, i.e. we start with the quantum mechanical description of an experiment and compare it with all possible realizations of a LRT experiment.

Let the observable $\hat{O}$ be the description of a quantum mechanical experiment. Then, as shown in subsection 3.3, we can find the diagonal representation of this observable to be

$$\hat{O} = \sum_{k=1}^{K} o_k \hat{\sigma}_k^A \otimes \hat{\sigma}_k^B \tag{7.3}$$

where $\{o_k\}$ are the uniquely determined and positive singular values of $\hat{O}$ and $K \leq \min\{N_A^2, N_B^2\}$ denotes the rank of $\hat{O}$. By using the positivity of the singular values we can introduce the local Hermitian operators

$$\hat{A}_k \equiv \sqrt{o_k}\hat{\sigma}_k^A \quad \text{and} \quad \hat{B}_k \equiv \sqrt{o_k}\hat{\sigma}_k^B \tag{7.4}$$

and hence, the observable $\hat{O}$ can be decomposed as

$$\hat{O} = \sum_{k=1}^{K} \hat{A}_k \otimes \hat{B}_k. \tag{7.5}$$

The expectation value of this operator

$$\left\langle \hat{O} \right\rangle = \sum_{k=1}^{K} \left\langle \hat{A}_k \otimes \hat{B}_k \right\rangle \tag{7.6}$$

now looks very similar to the CHSH-Bell correlation function, Eq. (2.22). In section 3.1 we have shown that for separable states this expectation value is confined in the interval $[c_{\min}, c_{\max}]$ and thus we arrive at

$$\left\langle \hat{O} \right\rangle_{sep} = \sum_{n=1}^{\infty} p_n \sum_{k=1}^{K} \langle a_n | \hat{A}_k | a_n \rangle \langle b_n | \hat{B}_k | b_n \rangle \leq c_{\max}. \tag{7.7}$$

In the case of a LRT description we have to replace the Hermitian operators $\hat{A}_k$ and $\hat{B}_k$ by observables A_k and B_k for which the experimental outputs are given by the eigenvalues of the corresponding operators. Moreover the pure states $|a_n\rangle$ and $|b_n\rangle$ have to be represented by probability densities a_n and b_n. As a consequence, the quantum inequality (7.7) translates into the classical inequality

$$\sum_{n=1}^{\infty} p_n \sum_{k=1}^{K} \langle A_k \rangle_{a_n} \langle B_k \rangle_{b_n} \leq C_{\max} \tag{7.8}$$

where a new upper bound $C_{\max}$ has been introduced. Hence we can ask the question:

> Are the quantum mechanical $c_{\max}$ and the classical $C_{\max}$ bounds equal?

A positive answer to this question would lead to the statement that *all* entangled states contain correlations which are stronger than correlations allowed by the local realistic theories because in the case of entangled states we can always find an entanglement indicator $\hat{O}_{\mathcal{E}}$ such that the inequality (7.7) is violated as shown in subsection 3.2.2.

7.2.3 Operations research

In section 5.3 we have seen that by using the methods of operations research, in particular the methods of linear programming, we can solve the discrete version of the Max-Min criterion. The inversion of this result yields an interesting question

> Is it possible to use quantum mechanical methods to solve problems of operations research? In particular, is it possible to find quantum algorithms which solve linear programs more efficiently than classical algorithms do?

Due to the fact that operations research plays an important role in many different fields of applications, the positive answer to this question would be a great stimulation for quantum information theory. We can already give an example which successfully uses quantum mechanical methods to solve a specific class of linear programs and thus indicates that in the future the question might in general be answered positively.

Example

Let $\mathcal{H}$ denote the entire Hilbert space of a 2×3 quantum system where the Peres-Horodecki criterion is necessary and sufficient. Thus by using this criterion we can decide whether the solution of the optimization problem, Eq. (5.10),

$$\eta_{\max} = \sup_{\{\hat{O}, \|\hat{O}\| \leq 1\}} \left(\min_{|a.b\rangle} \left(\mathrm{Tr} \left\{ \hat{O} \left(\hat{\rho} - |ab\rangle\langle ab| \right) \right\} \right) \right) \tag{7.9}$$

is given by $\eta_{\max} = 0$ ($\hat{\rho}$ is separable) or $\eta_{\max} > 0$ ($\hat{\rho}$ is entangled). On the other hand we have shown in section 5.3 that in the associated Hilbert-Schmidt vector space this optimization problem can be written in the form of a linear program with $72 = 2\left(\dim \mathcal{H}\right)^2$ variables and an infinitely large number of linear constraints. Hence, if a linear program can be mapped to the optimization problem, Eq. (7.9), we have a simple method to show whether a non-vanishing solution of this linear program exists.

A Appendix

> It is by logic that we prove, but by intuition that we discover.
>
> Henri Poincaré

A.1 Eigenvalue problem

Theorem:

Let $\mathcal{H}$ denote a Hilbert space with $\dim \mathcal{H} = N < \infty$ and let $\hat{O}$ be a Hermitian operator that acts on this space. Then the solution of the maximization problem

$$\lambda_{\max} = \max_{|\psi\rangle \in \mathcal{H}} \frac{\langle \psi | \hat{O} | \psi \rangle}{\langle \psi | \psi \rangle} \tag{A.1}$$

is given by the largest eigenvalue of $\hat{O}$.

Proof:
Let us introduce the complex function

$$f(\varepsilon) \equiv \frac{\left(\langle \psi_{\max}| + \varepsilon^* \langle \varphi| \right) \hat{O} \left(|\psi_{\max}\rangle + \varepsilon |\varphi\rangle \right)}{\left(\langle \psi_{\max}| + \varepsilon^* \langle \varphi| \right) \left(|\psi_{\max}\rangle + \varepsilon |\varphi\rangle \right)} \tag{A.2}$$

with $\varepsilon \in \mathbb{C}$. A necessary condition for $|\psi_{\max}\rangle$ to be the state that maximizes (A.1) is then

$$0 = \frac{\partial}{\partial \varepsilon^*} f(\varepsilon) \bigg|_{\varepsilon = 0} = \frac{\langle \varphi | \hat{O} | \psi_{\max} \rangle \langle \psi_{\max} | \psi_{\max} \rangle - \langle \psi_{\max} | \hat{O} | \psi_{\max} \rangle \langle \varphi | \psi_{\max} \rangle}{\langle \psi_{\max} | \psi_{\max} \rangle^2} \tag{A.3}$$

This condition must hold for all $|\varphi\rangle \in \mathcal{H}$ and therefore $|\psi_{\max}\rangle$ has to satisfy the

equation

$$\hat{O}|\psi_{\max}\rangle = \frac{\langle\psi_{\max}|\hat{O}|\psi_{\max}\rangle}{\langle\psi_{\max}|\psi_{\max}\rangle}|\psi_{\max}\rangle = \lambda|\psi_{\max}\rangle. \tag{A.4}$$

As a result, $|\psi_{\max}\rangle$ is an eigenvector of the operator $\hat{O}$ with eigenvalue $\lambda = \frac{\langle\psi_{\max}|\hat{O}|\psi_{\max}\rangle}{\langle\psi_{\max}|\psi_{\max}\rangle}$ and hence the largest eigenvalue $\lambda_{\max}$ maximizes the optimization problem (A.1).

□

Remarks:

1. In the same way it can be proven that the solution of the minimization problem

$$\lambda_{\min} = \min_{|\psi\rangle} \frac{\langle\psi|\hat{O}|\psi\rangle}{\langle\psi|\psi\rangle} \tag{A.5}$$

   is given by the smallest eigenvalue of $\hat{O}$.

2. If the largest and smallest eigenvalues of $\hat{O}$ are bounded

$$|\lambda_{\max}| < \infty \text{ and } |\lambda_{\min}| < \infty \tag{A.6}$$

   then $\hat{O}$ is bounded, too, which means that the inequality

$$\left|\langle\varphi|\hat{O}|\varphi\rangle\right| < \infty \tag{A.7}$$

   is valid for all normalized states with $\langle\varphi|\varphi\rangle = 1$.

A.2 Hilbert-Schmidt vector space

Theorem:

Hermitian operators acting on a N dimensional complex Hilbert space $\mathcal{H}$ constitute an Euclidian N^2-dimensional real vector space $V_{HS} = \mathbb{R}^{N^2}$. Moreover the trace operation over the product of two Hermitian operators defines a scalar product

$$\left\langle \hat{A}_1, \hat{A}_2 \right\rangle \equiv Tr\left\{ \hat{A}_1 \hat{A}_2 \right\}. \tag{A.8}$$

Proof:

In order for V_{HS} to be a vector space, the following conditions must hold for all elements $\hat{A}_1, \hat{A}_2, \hat{A}_3 \in V_{HS}$ and any scalars $a, b \in \mathbb{R}$ [51]:

1. Commutativity:
$$\hat{A}_1 + \hat{A}_2 = \hat{A}_2 + \hat{A}_1 \tag{A.9}$$

2. Associativity of vector addition:
$$\left(\hat{A}_1 + \hat{A}_2\right) + \hat{A}_3 = \hat{A}_1 + \left(\hat{A}_2 + \hat{A}_3\right) \tag{A.10}$$

3. Additive identity:
$$\hat{0} + \hat{A}_1 = \hat{A}_1 + \hat{0} = \hat{A}_1 \tag{A.11}$$
where $\hat{0}$ denotes the zero operator with
$$\langle \varphi | \hat{0} | \varphi \rangle = 0 \tag{A.12}$$
for all $|\varphi\rangle \in \mathcal{H}$.

4. Existence of additive inverse: For any $\hat{A}_1$, there exists $-\hat{A}_1$ such that
$$\hat{A}_1 + \left(-\hat{A}_1\right) = \hat{0} \tag{A.13}$$

5. Associativity of scalar multiplication:
$$a\left(b\hat{A}_1\right) = (ab)\,\hat{A}_1 \tag{A.14}$$

6. Distributivity of scalar sums:

$$(a+b)\,\hat{A}_1 = a\hat{A}_1 + b\hat{A}_1 \tag{A.15}$$

7. Distributivity of vector sums:

$$a\left(\hat{A}_1 + \hat{A}_2\right) = a\hat{A}_1 + a\hat{A}_2 \tag{A.16}$$

8. Scalar multiplication identity:

$$1\hat{A}_1 = \hat{A}_1 \tag{A.17}$$

It is obvious that all these conditions are fulfilled by Hermitian operators and hence they constitute a vector space.

For a real vector space the scalar product $\langle\cdot,\cdot\rangle$ has to satisfy the following properties [51]. Let $\hat{A}_1, \hat{A}_2, \hat{A}_3 \in V_{HS}$ be vectors and $a \in \mathbb{R}$ be a scalar, then the scalar product is:

1. Additive:
$$\left\langle \hat{A}_1 + \hat{A}_2, \hat{A}_3 \right\rangle = \left\langle \hat{A}_1, \hat{A}_2 \right\rangle + \left\langle \hat{A}_2, \hat{A}_3 \right\rangle \tag{A.18}$$

2. Homogeneous:
$$\left\langle a\hat{A}_1, \hat{A}_2 \right\rangle = a\left\langle \hat{A}_1, \hat{A}_2 \right\rangle \tag{A.19}$$

3. Symmetric:
$$\left\langle \hat{A}_1, \hat{A}_2 \right\rangle = \left\langle \hat{A}_2, \hat{A}_2 \right\rangle \tag{A.20}$$

4. non-negative:
$$\left\langle \hat{A}_1, \hat{A}_1 \right\rangle \geq 0 \tag{A.21}$$
and equal if and only if $\hat{A}_1 = \hat{0}$

Due to the linearity of the trace operation it is evident that the properties 1, 2 and 3 are fulfilled for the scalar product defined by

$$\left\langle \hat{A}_1, \hat{A}_2 \right\rangle \equiv \mathrm{Tr}\left\{\hat{A}_1\hat{A}_2\right\}. \tag{A.22}$$

Squared Hermitian operators are positive semidefinite because they satisfy the following inequality for all $|\psi\rangle \in \mathcal{H}$

$$\langle\psi|\hat{A}_1\hat{A}_1|\psi\rangle = \langle\tilde{\psi}|\tilde{\psi}\rangle \geq 0 \tag{A.23}$$

with $|\tilde{\psi}\rangle \equiv \hat{A}_1|\psi\rangle$. The trace over a positive operator vanishes only if the operator is the zero operator $\hat{0}$. Therefore the fourth property is also fulfilled and $\mathrm{Tr}\left\{\hat{A}_1\hat{A}_2\right\}$ defines a valid scalar product in the vector space V_{HS}.

Finally we prove that for $\dim\mathcal{H} = N$ we get $\dim V_{HS} = N^2$. Let the set $\{|\psi_n\rangle,\, n = 1 \ldots N\}$ be an orthonormal basis of $\mathcal{H}$. Then a Hermitian operator $\hat{A}$ can be decomposed in this basis as

$$\hat{A} = \sum_{n,m=1}^{N} a_{nm}|\psi_n\rangle\langle\psi_m| \tag{A.24}$$

where the $N \times N$ complex valued matrix (a_{nm}) contains the whole information about $\hat{A}$. Due to the Hermiticity of the operator $\hat{A}$ the N diagonal elements a_{nn} are real valued and the non-diagonal elements satisfy the equality

$$a_{nm} = a^*_{mn} \tag{A.25}$$

or equivalently

$$\mathrm{Re}\{a_{nm}\} = \mathrm{Re}\{a_{mn}\} \text{ and } \mathrm{Im}\{a_{nm}\} = -\mathrm{Im}\{a_{mn}\}. \tag{A.26}$$

Therefore, the n-tuple

$$\begin{aligned}(a_{11}, a_{22}, \ldots, a_{NN}, \mathrm{Re}\{a_{12}\}, \mathrm{Re}\{a_{13}\}, \ldots, \mathrm{Re}\{a_{N-1,N}\},\\ \mathrm{Im}\{a_{12}\}, \mathrm{Im}\{a_{13}\}, \ldots, \mathrm{Im}\{a_{N-1,N}\})\end{aligned} \tag{A.27}$$

with N^2 real components describes the operator $\hat{A}$ in a unique way. Hence the dimension of the vector space V_{HS} is N^2.

□

Remark:

The vector space presented in this theorem is called the Hilbert-Schmidt vector space [52].

A.3 Singular value decomposition

Theorem [51]:

If a complex valued $M \times N$ matrix $\mathbf{A}$ has rank K, then it may be written in the form

$$\mathbf{A} = \mathbf{V}\Sigma\mathbf{W}^{\dagger} \tag{A.28}$$

where $\mathbf{V}$ and $\mathbf{W}$ are $M \times M$ and $N \times N$ unitary matrices. The $M \times N$ matrix $\Sigma = (s_{nm})$ has $s_{nm} = 0$ for all $n \neq m$, and

$$s_{11} \geq s_{22} \geq \ldots \geq s_{KK} > s_{K+1,K+1} = \ldots = s_{qq} = 0, \tag{A.29}$$

where $q = \min\{M, N\}$. The numbers $\{s_{nn}\} \equiv \{s_n\}$ are the non-negative square roots of the eigenvalues of $\mathbf{A}\mathbf{A}^{\dagger}$, and hence are uniquely determined. The columns of $\mathbf{V}$ are eigenvectors of $\mathbf{A}\mathbf{A}^{\dagger}$ and the columns of $\mathbf{W}$ are the eigenvectors of $\mathbf{A}^{\dagger}\mathbf{A}$ (arranged in the same order as corresponding eigenvalues s_n^2). If $M = N = K$ then $\mathbf{V}$ is determined up to a right diagonal matrix $\mathbf{D} = diag\left(e^{i\vartheta_1}, e^{i\vartheta_2}, \ldots, e^{i\vartheta_N}\right)$ and $\mathbf{W}$ is uniquely determined. If $M < N$, then $\mathbf{W}$ is never uniquely determined. If $M > N$, the uniqueness of $\mathbf{V}$ and $\mathbf{W}$ is determined by considering $\mathbf{A}^{\dagger}$. If $\mathbf{A}$ is real, then $\mathbf{V}$ and $\mathbf{W}$ may all be taken to be real.

Proof:
See [51] theorem 7.3.5

□

A.4 Applications of the singular value decomposition

A.4.1 Schmidt decomposition

Theorem:

Let $\mathcal{H}_A$, $\mathcal{H}_B$ and $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$ be Hilbert spaces with $N_A = \dim \mathcal{H}_A$ and $N_B = \dim \mathcal{H}_B$ and let $|\Psi\rangle \in \mathcal{H}$ be an arbitrary state. Then there exist two sets of orthonormal states $\{|a_k\rangle \in \mathcal{H}_A\}$ and $\{|b_k\rangle \in \mathcal{H}_B\}$ such that

$$|\Psi\rangle = \sum_{k=1}^{K} s_k |a_k\rangle \otimes |b_k\rangle \tag{A.30}$$

with uniquely determined positive coefficients s_k.

Proof:
Let $\{|\psi_n\rangle,\, n = 1 \dots N_A\}$ be an orthonormal basis of $\mathcal{H}_A$ and $\{|\varphi_m\rangle,\, m = 1 \dots N_B\}$ be an orthonormal basis of $\mathcal{H}_B$. The state $|\Psi\rangle$ can be decomposed in these bases and is given by

$$|\Psi\rangle = \sum_{n=1}^{N_A} \sum_{m=1}^{N_B} c_{nm} |\psi_n\rangle \otimes |\varphi_m\rangle. \tag{A.31}$$

By identifying c_{nm} with coefficients of a $N_A \times N_B$ matrix $\mathbf{A}$ and by using the results of appendix A.3, two unitary $N_A \times N_A$ and $N_B \times N_B$ matrices $\mathbf{V}$ and $\mathbf{W}$ and a non-negative matrix Σ can be found such that

$$\mathbf{A} = \mathbf{V} \Sigma \mathbf{W}^\dagger \tag{A.32}$$

or equivalently

$$c_{nm} = \sum_{k=1}^{N_A} \sum_{l=1}^{N_B} v_{nk} s_k \delta_{kl} w^*_{ml} = \sum_{k=1}^{K} s_k v_{nk} w^*_{mk} \tag{A.33}$$

where s_k are the uniquely determined singular values of the matrix $\mathbf{A}$ and K denotes the rank of this matrix. The decomposition of the state $|\Psi\rangle$ is therefore

$$|\Psi\rangle = \sum_{k=1}^{K} s_k \left(\sum_{n=1}^{N_A} v_{nk} |\psi_n\rangle \right) \otimes \left(\sum_{m=1}^{N_B} w^*_{mk} |\varphi_m\rangle \right) \equiv \sum_{k=1}^{K} s_k |a_k\rangle \otimes |b_k\rangle. \tag{A.34}$$

The columns of the unitary matrices $\mathbf{V}$ and $\mathbf{W}^\dagger$ are orthonormal and hence the states $\{|a_n\rangle\}$ and $\{|b_n\rangle\}$ are orthonormal, too.

□

Remarks:

1. The decomposition of a state $|\Psi\rangle$ in the form of Eq. (A.30) is called Schmidt decomposition [64].

2. The uniquely determined positive coefficients s_k are called Schmidt factors.

A.4.2 Diagonal representation of Hermitian operators

Theorem:

Let $\mathcal{H}_A$, $\mathcal{H}_B$ and $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$ be Hilbert spaces with $N_A = \dim \mathcal{H}_A$ and $N_B = \dim \mathcal{H}_B$ and let $\hat{O}$ be an arbitrary Hermitian operator which acts on $\mathcal{H}$. Then there exists a set of Hermitian operators $\left\{\hat{\sigma}_k^A\right\}$ which act on $\mathcal{H}_A$ and a set of Hermitian operators $\left\{\hat{\sigma}_k^B\right\}$ which act on $\mathcal{H}_B$ such that the operator $\hat{O}$ has the diagonal representation

$$\hat{O} = \sum_{k=1}^{K} o_k \hat{\sigma}_k^A \otimes \hat{\sigma}_k^B \,, \quad o_1 \geq o_2 \geq \ldots \geq o_K. \tag{A.35}$$

Furthermore the $\hat{\sigma}$-operators are orthonormal with respect to the scalar product

$$Tr\{\hat{\sigma}_k \hat{\sigma}_l\} = \delta_{kl} \tag{A.36}$$

and the coefficients o_k are positive and uniquely determined.

Proof:
Let the sets

$$\overline{\Omega}_A = \left\{\hat{\overline{\sigma}}_n^A,\, n \in 1 \ldots N_A^2\right\} \text{ and } \overline{\Omega}_B = \left\{\hat{\overline{\sigma}}_m^B,\, m \in 1 \ldots N_B^2\right\} \tag{A.37}$$

be the complete orthonormal bases of the associated Hilbert-Schmidt vector spaces, see appendix A.2, of $\mathcal{H}_A$ and $\mathcal{H}_B$ respectively. Then the decomposition of the

operator $\hat{O}$ in these bases is given by

$$\hat{O} = \sum_{n=1}^{N_A^2} \sum_{m=1}^{N_B^2} \overline{o}_{nm} \hat{\overline{\sigma}}_n^A \otimes \hat{\overline{\sigma}}_m^B. \tag{A.38}$$

with real coefficients

$$\overline{o}_{nm} = \mathrm{Tr}\left\{ \hat{O}\, \hat{\overline{\sigma}}_n^A \otimes \hat{\overline{\sigma}}_m^B \right\}. \tag{A.39}$$

By identifying $\overline{o}_{nm}$ with the coefficients of a $N_A^2 \times N_B^2$ matrix $\mathbf{A}$ and by using the results of appendix A.3, two real valued unitary $N_A^2 \times N_A^2$ and $N_B^2 \times N_B^2$ matrices $\mathbf{V}$ and $\mathbf{W}$ and a diagonal non-negative matrix Σ can be found such that

$$\mathbf{A} = \mathbf{V} \Sigma \mathbf{W}^T \tag{A.40}$$

or

$$\overline{o}_{nm} = \sum_{k=1}^{N_A^2} \sum_{l=1}^{N_B^2} v_{nk} o_k \delta_{kl} w_{ml} = \sum_{k=1}^{K} o_k v_{nk} w_{mk}^* \tag{A.41}$$

where o_k are the uniquely determined singular values of the matrix $\mathbf{A}$ and K denotes the rank of this matrix. The decomposition of the Hermitian operator $\hat{O}$ is therefore given by

$$\hat{O} = \sum_{k=1}^{K} o_k \left(\sum_{n=1}^{N_A^2} v_{nk} \hat{\overline{\sigma}}_n^A \right) \otimes \left(\sum_{m=1}^{N_B^2} w_{mk}^* \hat{\overline{\sigma}}_m^B \right) \equiv \sum_{k=1}^{K} o_k \hat{\sigma}_k^A \otimes \hat{\sigma}_k^B. \tag{A.42}$$

The columns of the unitary matrices $\mathbf{V}$ and $\mathbf{W}^T$ are orthonormal and hence the sets of Hermitian operators $\left\{\hat{\sigma}_k^A\right\}$ and $\left\{\hat{\sigma}_k^B\right\}$ are orthonormal, too.

□

A.4.3 SVD-operator

Theorem:

Let $\mathcal{H}_A$, $\mathcal{H}_B$ and $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$ be Hilbert spaces with $N_A = \dim \mathcal{H}_A \leq \dim \mathcal{H}_B = N_B$ and let

$$\hat{\rho} = \sum_{k=1}^{K} r_k \hat{\sigma}_k^A \otimes \hat{\sigma}_k^B\,, \quad r_1 \geq r_2 \geq \ldots \geq r_K > 0 \tag{A.43}$$

be the diagonal representation, see appendix A.4.2, of the density operator. Furthermore let $\left\{\hat{\overline{O}}\right\}$ *denote a set of Hermitian operators which are defined as*

$$\hat{\overline{O}} = \sum_{n=1}^{N_A^2} \hat{\overline{\sigma}}_n^A \otimes \hat{\overline{\sigma}}_n^B$$

where the $\hat{\overline{\sigma}}$*-operators are orthonormal with respect to the scalar product*

$$\mathrm{Tr}\left\{\hat{\overline{\sigma}}_n^{A,B}\hat{\overline{\sigma}}_m^{A,B}\right\} = \delta_{nm}. \tag{A.44}$$

Then the maximum of the expectation value

$$\left\langle\hat{\overline{O}}\right\rangle_{\hat{\rho}} = Tr\left\{\hat{\overline{O}}\hat{\rho}\right\} \tag{A.45}$$

over all elements of the set $\left\{\hat{\overline{O}}\right\}$ *is reached by the operator*

$$\hat{O}_{SVD} \equiv \sum_{k=1}^{K} \hat{\sigma}_k^A \otimes \hat{\sigma}_k^B \tag{A.46}$$

and is equal to the sum over the singular values of $\hat{\rho}$*.*

Proof:
Let the sets

$$\Omega_A = \left\{\hat{\sigma}_n^A,\, n = 1 \ldots N_A^2\right\} \quad \text{and} \quad \Omega_B = \left\{\hat{\sigma}_n^B,\, n = 1 \ldots N_B^2\right\} \tag{A.47}$$

denote the bases of the associated Hilbert-Schmidt vector spaces of Alice and Bob, see appendix A.2, where the first K elements in each of these sets are equal to the $\hat{\sigma}$-operators of the diagonal representation of $\hat{\rho}$, Eq. (A.43). To fulfill the orthonormality condition of the $\hat{\overline{\sigma}}$-operators we introduce a $N_A^2 \times N_A^2$ unitary matrix $\mathbf{U} = (u_{nm})$ and a $N_B^2 \times N_B^2$ unitary matrix $\mathbf{V} = (v_{np})$. Then the $\hat{\overline{\sigma}}$-operators can be written as

$$\hat{\overline{\sigma}}_n^A = \sum_{m=1}^{N_A^2} u_{nm}\hat{\sigma}_m^A \quad \text{and} \quad \hat{\overline{\sigma}}_n^B = \sum_{p=1}^{N_B^2} v_{np}\hat{\sigma}_p^B \tag{A.48}$$

and the operator $\hat{\overline{O}}$ is given by

$$\hat{\overline{O}} = \sum_{n=1}^{N_A^2} \hat{\overline{\sigma}}_n^A \otimes \hat{\overline{\sigma}}_n^B = \sum_{n=1}^{N_A^2} \left(\sum_{m=1}^{N_A^2} u_{nm} \hat{\sigma}_m^A \right) \otimes \left(\sum_{p=1}^{N_B^2} v_{np} \hat{\sigma}_p^B \right). \tag{A.49}$$

The scalar product of $\hat{\overline{O}}$ and $\hat{\rho}$ yields

$$\begin{aligned} \left\langle \hat{\overline{O}} \right\rangle_{\hat{\rho}} = \mathrm{Tr}\left\{ \hat{\overline{O}} \hat{\rho} \right\} = \mathrm{Tr}\left\{ \left(\sum_{n=1}^{N_A^2} \sum_{m=1}^{N_A^2} \sum_{p=1}^{N_B^2} u_{nm} v_{np} \hat{\sigma}_m^A \otimes \hat{\sigma}_p^B \right) \left(\sum_{k=1}^{K} r_k \hat{\sigma}_k^A \otimes \hat{\sigma}_k^B \right) \right\} \\ = \sum_{k=1}^{K} \sum_{n=1}^{N_A^2} r_k u_{nk} v_{nk} \end{aligned} \tag{A.50}$$

where the orthonormality of the $\hat{\sigma}$-operators was used. By using the Cauchy-Schwarz inequality and the fact that the rows and columns of unitary matrices are unit vectors

$$\left| \sum_{n=1}^{N_A^2} u_{nk} v_{nk} \right| \leq \sum_{n=1}^{N_A^2} u_{nk}^2 \sum_{n=1}^{N_A^2} v_{nk}^2 \leq \sum_{n=1}^{N_A^2} u_{nk}^2 \sum_{n=1}^{N_B^2} v_{nk}^2 = 1 \tag{A.51}$$

the upper bound of the expectation value $\left\langle \hat{\overline{O}} \right\rangle_{\hat{\rho}}$ is given by

$$\left| \left\langle \hat{\overline{O}} \right\rangle_{\hat{\rho}} \right| = \left| \sum_{k=1}^{K} r_k \sum_{n=1}^{N_A^2} u_{nk} v_{nk} \right| \leq \sum_{k=1}^{K} |r_k| \left| \sum_{n=1}^{N_A^2} u_{nk} v_{nk} \right| \leq \sum_{k=1}^{K} |r_k| = \sum_{k=1}^{K} r_k \tag{A.52}$$

where in the last step the positivity of the singular values r_k was taken into account. This bound is sharp because the operator

$$\hat{O}_{SVD} \equiv \sum_{k=1}^{K} \hat{\sigma}_k^A \otimes \hat{\sigma}_k^B \tag{A.53}$$

reaches it. Hence, $\hat{O}_{SVD}$ maximizes the expectation value of the elements of the set $\left\{ \hat{\overline{O}} \right\}$ with respect to the density operator $\hat{\rho}$ and the maximum is equal to the sum over the singular values r_k of $\hat{\rho}$.

□

A.4.4 Kronecker product approximation

Theorem:

Let $\mathcal{H}_A$, $\mathcal{H}_B$ and $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$ be Hilbert spaces with $N_A = \dim \mathcal{H}_A$ and $N_B = \dim \mathcal{H}_B$ and let

$$\hat{O} = \sum_{k=1}^{K} o_k \hat{\sigma}_k^A \otimes \hat{\sigma}_k^B , \quad o_1 \geq o_2 \geq \ldots \geq o_K \tag{A.54}$$

be the diagonal representation, see appendix A.4.2, of an arbitrary Hermitian operator which acts on $\mathcal{H}$. Furthermore let $\left\{\hat{P}\right\}$ denote a set of Hermitian operators which are defined as a Kronecker product between two operators $\hat{A}$ and $\hat{B}$ acting on $\mathcal{H}_A$ and $\mathcal{H}_B$ respectively. Then the maximum of the scalar product

$$\chi = Tr\left\{\hat{O}\hat{P}\right\} \tag{A.55}$$

between $\hat{O}$ and the elements of the set $\left\{\hat{P}\right\}$ under the constraints

$$Tr\left\{\hat{A}^2\right\} = 1 \quad and \quad Tr\left\{\hat{B}^2\right\} = 1 \tag{A.56}$$

is reached by the operator

$$\hat{P}_{\max} \equiv \hat{\sigma}_1^A \otimes \hat{\sigma}_1^B \tag{A.57}$$

and is equal to the largest singular value of $\hat{O}$.

Proof:
Let the sets

$$\Omega_A = \left\{\hat{\sigma}_n^A,\, n = 1 \ldots N_A^2\right\} \quad \text{and} \quad \Omega_B = \left\{\hat{\sigma}_n^B,\, n = 1 \ldots N_B^2\right\} \tag{A.58}$$

denote the bases of the associated Hilbert-Schmidt vector spaces of Alice and Bob, see appendix A.2, where the first K elements in each of these sets are equal to the $\hat{\sigma}$-operators of the diagonal representation of $\hat{O}$, Eq. (A.54). Then all operators $\hat{A}$ and $\hat{B}$ can be written as

$$\hat{A} = \sum_{n=1}^{N_A^2} a_n \hat{\sigma}_n^A \quad \text{and} \quad \hat{B} = \sum_{n=1}^{N_B^2} b_n \hat{\sigma}_n^B . \tag{A.59}$$

The scalar product of $\hat{O}$ and $\hat{P}$ yields

$$\chi = \mathrm{Tr}\left\{\hat{O}\hat{P}\right\} = \mathrm{Tr}\left\{\hat{O}\,\hat{A}\otimes\hat{B}\right\} = \sum_{k=1}^{K} o_k a_k b_k \tag{A.60}$$

where the orthonormality of the $\hat{\sigma}$-operators was used. By using the Cauchy-Schwarz inequality and the normalization conditions

$$\mathrm{Tr}\left\{\hat{A}^2\right\} = \sum_{n=1}^{N_A^2} a_n^2 = 1 \quad \text{and} \quad \mathrm{Tr}\left\{\hat{B}^2\right\} = \sum_{n=1}^{N_B^2} b_n^2 = 1 \tag{A.61}$$

the upper bound of χ is given by

$$|\chi| = \left|\sum_{k=1}^{K} o_k a_k b_k\right| \leq \sqrt{\sum_{k=1}^{K} o_k^2 a_k^2 \sum_{n=1}^{K} b_n^2} \leq \sqrt{o_{\max}^2 \sum_{n=1}^{N_A^2} a_n^2 \sum_{m=1}^{N_B^2} b_m^2} = o_{\max} \tag{A.62}$$

where $o_{\max} = o_1$ is the largest singular value of $\hat{O}$. This bound is sharp because the operator

$$\hat{P}_{\max} = \hat{\sigma}_1^A \otimes \hat{\sigma}_1^B \tag{A.63}$$

reaches it. Hence, $\hat{P}_{\max}$ maximizes the scalar product χ.

□

Remark:

The Kronecker product approximation of a matrix is a common method which is used in computer science [65] to solve problems which involve large matrices.

A.5 Optimization problem

In this appendix we will present calculations which are dealing with the optimization problem: Find a pure product state $|ab\rangle$ which maximizes the expectation value of a bounded Hermitian operator

$$c = \langle ab|\hat{O}|ab\rangle \tag{A.64}$$

under the normalization conditions $\langle a|a\rangle = \langle b|b\rangle = 1$.

A.5.1 Projectors

Theorem:

Let $\mathcal{H}_A$, $\mathcal{H}_B$ and $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$ be Hilbert spaces with $N_A = \dim \mathcal{H}_A \leq N_B = \dim \mathcal{H}_B$ and let the Hermitian operator $\hat{O}$ be a projector

$$\hat{O} \equiv |\Psi\rangle\langle\Psi| \tag{A.65}$$

where $|\Psi\rangle \in \mathcal{H}$ denotes a potentially unnormalized state. Then the solution of the optimization problem

$$c_{\max} = \max_{|ab\rangle} \langle ab|\hat{O}|ab\rangle, \ |a\rangle \in \mathcal{H}_A, \ |b\rangle \in \mathcal{H}_B \tag{A.66}$$

is given by the square of the largest Schmidt factor, appendix A.4.1*, of the state $|\Psi\rangle$.*

Proof:
Let

$$|\Psi\rangle = \sum_{n=1}^{K} s_n |\psi_n \varphi_n\rangle \quad s_1 \geq s_s \geq \ldots \geq s_K \tag{A.67}$$

be the Schmidt decomposition of the state $|\Psi\rangle$. Then the upper bound of the

optimization problem is given by

$$\max_{|ab\rangle} |\langle ab|\Psi\rangle|^2 \leq \max_{|ab\rangle} \langle a| \left(\langle b|\Psi\rangle\langle\Psi|b\rangle + \sum_{n=2}^{N_B} \langle b_n|\Psi\rangle\langle\Psi|b_n\rangle \right) |a\rangle =$$

$$\max_{|a\rangle} \langle a|\mathrm{Tr}_B \left\{ |\Psi\rangle\langle\Psi| \right\} |a\rangle = \max_{|a\rangle} \langle a| \left(\sum_{n=1}^{K} s_n^2 |\psi_n\rangle\langle\psi_n| \right) |a\rangle \equiv \max_{|a\rangle} \langle a|\hat{A}|a\rangle$$

where $\{|b_n\rangle\}$ is an orthonormal set of states which are orthogonal to $|b\rangle$ and $\mathrm{Tr}_B\{\cdot\}$ denotes the trace over the Hilbert space $\mathcal{H}_B$. Due to appendix A.1 the solution of the final optimization problem corresponds to the largest eigenvalue of $\hat{A}$ which is equal to the square s_1^2 of the largest Schmidt factor of $|\Psi\rangle$. This bound is sharp because the pure product state

$$|ab\rangle \equiv |\psi_1\varphi_1\rangle \tag{A.68}$$

reaches it.

□

A.5.2 Necessary condition

Theorem:

Let $\mathcal{H}_A$, $\mathcal{H}_B$ and $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$ be Hilbert spaces with $N_A = \dim \mathcal{H}_A$ and $N_B = \dim \mathcal{H}_B$ and let $\hat{O}$ be a positive Hermitian operator which acts on $\mathcal{H}$. Furthermore let $|a_1b_1\rangle$ be a pure product state. Then $|a_1b_1\rangle$ maximizes the expectation value

$$c_{\max} = \max_{|ab\rangle} \langle ab|\hat{O}|ab\rangle, \ |a\rangle \in \mathcal{H}_A, \ |b\rangle \in \mathcal{H}_B \tag{A.69}$$

of $\hat{O}$ with respect to all pure product states only if it satisfies the relation

$$\hat{O}|a_1b_1\rangle = s_1|a_1b_1\rangle + \sum_{k=2}^{K} s_k|a_kb_k\rangle \ \ s_1 \geq s_2 \geq \ldots \geq s_K \tag{A.70}$$

where the Hilbert space vectors $\{|a_kb_k\rangle, \ k = 2 \ldots K\}$ are orthonormal pure product states, which are orthogonal to the state $|a_1b_1\rangle$.

Proof:
Let us introduce the unnormalized state

$$|\Psi\rangle = \hat{O}|a_1 b_1\rangle \tag{A.71}$$

with the Schmidt decomposition

$$|\Psi\rangle = \sum_{k=1}^{K} s_k |\psi_k \varphi_k\rangle \;\; s_1 \geq s_2 \geq \ldots \geq s_K. \tag{A.72}$$

Then as shown in appendix A.5.1 the product state corresponding to the largest Schmidt factor maximizes the overlap between $|\Psi\rangle$ and pure product states and therefore the inequality

$$s_1^2 = |\langle \psi_1 \varphi_1 | \Psi \rangle|^2 \geq |\langle a_1 b_1 | \Psi \rangle|^2 \tag{A.73}$$

or equivalently

$$\left| \langle \psi_1 \varphi_1 | \hat{O} | a_1 b_1 \rangle \right|^2 \geq \langle a_1 b_1 | \hat{O} | a_1 b_1 \rangle^2 \tag{A.74}$$

holds. Due to the positivity of the operator $\hat{O}$ there exists [51] an operator $\hat{A}$ such that

$$\hat{O} = \hat{A}^\dagger \hat{A}. \tag{A.75}$$

With the help of this operator and the Cauchy-Schwarz inequality the left hand side of inequality (A.74) is bounded by

$$\left| \langle \psi_1 \varphi_1 | \hat{O} | a_1 b_1 \rangle \right|^2 = \left| \langle \psi_1 \varphi_1 | \hat{A}^\dagger \hat{A} | a_1 b_1 \rangle \right|^2 \leq \langle \psi_1 \varphi_1 | \hat{A}^\dagger \hat{A} | \psi_1 \varphi_1 \rangle \langle a_1 b_1 | \hat{A}^\dagger \hat{A} | a_1 b_1 \rangle. \tag{A.76}$$

By combining this result with inequality (A.74) we arrive at

$$\langle \psi_1 \varphi_1 | \hat{O} | \psi_1 \varphi_1 \rangle \geq \langle a_1 b_1 | \hat{O} | a_1 b_1 \rangle. \tag{A.77}$$

Due to the assumption that the state $|a_1 b_1\rangle$ maximizes the expectation value of $\hat{O}$ with respect to all pure product states this inequality is an equality

$$\langle \psi_1 \varphi_1 | \hat{O} | \psi_1 \varphi_1 \rangle = \langle a_1 b_1 | \hat{O} | a_1 b_1 \rangle = s_1 \tag{A.78}$$

which yields[1]

$$|a_1 b_1\rangle = |\psi_1 \varphi_1\rangle. \tag{A.79}$$

Hence, $|a_1 b_1\rangle$ satisfies the relation

$$\hat{O}|a_1 b_1\rangle = |\Psi\rangle = s_1 |a_1 b_1\rangle + \sum_{k=2}^{K} s_k |a_k b_k\rangle \;\; s_1 \geq s_2 \geq \ldots \geq s_K \tag{A.80}$$

where the states $\{|a_k b_k\rangle,\ k = 2 \ldots K\}$ correspond to the remaining Schmidt factors $\{s_k,\ k = 2 \ldots K\}$ of $|\Psi\rangle$ and therefore are orthogonal to $|a_1 b_1\rangle$.

□

A.6 Transformations which preserve entanglement

Theorem:

Let $\mathcal{H}_A$, $\mathcal{H}_B$ and $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$ be Hilbert spaces with $N_A = \dim \mathcal{H}_A$ and $N_B = \dim \mathcal{H}_B$ and let $\hat{A}$ and $\hat{B}$ denote arbitrary but nonsingular[2] operators which act on $\mathcal{H}_A$ and $\mathcal{H}_B$. The quantum state is described by the density operator $\hat{\rho}$. Then the new density operator $\hat{\tilde{\rho}}$ which is constructed by the transformation

$$\hat{\tilde{\rho}} = \mathcal{N}\, \hat{A}^\dagger \otimes \hat{B}^\dagger\, \hat{\rho}\, \hat{A} \otimes \hat{B} \tag{A.81}$$

with the normalization constant

$$\mathcal{N} \equiv Tr\Big\{ \hat{A}^\dagger \otimes \hat{B}^\dagger\, \hat{\rho}\, \hat{A} \otimes \hat{B} \Big\}^{-1} \tag{A.82}$$

is inseparable if and only if the density operator $\hat{\rho}$ is inseparable.

Proof:

The only if case[3]: Let

$$\hat{\rho}_{sep} = \sum_n p_n |a_n b_n\rangle\langle a_n b_n| \tag{A.83}$$

[1] This statement is valid if the largest Schmidt factor s_1 is not degenerate. Otherwise if the first q Schmidt factors are equal $s_1 = s_2 = \ldots = s_q$ the pure product state $|a_1 b_1\rangle$ is equal to one of the corresponding states $\{|\psi_k \varphi_k\rangle,\ k = 1 \ldots q\}$ of the Schmidt decomposition of $|\Psi\rangle$.

[2] That is, none of the eigenvalues of $\hat{A}$ and $\hat{B}$ vanish.

[3] An alternative proof for the only if case is given in [54].

be a separable density operator. By applying the transformation, Eq. (A.81), we get a new density operator

$$\hat{\tilde{\rho}} = \mathcal{N} \sum_n p_n \hat{A}^\dagger |a_n\rangle\langle a_n| \hat{A} \otimes \hat{B}^\dagger |b_n\rangle\langle b_n| \hat{B} \tag{A.84}$$

$$\equiv \sum_n \tilde{p}_n |\psi_n\rangle\langle\psi_n| \otimes |\varphi_n\rangle\langle\varphi_n| \tag{A.85}$$

where the new states are given by

$$|\psi_n\rangle \equiv \frac{\hat{A}|a_n\rangle}{\sqrt{\langle a_n|\hat{A}^\dagger\hat{A}|a_n\rangle}} \text{ and } |\varphi_n\rangle \equiv \frac{\hat{B}|b_n\rangle}{\sqrt{\langle b_n|\hat{B}^\dagger\hat{B}|b_n\rangle}}. \tag{A.86}$$

Due to Eq. (A.85) the new density operator $\hat{\tilde{\rho}}$ is by definition separable. Hence, it is impossible to create entanglement by applying the transformation, Eq. (A.81) and therefore $\hat{\tilde{\rho}}$ is inseparable only if $\hat{\rho}$ is.

The if case:

Let $\hat{\rho}$ be an inseparable state. Then, as discussed in subsection 3.2.2, there exists at least one entanglement indicator $\hat{O}$ such that the inequality

$$\mathrm{Tr}\left\{\hat{O}\hat{\rho}\right\} > \langle ab|\hat{O}|ab\rangle \tag{A.87}$$

holds for all pure product states $|ab\rangle \in \mathcal{H}$. With the help of the operator $\hat{O}$ we can define a new operator

$$\hat{O}_{pos} \equiv \hat{O} - c_{\max}\hat{\mathbb{1}} \tag{A.88}$$

where $c_{\max}$ denotes the maximal expectation value of $\hat{O}$ with respect to pure product states. This new operator fulfills the inequality

$$\mathrm{Tr}\left\{\hat{O}_{pos}\hat{\rho}\right\} > 0 \geq \langle ab|\hat{O}_{pos}|ab\rangle \quad \forall |ab\rangle \in \mathcal{H} \tag{A.89}$$

and therefore detects entanglement of $\hat{\rho}$.

By applying the transformation, Eq. (A.81), a new density operator $\hat{\tilde{\rho}}$ can be constructed. Due to the fact that $\hat{A}$ and $\hat{B}$ are nonsingular the inverse operators $\hat{A}^{-1}$ and $\hat{B}^{-1}$ exist. By using these operators we define the new entanglement indicator

$$\hat{\tilde{O}} = \left(\hat{A} \otimes \hat{B}\right)^{-1} \hat{O}_{pos} \left(\hat{A}^\dagger \otimes \hat{B}^\dagger\right)^{-1} \tag{A.90}$$

which fulfills the inequality

$$\mathrm{Tr}\left\{\hat{\tilde{O}}\hat{\tilde{\rho}}\right\} = \mathcal{N}\mathrm{Tr}\left\{\left(\hat{A}\otimes\hat{B}\right)^{-1}\hat{O}_{pos}\left(\hat{A}^{\dagger}\otimes\hat{B}^{\dagger}\right)^{-1}\hat{A}^{\dagger}\otimes\hat{B}^{\dagger}\,\hat{\rho}\,\hat{A}\otimes\hat{B}\right\} = \mathcal{N}\mathrm{Tr}\left\{\hat{O}_{pos}\hat{\rho}\right\} > 0.$$

The calculation of the expectation value of this operator with respect to arbitrary pure product states $|ab\rangle$ yields

$$\langle ab|\hat{\tilde{O}}|ab\rangle = \langle ab|\left(\hat{A}\otimes\hat{B}\right)^{-1}\hat{O}_{pos}\left(\hat{A}^{\dagger}\otimes\hat{B}^{\dagger}\right)^{-1}|ab\rangle \equiv \langle\psi\varphi|\hat{O}_{pos}|\psi\varphi\rangle \leq 0 \quad \text{(A.91)}$$

where the generally unnormalized pure product states

$$|\psi\varphi\rangle \equiv \left(\hat{A}^{\dagger}\otimes\hat{B}^{\dagger}\right)^{-1}|ab\rangle \quad \text{(A.92)}$$

have been introduced. Therefore the inequality

$$\mathrm{Tr}\left\{\hat{\tilde{O}}\hat{\tilde{\rho}}\right\} > \langle ab|\hat{\tilde{O}}|ab\rangle \quad \text{(A.93)}$$

holds for all pure product states and is sufficient to verify entanglement of $\hat{\tilde{\rho}}$. Hence, $\hat{\tilde{\rho}}$ is inseparable if $\hat{\rho}$ is.

□

Remarks:

1. The only if case of the theorem is equivalent to the well known statement [54], that entanglement cannot be created by local operations and classical communication.

2. The if case is an interesting extension of this statement, namely the entanglement of a quantum state *cannot be destroyed* by applying local operations which correspond to nonsingular operators $\hat{A}$ and $\hat{B}$.

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