The role of quantum correlations beyond entanglement in quantum information theory

Inaugural-Dissertation

zur Erlangung des Doktorgrades
der Mathematisch-Naturwissenschaftlichen Fakultät
der Heinrich-Heine-Universität Düsseldorf

vorgelegt von

Alexander Streltsov
aus Taganrog

Düsseldorf, Januar 2013

Aus dem Institut für Theoretische Physik, Lehrstuhl III
der Heinrich-Heine-Universität Düsseldorf

Gedruckt mit der Genehmigung der
Mathematisch-Naturwissenschaftlichen Fakultät der
Heinrich-Heine-Universität Düsseldorf

Referent: Prof. Dr. Dagmar Bruß
1. Koreferent: Prof. Dr. Dr. Carsten Müller
2. Koreferent: Prof. Dr. Norbert Lütkenhaus

Tag der mündlichen Prüfung: 14. Juni 2013

Acknowledgements

I thank the following persons:

- Prof. Dr. Dagmar Bruß for the supervision,
- Dr. Hermann Kampermann for useful criticism,
- Prof. Dr. Otfried Gühne, Dr. Tobias Moroder, and Dr. Matthias Kleinmann for useful comments,
- Silvestre Abruzzo, Sylvia Bratzik, Matteo Rossi, Dr. Zahra Shadman, Dr. Colin Wilmott, Junyi Wu, Michael Epping and all the other group members for discussion.

List of included publications

A. Streltsov, H. Kampermann, and D. Bruß, New J. Phys. **12**, 123004 (2010).

A. Streltsov, H. Kampermann, and D. Bruß, Phys. Rev. Lett. **107**, 170502 (2011).

A. Streltsov, H. Kampermann, and D. Bruß, Phys. Rev. Lett. **106**, 160401 (2011).

A. Streltsov, H. Kampermann, and D. Bruß, Phys. Rev. A **84**, 022323 (2011).

A. Streltsov, G. Adesso, M. Piani, and D. Bruß, Phys. Rev. Lett. **109**, 050503 (2012).

A. Streltsov, H. Kampermann, and D. Bruß, Phys. Rev. Lett. **108**, 250501 (2012).

Abstract

Quantum entanglement is the most popular kind of quantum correlations. Its role in several tasks in quantum information theory like quantum cryptography, quantum dense coding and quantum teleportation is indisputable. The role of entanglement in quantum algorithms has also attracted enormous amount of attention in the literature. The research in this direction is motivated by the finding that a quantum computer can efficiently factorize arbitrary integer numbers. Since no classical algorithm is known today that can solve this problem efficiently, this example clearly demonstrates the superiority of a quantum computer compared to its classical counterpart. In this context, entanglement also plays a crucial role: if the quantum computer operates on a pure state without entanglement, then the computational process can be simulated efficiently on a classical computer. In this case entanglement is the key ingredient that makes the difference between a quantum and a classical computer.

However, the situation is more involved if the computational process is not perfect. In this case the quantum computer operates on a mixed state, and the role of entanglement is less obvious. A seminal result in this direction is a quantum algorithm known under the acronym DQC1. This algorithm operates on an almost maximally mixed state with vanishingly little entanglement. However, DQC1 can still perform tasks efficiently for which no efficient classical algorithm is known today. Thus, it is reasonable to assume that entanglement in general is not related to the efficiency of a quantum algorithm.

Triggered by this observation other kinds of quantum correlations have been studied. In this context a particular measure of quantum correlations known as quantum discord is referred to frequently in the literature. Quantum discord is a measure of quantum correlations beyond entanglement, i.e., a quantum state can have no entanglement, but nonvanishing quantum discord. Quantum discord is also regarded as the key resource in the DQC1 algorithm. Although this statement is still controversial, it was shown under very general assumptions that quantum discord is required if a quantum computer is to show an exponential speedup over any classical algorithm.

In this thesis we give a short introduction into the theory of entanglement and general quantum correlations, and further discuss our results. In particular, we show that two different kinds of entanglement measures can coincide. This result is used to build an algorithm for computing entanglement. We also consider the role of quantum correlations for the distribution of entanglement and for the quantum measurement process. We further discuss the behavior of quantum correlations under local noise, and their monogamy properties.

Zusammenfassung

Quantenverschränkung ist zweifelsfrei die bekannteste Art von Quantenkorrelationen. In diversen Anwendungen der Quanteninformationstheorie, wie Quantenkryptographie, superdichte Kodierung und Quantenteleportation, ist die Rolle von Quantenverschränkung unumstritten. Die Bedeutung von Verschränkung in Quantenalgorithmen wird auch heute noch intensiv erforscht. Dies wurde insbesondere durch die Entdeckung gefördert, dass ein Quantencomputer beliebige Zahlen effizient faktorisieren kann. Da bis heute kein klassischer Algorithmus bekannt ist, der diese Aufgabe effizient lösen kann, demonstriert dieses Beispiel deutlich die Überlegenheit eines Quantencomputers gegenüber einem klassischen Computer. Dabei spielt auch die Verschränkung eine wesentliche Rolle: wird der Quantencomputer mit einem reinen Zustand ohne Verschränkung betrieben, so kann der gesamte Rechenprozess effizient auf einem klassischen Computer simuliert werden. Die Verschränkung ist also in diesem Fall die wesentliche Zutat, die einen Quantencomputer von einem klassischen unterscheidet.

Jedoch ist die Rolle der Verschränkung weniger offensichtlich, wenn der Quantencomputer auf einem gemischten Zustand arbeitet. Ein bahnbrechendes Ergebnis in diesem Zusammenhang ist ein Quantenalgorithmus, der unter der Abkürzung DQC1 bekannt ist. Dieser Algorithmus arbeitet auf einem fast vollständig gemischten Zustand mit verschwindend geringer Verschränkung. Trotzdem kann DQC1 bestimmte Aufgaben effizient lösen, für die heute kein effizientes klassisches Lösungsverfahren bekannt ist. Deswegen muss davon ausgegangen werden, dass Verschränkung im Allgemeinen wenig über die Effizient eines Quantenalgorithmus aussagt.

Diese Beobachtung führte zur Untersuchung anderer Arten von Quantenkorrelationen. Insbesondere wird dabei häufig Quantum Discord (dt.: Missklang) genannt. Quantum Discord ist ein Quantenkorrelationsmaß, welches über die Verschränkung hinausgeht. Obwohl nicht unumstritten, wird Quantum Discord als der essenzielle Parameter im DQC1 Algorithmus angesehen. Zudem wurde unter sehr allgemeinen Voraussetzungen gezeigt, dass Quantum Discord notwendig ist, sollte ein Quantenalgorithmus Probleme effizient lösen können, die nicht in polynomieller Zeit auf einem klassischen Computer lösbar sind.

In dieser Arbeit gehen wir kurz auf die Grundlagen der Quantenverschränkung und allgemeiner Quantenkorrelationen ein. Anschließend diskutieren wir unsere Ergebnisse. Zunächst stellen wir unsere Beiträge zur Theorie der Verschränkung dar. Dabei zeigen wir, dass zwei verschiedene Arten von Verschränkungsmaßen zusammenfallen können. Dieses Ergebnis wird benutzt, um Algorithmen zur Berechnung von Verschränkung zu finden. Danach betrachten wir die Rolle der Quantenkorrelationen beim Verteilen von Verschränkung und im Messprozess. Ferner diskutieren wir das Verhalten von Quantenkorrelationen unter lokalem Rauschen und ihre Monogamieeigenschaften.

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1 Introduction

Quantum entanglement has fascinated the minds of physicists since the very inception of quantum theory (Schrödinger, 1935). Entangled quantum systems can behave in a bizarre way, exhibiting features which seem to contradict "our common sense notions of how the world works" (Nielsen and Chuang, 2000, p. 114). This was first pointed out in a seminal work by Einstein, Podolsky, and Rosen, who concluded that the quantum theory must be incomplete (Einstein *et al.*, 1935). In a later correspondence to Max Born, Einstein even called entanglement a "spooky action at a distance".

However, about 30 years after Einstein's objection, Bell proposed an experiment, which aimed to distinguish between predictions made by quantum theory on the one hand, and Einstein's arguments on the other hand (Bell, 1964). Bell's ideas served as a starting point for Clauser, Horne, Shimony, and Holt, who formulated an inequality which is known today as the CHSH inequality (Clauser *et al.*, 1969). Following Einstein *et al.*, Nature should respect the CHSH inequality, and the fact that it can be violated in quantum theory demonstrates the incompleteness of quantum mechanics.

Due to its simplicity, the CHSH inequality could be tested experimentally by Freedman and Clauser already short time after its discovery (Freedman and Clauser, 1972). The data showed a violation of the CHSH inequality, thus invalidating Einstein's arguments, in favor of the quantum mechanical description of Nature. Later in the years 1981/82 Aspect *et al.* performed three experiments (Aspect *et al.*, 1981, 1982a,b), confirming the results of Freedman and Clauser. Since that time, several experiments have demonstrated violation of the CHSH inequality, although some loopholes still remained open (Horodecki *et al.*, 2009).

The formal definition of entanglement as we use it today can be dated back to the year 1989, when Werner extended the concept of entanglement to all mixed quantum states (Werner, 1989). Werner's work can be regarded as the starting point for the theory of entanglement, which studies properties and implications of entanglement, and its role in such fundamental tasks like quantum cryptography (Ekert, 1991), quantum dense coding (Bennett and Wiesner, 1992) and quantum teleportation (Bennett *et al.*, 1993). Several important contributions to the theory of entanglement also came from the Horodecki family: one example is the discovery of "bound" entanglement (Horodecki *et al.*, 1998). Bound entangled states need some amount of entanglement to be created, but cannot be used for the extraction of any pure entangled state. A comprehensive review on this topic can be found in (Horodecki *et al.*, 2009).

The role of entanglement in quantum algorithms is still subject of extensive debate. This is due to the results by Jozsa and Linden, who showed that a quantum computer operating on a pure state needs entanglement in order to have an exponential speedup compared to classical computation (Jozsa, 1997; Jozsa and Linden, 2003). Although exponential speedup of a quantum computer is not yet rigorously proven, there is strong evidence for its existence. One of the most prominent examples pointing in this direction is Shor's prime factorization algorithm proposed in (Shor, 1994). The algorithm is able to find the prime factors for any product of two primes on a quantum computer, where the time for the computation grows polynomially in the number of input bits. This is significantly faster, compared to the best known classical algorithm, which exhibits an exponential increase of the running time.

Due to the presence of entanglement in Shor's algorithm (Jozsa and Linden, 2003) one might be tempted to see entanglement as the key resource for quantum computation. While for *pure state* quantum computation this is indeed the case, the situation becomes more involved if *mixed state* quantum computation is considered (Jozsa and Linden, 2003). A popular example for mixed state quantum computation has been presented by Knill and Laflamme (Knill and Laflamme, 1998). Surprisingly, their algorithm does not require any entanglement, while still being able to solve certain problems efficiently, for which no efficient classical algorithm is known (Datta *et al.*, 2005). This finding triggered the search for quantum correlations beyond entanglement, which should be responsible for the efficiency of a quantum computer.

Quantum discord, introduced by Zurek in the year 2000, has been recognized as a possible candidate for those general quantum correlations (Zurek, 2000; Ollivier and Zurek, 2001). On the one hand, quantum discord can even exist in systems which are not entangled. On the other hand, it has been shown that the algorithm presented by Knill and Laflamme exhibits nonvanishing amount of discord (Datta *et al.*, 2008). An even stronger statement has been made by Eastin, who showed that mixed state quantum computation with zero discord in each step can be simulated efficiently on a classical computer (Eastin, 2010).

In the light of these results, it is not surprising that an enormous amount of research has been devoted to this topic in the last few years. Three years after Zurek has proposed quantum discord as a new kind of quantum correlations beyond entanglement, he gave it an alternative thermodynamical interpretation (Zurek, 2003). He considered the amount of work which can be extracted from a quantum system by a classical and a quantum Maxwell's demon. He showed that the quantum demon is more powerful, since it can operate on the whole quantum state, while the classical demon is restricted to local subsystems only. Zurek concluded that more work can be extracted in the quantum case, and this quantum advantage is related to the quantum discord.

Approximately at the same time when Zurek defined quantum discord, a closely related quantity has been proposed by Henderson and Vedral (Henderson and Vedral, 2001). The authors aim to separate correlations into quantum and purely classical parts by postulating several reasonable properties. This approach is significantly different from Zurek's, and the fact that both arrive at the same result is surprising. Another related quantity is the *information deficit*, presented in (Oppenheim *et al.*, 2002). The authors study the amount of work, which can be extracted from a heat bath using a mixed quantum state. If the mixed state is shared by two parties, the amount of extractable work is usually smaller, compared to the case where the whole state is in possession of a single party. The difference of these two quantities is the information deficit.

In the following years several interpretations for quantum discord and related quantities have been presented by different authors. They range from the role of quantum discord in the task known as *quantum state merging* (Madhok and Datta, 2011; Cavalcanti *et al.*, 2011) to the generation of entanglement between the system and the measurement apparatus in the measurement process (Streltsov *et al.*, 2011b; Piani *et al.*, 2011). Quantum correlations like the information deficit were also shown to be the key resource for the task of entanglement distribution (Streltsov *et al.*, 2012b; Chuan *et al.*, 2012). Experiments demonstrating the role of quantum discord for remote state preparation (Dakić *et al.*, 2012) and information encoding (Gu *et al.*, 2012) have also been devised. More references can be found in the recent review article on this topic (Modi *et al.*, 2012).

This thesis is organized as follows:

- in Chapter 2 we present the basic mathematical framework used in this work,
- in Chapter 3 we give an introduction into the theory of quantum entanglement,
- in Chapter 4 we present the definition and basic properties of general quantum correlations beyond entanglement,
- in Chapter 5 we summarize our contributions to the discussion on quantum entanglement and general quantum correlations beyond entanglement,
- in Chapter 6 we give an outlook for possible future research,
- in Chapter 7 we give a short list of main results.

All six publications which are referred to in Chapter 5 can be found in the attachment of this thesis.

2 Mathematical framework

In this chapter we present the mathematical framework which will be used in this thesis. If not otherwise stated, the material presented in this chapter is taken from (Nielsen and Chuang, 2000).

2.1 Quantum states

In quantum mechanics, any physical system is completely described by a state vector $|\Psi\rangle$ in a Hilbert space $\mathcal{H}$. A system with a two-dimensional Hilbert space is also called a *qubit* (quantum bit). If not otherwise stated, we consider a Hilbert space with an arbitrary but finite dimension. For two parties, Alice (A) and Bob (B), with Hilbert spaces $\mathcal{H}_A$ and $\mathcal{H}_B$ the total Hilbert space is a tensor product of the subsystem spaces: $\mathcal{H}_{AB} = \mathcal{H}_A \otimes \mathcal{H}_B$.

Any system which is described by a single state vector is said to be in a *pure state*. However, in a realistic experimental setup the physical state of the considered system is not completely known. If the system is in the pure state $|\psi_i\rangle$ with probability p_i, the physical state of the system can be described using the *density operator*

$$\rho = \sum_i p_i \, |\psi_i\rangle \langle\psi_i| \, . \tag{2.1}$$

The state of such a system is called *mixed state*. In the following, whenever we talk about quantum states, we usually mean mixed states.

In order to have a meaningful physical interpretation, any density operator has the following two properties:

- ρ has trace equal to one:
$$\mathrm{Tr}[\rho] = 1, \tag{2.2}$$
- ρ is a positive operator:
$$\langle\psi|\rho|\psi\rangle \geq 0 \tag{2.3}$$
  for any vector $|\psi\rangle$.

Note that the second property also implies that ρ is Hermitian: $\rho^\dagger = \rho$. These two condition are essential for the definition of quantum measurements and operations, which is presented in the following.

2.2 Quantum measurements and operations

Quantum measurement is one of the most important concepts in quantum theory. Most physicists are familiar with the *projective measurement*: for a spin-$\frac{1}{2}$ particle in the state

$$|\psi\rangle = a\,|\!\uparrow\rangle + b\,|\!\downarrow\rangle\,, \tag{2.4}$$

the probability to measure "spin up" or "spin down" is given by $p(\uparrow) = |a|^2$ or $p(\downarrow) = |b|^2 = 1 - p(\uparrow)$. Moreover, the measurement postulate of quantum mechanics tells us that the quantum state after the measurement is either $|\!\uparrow\rangle$ or $|\!\downarrow\rangle$, depending on the outcome of the measurement.

In quantum information theory, a more general definition is considered. A general quantum measurement is described by a collection $\{E_i\}$ of *measurement operators* that satisfy the completeness equation:

$$\sum_i E_i^\dagger E_i = \mathbb{1}, \tag{2.5}$$

where $\mathbb{1}$ is the identity operator. Given a density operator ρ and the set of measurement operators $\{E_i\}$, the probability that the result i occurs is given by

$$p(i) = \mathrm{Tr}[E_i^\dagger E_i \rho]. \tag{2.6}$$

After the measurement with outcome i, the state of the system is described by the following density operator:

$$\frac{E_i \rho E_i^\dagger}{\mathrm{Tr}[E_i^\dagger E_i \rho]}. \tag{2.7}$$

The positivity of the density operator ρ in Eq. (2.3) implies that all probabilities are nonnegative: $p(i) \geq 0$. The completeness equation (2.5) together with Eq. (2.2) implies that the probabilities sum up to one: $\sum_i p(i) = 1$.

For a projective measurement, the operators E_i are orthogonal projectors: $E_i E_j = \delta_{ij} E_i$. Such a measurement was considered below Eq. (2.4), there the measurement operators are $E_\uparrow = |\!\uparrow\rangle\langle\uparrow\!|$, and $E_\downarrow = |\!\downarrow\rangle\langle\downarrow\!|$. *Von Neumann measurement* is a special projective measurement, where the measurement operators E_i are orthogonal projectors with rank one. In general, the measurement operators do not have to be projectors, they only need to satisfy the completeness equation (2.5). However, any general quantum measurement on a state described by the density operator ρ can be seen as a projective measurement on a larger system with the density operator $\rho \otimes \rho_{\mathrm{aux}}$, where ρ_{aux} is the density operator of an auxiliary system (Peres, 1995, p. 282ff.). General measurements are also called *POVMs* (Positive Operator-Valued Measure).

For composite systems consisting of two subsystems, Alice and Bob, it is possible to perform *local measurements* on one of the subsystems. If a local measurement is done on Alice's subsystem, the subsystem of Bob remains unchanged. In this case, the measurement operators have the form $E_i = E_i^A \otimes \mathbb{1}^B$, with the identity operator $\mathbb{1}^B$ on Bob's Hilbert space. Similarly, measurement operators corresponding to local measurement on Bob's subsystem have the form $E_i = \mathbb{1}^A \otimes E_i^B$.

Finally, we also mention the concept of *quantum operations*, which is closely related to quantum measurements. Any set of measurement operators $\{E_i\}$ can also be called a quantum operation. The corresponding operators E_i are then called *Kraus operators*. The action of a quantum operation $\{E_i\}$ on a density operator ρ is given by

$$\Lambda(\rho) = \sum_i E_i \rho E_i^\dagger. \tag{2.8}$$

For composite systems, *local quantum operations* can be defined in the same way as it was done for local measurements. The importance of quantum operations lies in the fact that they describe the most general change of a quantum state possible in experiments. Quantum operations also play an important role in the study of noisy systems: noise is usually modeled as a quantum operation. They are also essential for the theory of quantum entanglement and general quantum correlations, as will be discussed later in this thesis.

2.3 Reduced density operator

Sometimes one is only interested in one of the subsystems, e.g., A. This situation is captured by the concept of the *reduced density operator*. If the total system is described by the density operator ρ^{AB}, then the system of A is described by the reduced density operator

$$\rho^A = \mathrm{Tr}_B[\rho^{AB}], \tag{2.9}$$

where Tr_B is called *partial trace* over subsystem B. The partial trace is defined by

$$\mathrm{Tr}_B[|a_1\rangle\langle a_2| \otimes |b_1\rangle\langle b_2|] = |a_1\rangle\langle a_2| \,\mathrm{Tr}[|b_1\rangle\langle b_2|], \tag{2.10}$$

where $|a_1\rangle$ and $|a_2\rangle$ are any two vectors in $\mathcal{H}_A$, and $|b_1\rangle$ and $|b_2\rangle$ are any two vectors in $\mathcal{H}_B$. The trace on the right hand side is the usual trace for the subsystem B: $\mathrm{Tr}[|b_1\rangle\langle b_2|] = \langle b_2|b_1\rangle$. In addition to Eq. (2.10), we also require that the partial trace is linear, i.e., $\mathrm{Tr}_B[M^{AB} + N^{AB}] = \mathrm{Tr}_B[M^{AB}] + \mathrm{Tr}_B[N^{AB}]$ for any two operators M^{AB} and N^{AB}. In this way, the partial trace is defined for all density operators. The physical meaning of the partial trace lies in the fact that it is the unique operation for obtaining correct measurement statistics for the subsystem A (Nielsen and Chuang, 2000, p. 105ff.).

2.4 Entropy and mutual information

The *von Neumann entropy* of a quantum state with density operator ρ is defined as

$$S(\rho) = -\mathrm{Tr}[\rho \log_2 \rho], \tag{2.11}$$

where the logarithm of the density operator ρ is defined via its eigenvalues λ_i and eigenstates $|i\rangle$ in the following way: $\log_2 \rho = \sum_i \log_2(\lambda_i) |i\rangle \langle i|$. With this definition, the entropy can be written as

$$S(\rho) = -\sum_i \lambda_i \log_2 \lambda_i, \tag{2.12}$$

where it is defined that $0 \log_2 0 = 0$.

The von Neumann entropy is the quantum version of the classical *Shannon entropy*. For a discrete random variable X which can take a value x with probability p_x, the Shannon entropy is defined as

$$H(X) = -\sum_x p_x \log_2 p_x. \tag{2.13}$$

Similar to the Shannon entropy, which measures the uncertainty of a classical random variable, the von Neumann entropy measures the uncertainty of a quantum state. Pure states represent full knowledge about a quantum system: their von Neumann entropy is zero. On the other hand, for a d-dimensional Hilbert space, maximal uncertainty is represented by the completely mixed density operator $\mathbb{1}/d$ with the von Neumann entropy $\log_2 d$.

For two parties, the von Neumann entropy can be used to define the *mutual information* between the parties. If the total state is given by the density operator ρ^{AB} with reduced density operators ρ^A and ρ^B, the mutual information is defined as

$$I(\rho^{AB}) = S(\rho^A) + S(\rho^B) - S(\rho^{AB}). \tag{2.14}$$

The mutual information is zero if the state is completely uncorrelated, i.e., if the density operator has the form $\rho^{AB} = \rho^A \otimes \rho^B$. Otherwise, the mutual information is greater than zero: it measures the amount of correlations between A and B.

Closely related to the von Neumann entropy is the *quantum relative entropy*. For two density operators ρ and σ it is defined as

$$S(\rho\|\sigma) = \mathrm{Tr}[\rho \log_2 \rho] - \mathrm{Tr}[\rho \log_2 \sigma]. \tag{2.15}$$

The quantum relative entropy is zero if $\rho = \sigma$, and greater than zero otherwise. As a fundamental quantity, relative entropy is frequently used in quantum information theory, especially in the study of quantum entanglement and quantum correlations, as will be shown later in this thesis. At this point we only mention that the mutual information defined in Eq. (2.14) can be written as the relative entropy between the density operator ρ^{AB} and the tensor product of the reduced density operators $\rho^A \otimes \rho^B$ (Vedral, 2002):

$$I(\rho^{AB}) = S(\rho^{AB}\|\rho^A \otimes \rho^B). \tag{2.16}$$

2.5 Distance between density operators

Given two quantum states, how "close" are they to each other? This question, posed in (Nielsen and Chuang, 2000, p. 403), can be answered by defining an appropriate distance onto the set of density operators. One important and frequently used distance is the *trace distance*

$$D_t(\rho, \sigma) = \frac{1}{2}\mathrm{Tr}|\rho - \sigma|, \tag{2.17}$$

where ρ and σ are any two density operators, $|M| = \sqrt{M^\dagger M}$ is the trace norm of an operator M, and the square root of a Hermitian operator $M^\dagger M$ with nonnegative eigenvalues λ_i and eigenstates $|i\rangle$ is defined as $\sqrt{M^\dagger M} = \sum_i \sqrt{\lambda_i} |i\rangle \langle i|$. The trace distance satisfies all properties of a general mathematical distance D:

- $D(\rho, \sigma) \geq 0$, and $D(\rho, \sigma) = 0$ holds if and only if $\rho = \sigma$,
- D is symmetric: $D(\rho, \sigma) = D(\sigma, \rho)$,
- D satisfies the triangle inequality: $D(\rho, \tau) \leq D(\rho, \sigma) + D(\sigma, \tau)$ for any three density operators ρ, σ, and τ.

In quantum information theory, the trace distance has an important interpretation: $\frac{1}{2} + \frac{1}{2}D_t(\rho, \sigma)$ is the optimal probability of success for distinguishing two quantum states with density operators ρ and σ (Fuchs and van de Graaf, 1997).

Another frequently used quantity is the *fidelity*. For two density operators ρ and σ it is defined as

$$F(\rho, \sigma) = \left(\mathrm{Tr}\sqrt{\sqrt{\rho}\sigma\sqrt{\rho}}\right)^2. \tag{2.18}$$

The fidelity itself is not a distance, since it is one if and only if $\rho = \sigma$, and smaller than one otherwise. However, the fidelity can be used to define the *Bures distance*: $D_B(\rho, \sigma) = 2(1 - \sqrt{F(\rho, \sigma)})$, which satisfies all properties of a mathematical distance.

Both, the trace distance and the Bures distance have also another important property, namely they are *nonincreasing under quantum operations*:

$$D(\Lambda(\rho), \Lambda(\sigma)) \leq D(\rho, \sigma), \tag{2.19}$$

where ρ and σ are any two density operators, and Λ is any quantum operation. This property is frequently used in quantum information theory, especially in studying entanglement and other quantum correlations.

Note that inequality (2.19) does not follow from the general properties of a mathematical distance, and thus there exist distances which violate it. One such distance is the *Hilbert-Schmidt distance*

$$D_{HS}(\rho, \sigma) = \|\rho - \sigma\|^2, \tag{2.20}$$

where $||M|| = \sqrt{\mathrm{Tr}[M^\dagger M]}$ is the square norm, or the Hilbert-Schmidt norm of an operator M. For the Hilbert-Schmidt distance violation of Eq. (2.19) was shown in (Ozawa, 2000; Piani, 2012).

Finally, the relative entropy introduced in Eq. (2.15) is not a distance in the mathematical sense since it is not symmetric, and also does not satisfy the triangle inequality. However, the relative entropy is nonincreasing under quantum operations, i.e., it satisfies the inequality (2.19) (Vedral, 2002).

3 Quantum entanglement

In this chapter we will discuss basic definition and properties of quantum entanglement. A detailed review on this topic can be found in (Horodecki *et al.*, 2009). If not otherwise stated, the material presented in this chapter is taken from (Horodecki *et al.*, 2009).

3.1 Definition

For two parties, Alice (A) and Bob (B), states of the total quantum system can have product form[1]:

$$|\Psi\rangle = |a\rangle \otimes |b\rangle\,, \tag{3.1}$$

where the states $|a\rangle$ and $|b\rangle$ are elements of the corresponding local Hilbert spaces $\mathcal{H}_A$ and $\mathcal{H}_B$. States of the form given in Eq. (3.1) are not entangled, they are also called *separable*. However, not all states are separable, since quantum mechanics also allows superpositions which are not necessarily product:

$$|\Phi\rangle = \frac{1}{N}(|a_1\rangle \otimes |b_1\rangle + |a_2\rangle \otimes |b_2\rangle), \tag{3.2}$$

where N assures normalization such that $\langle\Phi|\Phi\rangle = 1$. If $|\Phi\rangle$ cannot be written as a product, i.e., $|\Phi\rangle \neq |a\rangle \otimes |b\rangle$, the state is called *entangled*.

Example. The singlet state $|\Phi\rangle = \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle)$ is entangled, it cannot be written as a product.

A mixed state is separable if the corresponding density operator can be written as a convex combination of pure product states (Werner, 1989):

$$\rho_{\mathrm{sep}} = \sum_i p_i\, |a_i\rangle\langle a_i| \otimes |b_i\rangle\langle b_i|\,. \tag{3.3}$$

The pure states $|a_i\rangle$ and $|b_i\rangle$ are elements of the local Hilbert spaces $\mathcal{H}_A$ and $\mathcal{H}_B$, and $p_i \geq 0$ are probabilities summing up to one: $\sum_i p_i = 1$. If the density operator cannot be written in this form, the state is called entangled.

The idea behind this definition of entanglement is the following: suppose that Alice and Bob are able to produce any quantum state locally. In addition, they have access to a classical communication channel, such as a telephone. Then, Alice and Bob can produce any separable state

[1] Sometimes we write $|a\rangle|b\rangle$ or $|ab\rangle$ instead of $|a\rangle \otimes |b\rangle$.

with density operator as given in Eq. (3.3) by the following procedure: Alice prepares the state $|a_i\rangle$ with the probability p_i, and lets Bob know which state she prepared. Depending on this information, Bob prepares the corresponding state $|b_i\rangle$. On the other hand, it is not possible to create entangled states such as the singlet state in this way.

3.2 Local operations and classical communication (LOCC)

The process for creating separable states presented above belongs to the class of *local operations and classical communication* (LOCC), first introduced in (Bennett *et al.*, 1996c). This class of operations describes the most general procedure Alice and Bob can apply in quantum theory, if they are limited to classical communication only. The full mathematical description of these operations is demanding, and still subject of extensive research (Chitambar *et al.*, 2012). However, the general idea is simple, and will be explained in the following.

For two parties, Alice and Bob, a quantum operation Λ_{LOCC} belongs to the class of LOCC, if it can be decomposed into the following steps:

1. One of the parties, e.g. Alice, performs a local measurement on her subsystem.
2. The outcome of the measurement is communicated *classically* to the other party, here Bob.
3. Depending on the received information, Bob performs a local measurement on his subsystem.
4. The outcome of Bob's measurement is communicated *classically* to Alice.
5. Depending on the received information, Alice performs a local measurement on her subsystem, and the process starts over at step 2.

The class of LOCC plays an important role in quantum information theory, especially when studying entanglement. As we have mentioned above, any separable state can be created with LOCC. On the other hand, LOCC cannot be used to create entangled states (Horodecki *et al.*, 2009).

3.3 Entanglement as a resource

Until the 1990s, quantum entanglement was mainly regarded as a physical curiosity: an exotic feature with no practical use. This situation started to change in 1991, when Ekert presented the first task in quantum information theory which based on entanglement (Ekert, 1991). In his work, Ekert showed that if two parties, Alice and Bob, share a large amount of entangled singlet states, they can communicate in a completely secure way. This task is referred to as *quantum* *cryptography*, or *quantum key distribution*. This strong result should be compared to the classical cryptography as we use it today. The security of classical cryptography is mainly based on the conjecture that a large number is hard to factorize, whereas the quantum cryptography protocol presented by Ekert is provably secure.

Motivated by Ekert's result, several tasks involving entanglement have been presented in the following years. In 1992 Bennett and Wiesner showed that two entangled parties can communicate two classical bits by sending only one qubit, i.e., one quantum system on a two-dimensional Hilbert space (Bennett and Wiesner, 1992). This task is also known as *quantum dense coding*, since it suggests that two classical bits can be coded into one quantum bit.

Another application for entanglement has been proposed in (Bennett *et al.*, 1993). The authors studied the task of communicating an unknown quantum state between two parties. An unknown quantum state cannot be communicated by classical means, which is a direct consequence of the fact that such a state cannot be cloned (Wootters and Zurek, 1982). However, if the two parties share an entangled singlet, Bennett *et al.* showed that any unknown quantum bit can be perfectly communicated. This task is also known as *quantum teleportation*.

Entanglement was also proposed to be the resource for quantum computation. In particular, Jozsa claimed in 1997 that entanglement is essential, if a quantum computer is to show an exponential speed-up over its classical counterpart (Jozsa, 1997). This statement was studied in greater detail in (Jozsa and Linden, 2003). The authors considered the scenario of *pure state* quantum computation, where the state of the quantum computer remains pure during the entire computational process. The authors proved that a quantum computation can be simulated efficiently on a classical computer if the amount of entanglement in the computational process does not depend on the length of the input. This was the first quantitative result, proving that entanglement must grow in the input length, if a pure state quantum computer is to show an exponential speed-up over classical computation.

However, the role of entanglement is less clear if the quantum computer is not restricted to pure states, but is also allowed to operate on *mixed states*. One such algorithm was devised in (Knill and Laflamme, 1998). The authors considered the scenario where the initial state consists of one qubit in a pure state, together with an arbitrary amount of completely mixed qubits. The authors called their procedure *deterministic quantum computation with one quantum bit* (*DQC1*). Surprisingly, DQC1 is able to perform useful tasks, like the computation of the trace of a large unitary matrix (Laflamme *et al.*, 2002) exponentially faster than any known classical algorithm even with a vanishing amount of entanglement (Datta *et al.*, 2005). This finding triggered the research of quantum correlations beyond entanglement, which should be responsible for the power of a quantum computer. We will come back to these general quantum correlations and the DQC1 algorithm in Chapter 4.

3.4 Entanglement measures

The tasks presented above, namely quantum cryptography, dense coding and teleportation demonstrate the role of entanglement for a very special case. In particular, two parties, Alice and Bob, need to share entangled singlets in order to perform these tasks. However, a pure quantum state is not necessarily a singlet, and in a realistic scenario the quantum state is usually mixed. For this reason it is natural to ask whether a general mixed quantum state can also be used for some of these tasks.

The "usefulness" of a quantum state for one of the tasks presented above is usually quantified by the amount of entanglement contained in the state. One of the most popular quantifiers is the *distillable entanglement* (Bennett *et al.*, 1996b): it is defined as the number of singlets that can be obtained per copy of a given mixed state via local operations and classical communication, if the number of copies goes to infinity[2]. The major disadvantage of the distillable entanglement is the fact that it is hard to evaluate. Thus, exact expressions are only known in a few special cases. For this reason, other quantifiers, known as *entanglement measures*, have been proposed in the literature. Any entanglement measure E fulfills the following two properties (Horodecki *et al.*, 2009):

1. E does not increase under local operations and classical communication,

2. E vanishes on separable states.

Before we present entanglement measures for general mixed states, we consider the case of pure states in the following section.

3.4.1 Pure states

For a pure state $|\psi\rangle^{AB}$ distributed between two parties, Alice and Bob, entanglement is usually quantified by the von Neumann entropy of the reduced density operator $\rho^A = \mathrm{Tr}_B[|\psi\rangle\langle\psi|^{AB}]$:

$$E(|\psi\rangle^{AB}) = S(\rho^A) = -\sum_i \lambda_i \log_2 \lambda_i, \tag{3.4}$$

where λ_i are the eigenvalues of ρ^A. The importance of this quantity in quantum information theory comes from the fact that it is equal to the distillable entanglement for all pure states (Bennett *et al.*, 1996a).

So far we considered bipartite scenario, where the state was distributed between two parties. For *multipartite* pure states, i.e., states which are distributed between more than two parties, the situation becomes more involved. Similar to the definition of a bipartite separable state in Eq.

[2]See also (Horodecki *et al.*, 2009) for a formal definition.

(3.1) on page 10, an n-partite pure state on a Hilbert space $\mathcal{H}_1 \otimes \ldots \otimes \mathcal{H}_n$ is separable, if it can be written as a tensor product of n states:

$$|\phi\rangle = |\phi^1\rangle \otimes |\phi^2\rangle \otimes \ldots \otimes |\phi^n\rangle\,, \tag{3.5}$$

where each state $|\phi^i\rangle$ is element of the corresponding Hilbert space $\mathcal{H}_i$. Otherwise the state is n-partite entangled. The amount of entanglement in a multipartite pure state can be quantified using the *geometric measure of entanglement* (Shimony, 1995; Barnum and Linden, 2001; Wei and Goldbart, 2003):

$$E_G(|\psi\rangle) = \min_{|\phi\rangle\in\mathcal{S}} \left(1 - |\langle\psi|\phi\rangle|^2\right), \tag{3.6}$$

where the minimum is taken over the set of separable states $\mathcal{S}$, i.e., over states $|\phi\rangle$ of the form (3.5). The geometric measure of entanglement plays an important role in entanglement theory, in particular for studying multipartite systems. Moreover, its role for quantum computation has also been investigated: Gross *et al.* used this quantity to show that "most quantum states are too entangled to be useful as computational resources" (Gross *et al.*, 2009).

3.4.2 Mixed states

Two main classes of entanglement measures for mixed states are considered in the literature. These are

- convex roof measures and
- distance-based measures.

Any measure of entanglement E which is defined on all pure states can be extended to mixed states via the following *convex roof* construction (Uhlmann, 1998):

$$E(\rho) = \inf_{\{p_i,|\psi_i\rangle\}} \sum_i p_i E(|\psi_i\rangle), \tag{3.7}$$

where the infimum is taken over all decompositions $\{p_i, |\psi_i\rangle\}$ of the given density operator ρ with nonnegative probabilities p_i, i.e., $\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$.

For bipartite systems, the *entanglement of formation* defined in (Bennett *et al.*, 1996c) is one of the most popular and frequently used convex roof measures. For pure states it is defined as the von Neumann entropy of the reduced density operator in Eq. (3.4). The extension to mixed states is done via the convex roof construction in Eq. (3.7). Although the infimum in Eq. (3.7) is hard to evaluate in general, Wootters presented a closed expression for the entanglement of formation for all mixed states of two qubits (Wootters, 1998). For any such state, the entanglement of formation E_f is given by

$$E_f(\rho) = h\left(\frac{1}{2} + \frac{1}{2}\sqrt{1 - C^2(\rho)}\right) \tag{3.8}$$

with the binary entropy $h(x) = -x\log_2 x - (1-x)\log_2(1-x)$, and the concurrence $C(\rho) = \max\{0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4\}$, where λ_i are the square roots of the eigenvalues of $\rho\tilde{\rho}$ in decreasing order, and $\tilde{\rho}$ is defined as $\tilde{\rho} = (\sigma_y \otimes \sigma_y)\rho^*(\sigma_y \otimes \sigma_y)$ with the Pauli matrix $\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$.

The geometric measure of entanglement, defined for pure states in Eq. (3.6), can also be extended to mixed states via the convex roof construction (Wei and Goldbart, 2003). In contrast to the entanglement of formation, which is only defined for two parties, the geometric measure of entanglement can also be used to quantify multipartite entanglement in mixed states. Similar to the definition of a bipartite separable mixed state in Eq. (3.3) on page 10, a mixed state on a Hilbert space $\mathcal{H} = \mathcal{H}_1 \otimes \ldots \otimes \mathcal{H}_n$ is n-partite separable if the corresponding density operator can be written as a convex combination of pure n-partite product states:

$$\rho_{\mathrm{sep}} = \sum_i p_i \left|\phi_i^1\right\rangle\left\langle\phi_i^1\right| \otimes \left|\phi_i^2\right\rangle\left\langle\phi_i^2\right| \otimes \ldots \otimes \left|\phi_i^n\right\rangle\left\langle\phi_i^n\right|, \tag{3.9}$$

where each pure state $|\phi_i^j\rangle$ is an element of the corresponding Hilbert space $\mathcal{H}_j$. Otherwise the state is called n-partite entangled.

Both entanglement measures presented so far, the entanglement of formation and the geometric measure of entanglement, satisfy the criteria for a proper entanglement measure given on page 13: they do not increase under local operations and classical communication and vanish on separable states. While the second property is easy to verify for both measures, the first property was shown in (Bennett *et al.*, 1996c) for the entanglement of formation and in (Wei and Goldbart, 2003) for the geometric measure of entanglement.

The second main class of entanglement measures are measures based on distance proposed in (Vedral *et al.*, 1997). All those measures can be written as

$$E(\rho) = \inf_{\sigma \in \mathcal{S}} D(\rho, \sigma), \tag{3.10}$$

where D is a distance, and the infimum is taken over the set of density operators $\mathcal{S}$ corresponding to separable states. If the distance D does not increase under quantum operations, i.e.,

$$D(\rho, \sigma) \geq D(\Lambda(\rho), \Lambda(\sigma)) \tag{3.11}$$

for any quantum operation Λ and any two density operators ρ and σ, then the corresponding measure of entanglement does not increase under local operations and classical communication (Vedral *et al.*, 1997). This property is satisfied by the relative entropy $S(\rho\|\sigma) = \mathrm{Tr}[\rho\log_2\rho] - \mathrm{Tr}[\rho\log_2\sigma]$, although the relative entropy is not a distance in the mathematical sense. The corresponding measure of entanglement is called *relative entropy of entanglement*:

$$E_R(\rho) = \min_{\sigma \in \mathcal{S}} S(\rho\|\sigma). \tag{3.12}$$

The relative entropy of entanglement is one of the most popular and widely studied measures of entanglement. One reason is the fact that the relative entropy itself plays an important role in quantum information theory (Vedral, 2002). Moreover, the relative entropy of entanglement is a powerful upper bound for the distillable entanglement (Horodecki *et al.*, 2000).

As already mentioned in Section 2.5, the Bures distance defined as $D_B(\rho,\sigma) = 2(1 - \sqrt{F(\rho,\sigma)})$ with the fidelity $F(\rho,\sigma) = \left(\mathrm{Tr}\sqrt{\sqrt{\rho}\sigma\sqrt{\rho}}\right)^2$ also satisfies Eq. (3.11). The corresponding measure is called *Bures measure of entanglement* (Vedral *et al.*, 1997; Vedral and Plenio, 1998). One of our results presented in Section 5.1.1 is the finding that the Bures measure of entanglement is closely related to the geometric measure of entanglement. In particular, both measures are simple functions of each other. This result also allows to give a closed formula for the Bures measure of entanglement for any mixed state of two qubits.

We have already mentioned above that all distance-based entanglement measures do not increase under local operations and classical communication, if the distance satisfies Eq. (3.11). This is one of the properties any reasonable measure of entanglement should satisfy. Moreover, any entanglement measure should also vanish on separable states. This is also easily seen to be true for any distance $D(\rho,\sigma)$ which is zero if and only if $\rho = \sigma$, and larger than zero otherwise.

Finally, we mention the relationship between three of the measures presented in this section, namely between the distillable entanglement E_d, the relative entropy of entanglement E_R, and the entanglement of formation E_f. As was shown in (Horodecki *et al.*, 2000), these measures satisfy the inequality

$$E_d \leq E_R \leq E_f \tag{3.13}$$

for all mixed states, i.e., the relative entropy of entanglement is always between E_d and E_f.

4 Quantum correlations beyond entanglement

The concept of quantum correlations beyond entanglement is similar to the concept of entanglement presented in the previous chapter. In particular, both concepts coincide on pure states and differences arise on mixed states only. In this chapter we discuss basic definitions and properties of these general quantum correlations. A detailed review on this topic can be found in (Modi *et al.*, 2012).

4.1 Definition

A mixed state shared by two parties, Alice and Bob, is called *classically correlated*, if the corresponding density operator can be written as (Oppenheim *et al.*, 2002)

$$\rho_{\mathrm{cc}} = \sum_{i,j} p_{ij} \left|i\right\rangle\left\langle i\right|^A \otimes \left|j\right\rangle\left\langle j\right|^B, \tag{4.1}$$

where $\{\left|i\right\rangle^A\}$ are orthogonal states on Alice's Hilbert space $\mathcal{H}_A$ and $\{\left|j\right\rangle^B\}$ are orthogonal states on Bob's Hilbert space $\mathcal{H}_B$. The probabilities p_{ij} are nonnegative, and sum up to one: $\sum_{i,j} p_{ij} = 1$. Otherwise the state is called *quantum correlated*.

Note that every classically correlated state is also separable. On the other hand, a separable state with the density operator $\rho_{\mathrm{sep}} = \sum_i p_i \left|a_i\right\rangle\left\langle a_i\right| \otimes \left|b_i\right\rangle\left\langle b_i\right|$ is not necessarily classically correlated, since the states $\{\left|a_i\right\rangle\}$ and $\{\left|b_i\right\rangle\}$ do not have to be orthogonal. Moreover, a pure state is quantum correlated if and only if the state is entangled, i.e., both concepts are equivalent for pure states. For this reason, we will discuss mixed states in the following.

The intuition behind this definition of classically correlated states comes from the fact that these states are not disturbed by certain local von Neumann measurements on Alice's and Bob's subspaces. The measurement operators corresponding to these non-disturbing von Neumann measurements are given by $E_i^A = \left|i\right\rangle\left\langle i\right|^A$ and $E_j^B = \left|j\right\rangle\left\langle j\right|^B$. In a similar way we can also define a class of quantum states which is not disturbed under certain von Neumann measurements on the subspace of one party (e.g. Alice) only. In this case, the density operator has the form

$$\rho_{\mathrm{cq}} = \sum_i p_i \left|i\right\rangle\left\langle i\right|^A \otimes \rho_i^B, \tag{4.2}$$

where $|i\rangle^A$ are orthogonal states on Alice's Hilbert space $\mathcal{H}_A$, ρ_i^B are density operators on Bob's Hilbert space $\mathcal{H}_B$ and the nonnegative probabilities p_i sum up to one. These states are called *classical-quantum* states (Horodecki *et al.*, 2005a; Piani *et al.*, 2008). The corresponding von Neumann measurement on Alice's subsystem which does not disturb the total state is given by the measurement operators $E_i^A = |i\rangle\langle i|^A$. Similarly, the density operator of a *quantum-classical* state has the form $\rho_{\mathrm{qc}} = \sum_i p_i \rho_i^A \otimes |i\rangle\langle i|^B$. Such a state is not disturbed by a local von Neumann measurement on Bob's subspace with measurement operators $E_i^B = |i\rangle\langle i|^B$.

In contrast to entanglement, which cannot be created by local operations and classical communication, quantum correlations beyond entanglement can even be created by local operations without any communication. This will be discussed in more detail in the Section 5.2.3 of this thesis.

4.2 Measures of quantum correlations

In Section 3.4 we argued that a measure of entanglement can be defined via the usefulness of a quantum state to perform certain tasks. The figure of merit is the distillable entanglement, which quantifies how many singlets can be extracted from a given quantum state via local operations and classical communication, if many copies of the same state are available. Since singlets can be used for many tasks in quantum information, e.g., quantum cryptography, dense coding and teleportation, the distillable entanglement is directly related to the performance of these tasks.

For general quantum correlations the situation is less clear, since the definition of "distillable quantum correlations" is meaningless. The reason for this will be studied in more detail in Section 5.2.3. The results presented there imply that local operations and classical communication can create an arbitrary amount of quantum correlations. This means that a measure of "distillable quantum correlations" would be infinite for all quantum states. However, several other approaches to quantify quantum correlations have been proposed in the literature. The most important measures of quantum correlations will be presented in this section.

4.2.1 Quantum discord

Quantum discord is historically the first measure of quantum correlations beyond entanglement (Zurek, 2000; Ollivier and Zurek, 2001; Henderson and Vedral, 2001). The definition of quantum discord is based on the fact that in classical information theory the mutual information between two random variables X and Y can be expressed in two different ways, namely

$$\begin{aligned} I(X:Y) &= H(X) + H(Y) - H(X,Y), \\ J(X:Y) &= H(X) - H(X|Y). \end{aligned} \tag{4.3}$$

Here, $H(X) = -\sum_x p_x \log_2 p_x$ is the classical Shannon entropy of the random variable X, where p_x is the probability that the random variable X takes the value x. $H(X, Y)$ is the joint entropy of both variables X and Y. The conditional entropy $H(X|Y)$ is defined as

$$H(X|Y) = \sum_y p_y H(X|y), \tag{4.4}$$

where p_y is the probability that the random variable Y takes the value y, and $H(X|y)$ is the entropy of the variable X conditioned on the variable Y taking the value y: $H(X|y) = -\sum_x p_{x|y} \log_2 p_{x|y}$, and $p_{x|y}$ is the probability of x given y.

The equality of I and J for classical random variables follows from Bayes' rule $p_{x|y} = p_{xy}/p_y$, which can be used to show that $H(X|Y) = H(X, Y) - H(Y)$. However, as was noticed in (Ollivier and Zurek, 2001), I and J are no longer equal if quantum theory is applied. In particular, for a quantum state with the density operator ρ^{AB}, the mutual information between A and B is given by

$$I(\rho^{AB}) = S(\rho^A) + S(\rho^B) - S(\rho^{AB}) \tag{4.5}$$

with the von Neumann entropy S, and the reduced density operators $\rho^A = \mathrm{Tr}_B[\rho^{AB}]$ and $\rho^B = \mathrm{Tr}_A[\rho^{AB}]$. This expression is the generalization of the classical mutual information $I(X : Y)$ to the quantum theory.

On the other hand, the generalization of $J(X : Y)$ is not completely straightforward. Ollivier and Zurek have proposed the following way to generalize J to quantum theory (Ollivier and Zurek, 2001): for a bipartite quantum state with the density operator ρ^{AB}, they defined the conditional entropy of A conditioned on a measurement on B:

$$S(A|\{\Pi_i^B\}) = \sum_i p_i S(\rho_i^A), \tag{4.6}$$

where $\{\Pi_i^B\}$ are measurement operators corresponding to a von Neumann measurement on the subsystem B, i.e., orthogonal projectors with rank one. The probability p_i for obtaining the outcome i is given by $p_i = \mathrm{Tr}[\Pi_i^B \rho^{AB}]$, and the corresponding post-measurement state of the subsystem A is represented by the density operator $\rho_i^A = \mathrm{Tr}_B[\Pi_i^B \rho^{AB}]/p_i$. The quantity J can now be extended to quantum states as follows (Ollivier and Zurek, 2001):

$$J(\rho^{AB})_{\{\Pi_i^B\}} = S(\rho^A) - S(A|\{\Pi_i^B\}), \tag{4.7}$$

where the index $\{\Pi_i^B\}$ clarifies that the value depends on the choice of the measurement operators Π_i^B. The quantity J represents the amount of information gained about the subsystem A by measuring the subsystem B (Ollivier and Zurek, 2001).

Quantum discord is the difference of these two inequivalent expressions for the mutual information, minimized over all von Neumann measurements:

$$\delta^{A|B}(\rho^{AB}) = \min_{\{\Pi_i^B\}} \left[I(\rho^{AB}) - J(\rho^{AB})_{\{\Pi_i^B\}} \right], \tag{4.8}$$

where the minimization over all von Neumann measurements is done in order to have a measurement-independent expression (Ollivier and Zurek, 2001). As was also shown in (Ollivier and Zurek, 2001), quantum discord is nonnegative, and is equal to zero on quantum-classical states only. These are states with the density operator of the form $\rho_{\mathrm{qc}} = \sum_i p_i \rho_i^A \otimes |i\rangle\langle i|^B$.

A closely related quantity was proposed in (Henderson and Vedral, 2001). The authors aimed to quantify *classical correlations* in quantum states by defining a measure of classical correlations C_B which is equal to J given in Eq. (4.7), maximized over all general quantum measurements on the subsystem B:

$$C_B(\rho^{AB}) = \max_{\{E_i^B\}} J(\rho^{AB})_{\{E_i^B\}}. \tag{4.9}$$

Here, E_i^B are measurement operators acting on the subsystem B, and $J(\rho^{AB})_{\{E_i^B\}}$ is the generalization of Eq. (4.7) to all quantum measurements:

$$J(\rho^{AB})_{\{E_i^B\}} = S(\rho^A) - S(A|\{E_i^B\}) \tag{4.10}$$

with $S(A|\{E_i^B\}) = \sum_i p_i S(\rho_i^A)$. The measurement probabilities are now given by $p_i = \mathrm{Tr}[\left(E_i^B\right)^\dagger E_i^B \rho^{AB}]$, and the corresponding post-measurement state of the subsystem A is now represented by the density operator $\rho_i^A = \mathrm{Tr}_B[\left(E_i^B\right)^\dagger E_i^B \rho^{AB}]/p_i$.

In today's literature, quantum discord is frequently defined as the difference between the mutual information I, and the amount of classical correlations C_B (Datta, 2008):

$$D^{A|B}(\rho^{AB}) = I(\rho^{AB}) - C_B(\rho^{AB}). \tag{4.11}$$

This measure is in general different from the original quantum discord $\delta^{A|B}$ proposed by Ollivier and Zurek. However, this quantity is also nonnegative, and vanishes on quantum-classical states only (Datta, 2010).

The second version of quantum discord, defined in Eq. (4.11), is related to the entanglement of formation E_f via the Koashi-Winter relation (Koashi and Winter, 2004; Fanchini *et al.*, 2011):

$$E_f(\rho^{AB}) = D^{A|C}(\rho^{AC}) + S(\rho^{AC}) - S(\rho^C), \tag{4.12}$$

where the total state with density operator ρ^{ABC} is pure, i.e., $\rho^{ABC} = |\psi\rangle\langle\psi|^{ABC}$. The reduced states are defined as $\rho^{AB} = \mathrm{Tr}_C[\rho^{ABC}]$, $\rho^{AC} = \mathrm{Tr}_B[\rho^{ABC}]$, $\rho^C = \mathrm{Tr}_{AB}[\rho^{ABC}]$, and S is the von Neumann entropy. We will come back to the Koashi-Winter relation in Section 4.3, where the role of quantum discord and other quantum correlations in quantum information theory will be discussed.

4.2.2 General measures of quantum correlations

Postulates for a reasonable measure of general quantum correlations have been proposed recently in (Brodutch and Modi, 2012). There the authors identify three necessary conditions every measure of quantum correlations Q should satisfy. These conditions are:

1. Q is nonnegative,

2. Q is invariant under local unitary operations,

3. Q is zero on classically correlated states.

All measures of quantum correlations considered in this thesis satisfy these three criteria. Note that both versions of quantum discord, $\delta^{A|B}$ and $D^{A|B}$, also satisfy all these criteria, although they are zero on all quantum-classical states with density operator of the form $\rho_{\mathrm{qc}} = \sum_i p_i \rho_i^A \otimes |i\rangle\langle i|^B$. In this section we will present main measures of general quantum correlations apart from quantum discord.

Information deficit is a measure of quantum correlations which was originally based on the task of extracting work from a heat bath using a quantum state (Oppenheim *et al.*, 2002; Horodecki *et al.*, 2005a). In particular, the amount of extractable work from a heat bath of temperature T using a mixed state of n qubits with the density operator ρ is given by

$$W = kT\{n - S(\rho)\}, \tag{4.13}$$

where k is the Boltzmann constant and S is the von Neumann entropy. However, if the state is shared by two parties, Alice and Bob, each of them having access to the local subsystem only, the amount of extractable work W' will in general be different from W. If Bob is allowed to perform a single von Neumann measurement on his local system, and send the resulting state to Alice, the maximal amount of work which Alice can extract from the resulting state in this way is given by

$$W' = W - kT \cdot \Delta^{A|B}(\rho^{AB}), \tag{4.14}$$

where $\Delta^{A|B}$ is known as the *one-way information deficit* (Horodecki *et al.*, 2005a; Modi *et al.*, 2012):

$$\Delta^{A|B}(\rho^{AB}) = \min_{\sigma^{AB} \in QC} S(\rho^{AB} \| \sigma^{AB}). \tag{4.15}$$

$S(\rho\|\sigma)$ is the relative entropy between the density operators ρ and σ, and the minimum is taken over the set of density operators QC corresponding to quantum-classical states. These are states with density operator of the form $\sigma^{AB} = \sum_i p_i \sigma_i^A \otimes |i\rangle\langle i|^B$. Similar to quantum discord, the one-way information deficit is zero on quantum-classical states only. For this reason, this quantity is also called *relative entropy of discord* (Modi *et al.*, 2010).

The *zero-way information deficit* is obtained in the same way, if Alice and Bob both perform a local von Neumann measurement, before Bob sends his system to Alice (Horodecki *et al.*, 2005a). The maximal amount of work which Alice can extract in this procedure is given by $W' = W - kT \cdot Q_R(\rho^{AB})$, where Q_R is defined as

$$Q_R(\rho^{AB}) = \min_{\sigma^{AB} \in CC} S(\rho^{AB} \| \sigma^{AB}), \tag{4.16}$$

and the minimum is taken over the set of density operators CC corresponding to classically correlated states. Q_R is also known as the *relative entropy of quantumness* (Piani *et al.*, 2011; Modi *et al.*, 2010).

Inspired by the expression of the one-way information deficit as the minimal relative entropy between a given density operator and the set of density operators QC corresponding to quantum-classical states, Dakić *et al.* defined the *geometric measure of discord* as the minimal Hilbert-Schmidt distance between a given density operator ρ^{AB} and QC (Dakić *et al.*, 2010):

$$D_G^{A|B}(\rho^{AB}) = \min_{\sigma^{AB}\in QC} \left\|\rho^{AB} - \sigma^{AB}\right\|^2 \tag{4.17}$$

with the square norm $\|M\| = \sqrt{\mathrm{Tr}[M^\dagger M]}$. The main advantage of the geometric measure of discord was already presented in the original work by Dakić *et al.*: this measure has an analytical expression for all two-qubit states (Dakić *et al.*, 2010). If ρ^{AB} is a density operator representing a two-qubit state, then the geometric measure of discord can be written as (Dakić *et al.*, 2010)

$$D_G^{A|B}(\rho^{AB}) = \frac{1}{4}(\left\|\vec{y}\right\|^2 + \|T\|^2 - k_{\max}), \tag{4.18}$$

where $\vec{y}$ is a 3-dimensional vector with entries $y_i = \mathrm{Tr}[(\mathbb{1}\otimes\sigma_i)\rho^{AB}]$, and T is the 3×3 correlation tensor with components $T_{ij} = \mathrm{Tr}[(\sigma_i \otimes \sigma_j)\rho^{AB}]$. The Pauli operators σ_i are given as $\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $\sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$, and $\sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$. Finally, $k_{\max}$ is the largest eigenvalue of the real matrix $K = \vec{y}\vec{y}^T + TT^T$.

4.3 Role of quantum correlations in quantum information

Enormous amount of research in the last years has been devoted to the understanding of the role of quantum correlations beyond entanglement in quantum information theory. Main reason for this development was the finding that quantum discord is present in the quantum computational model known as *deterministic quantum computation with one quantum bit* (DQC1) (Knill and Laflamme, 1998; Laflamme *et al.*, 2002; Datta *et al.*, 2008). In the following section we will present this algorithm and discuss the role of quantum discord in it. A detailed discussion can also be found in (Modi *et al.*, 2012).

4.3.1 Deterministic quantum computation with one quantum bit (DQC1)

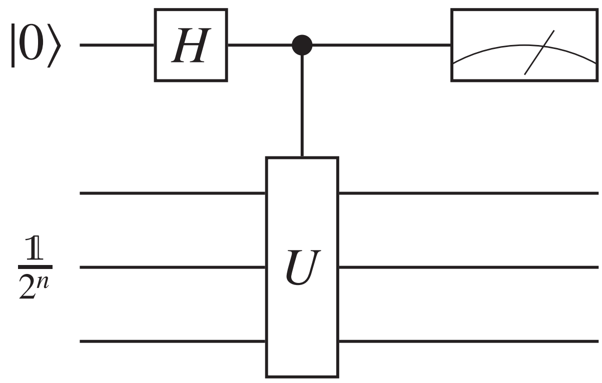

Figure 4.1: DQC1 circuit, as presented in (Laflamme *et al.*, 2002). The control qubit is initially in the pure state $|0\rangle$, while the target n-qubit system is in the maximally mixed state. After a Hadamard gate on the control qubit the total system undergoes a controlled unitary operation ending up in the final state with density operator ρ_f given in Eq. (4.20). A measurement on the control qubit reveals the trace of $U/2^n$.

The DQC1 model was first presented in (Knill and Laflamme, 1998). It can be explained using the circuit shown in Fig. 4.1, which was first presented in (Laflamme *et al.*, 2002): the initial state of the system is given by one single qubit in the pure state $|0\rangle$ together with n qubits in the maximally mixed state, represented by the density operator $\mathbb{1}/2^n$. The density operator of the total initial state is thus given by

$$\rho_i = |0\rangle\langle 0| \otimes \frac{\mathbb{1}}{2^n}. \tag{4.19}$$

A Hadamard gate $H = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$ is applied on the first qubit, followed by a controlled unitary operation with the first qubit as the control qubit, and the n remaining qubits in the maximally mixed state as the target. The density operator of the final state is given by

$$\rho_f = \frac{1}{2}\left(\mathbb{1} \otimes \frac{\mathbb{1}}{2^n} + |0\rangle\langle 1| \otimes \frac{U^\dagger}{2^n} + |1\rangle\langle 0| \otimes \frac{U}{2^n}\right). \tag{4.20}$$

Measuring the expectation values of the Pauli operators $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ and $\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$ on the first qubit in the final state gives us the real and the imaginary part of the trace of the unitary U divided by 2^n: $\langle\sigma_x\rangle = \mathrm{Re}\,(\mathrm{Tr}[U/2^n])$ and $\left\langle\sigma_y\right\rangle = \mathrm{Im}\,(\mathrm{Tr}[U/2^n])$. This shows that the DQC1 circuit is able to compute the normalized trace of any 2^n-dimensional unitary. The computation is efficient, i.e., the number of steps grows at most polynomially with the number of qubits n as long as the unitary can be implemented using a polynomial number of two-qubit gates (Datta *et al.*, 2005). Since no classical algorithm is known so far that can solve this problem efficiently, DQC1 is said to have an exponential speedup over any known classical algorithm. In (Datta *et al.*, 2005) the authors relate the computation of the trace of a unitary matrix to a number of different problems for which no efficient solution on a classical computer is known so far. The authors conclude that the DQC1 model is probable to show exponential speedup over classical computation in general.

The role of entanglement in the DQC1 model has been studied in (Poulin *et al.*, 2004; Datta *et al.*, 2005). As was shown in (Poulin *et al.*, 2004), the control qubit is never entangled with the remaining target system. More general results have been presented in (Datta *et al.*, 2005). There the authors investigated the amount of entanglement generated by the protocol in a general bipartite cut. They found that the amount of entanglement, as measured by the so called negativity (Vidal and Werner, 2002), is vanishingly small for large n. Although entanglement was believed to be the key resource for the quantum computational speedup, the authors of (Datta *et al.*, 2005) claim that for DQC1 this is not the case.

Trying to identify the reason for the power of DQC1, Datta *et al.* suggested that quantum discord is the figure of merit in this computational model (Datta *et al.*, 2008). Datta's arguments are based on the finding that the final state with density operator ρ_f is typically quantum correlated, i.e., if the unitary U is sampled at random, then the final state always has a nonzero amount of quantum discord between the n target qubits and the control qubit. This result has led to a debate about the role of quantum discord in quantum computation, which continues until the present day. On the one hand, Eastin found that a quantum computational process consisting of one- and two-qubit gates requires quantum discord in some steps of the protocol in order to show an exponential speedup over any classical algorithm (Eastin, 2010). On the other hand, Dakić *et al.* claimed that DQC1 might show exponential speedup over classical computation even without any quantum discord in the final state (Dakić *et al.*, 2010). These results do not contradict each other: Eastin's statement cannot be applied to DQC1 directly, since the description of DQC1 given above requires gates on more than two qubits. However, these results show that the role of quantum discord in quantum computational processes is still not completely understood, and more work has to be done in this direction.

Experimental realizations of DQC1 have also been presented. Lanyon *et al.* proposed an optical implementation of DQC1 with two qubits (Lanyon *et al.*, 2008). In accordance with the theoretical prediction, the authors found that the implemented quantum state does not have any entanglement, but has nonvanishing quantum discord. An NMR implementation of DQC1 with four qubits has been presented by Passante *et al.*, where the presence of quantum discord has also been confirmed (Passante *et al.*, 2011).

4.3.2 Quantum state merging

Another interpretation for quantum discord was presented in (Madhok and Datta, 2011; Cavalcanti *et al.*, 2011). The authors related quantum discord to the task known as *quantum state* *merging* (Horodecki *et al.*, 2005b). In this task, three parties, Alice, Bob and Charlie share a total pure state $|\psi\rangle^{ABC}$. The aim of Alice and Bob is to merge their states, such that the final state $|\psi\rangle^{B'BC}$ is the same as the initial state $|\psi\rangle^{ABC}$, but both subsystems B' and B are in Bob's possession. Entanglement can be seen as a resource in this process: if Alice and Bob additionally share sufficiently many singlets, they can always merge their states by local operations and classical communication in the asymptotic case, where many copies of the initial state $|\psi\rangle^{ABC}$ are available (Horodecki *et al.*, 2005b). The authors of (Horodecki *et al.*, 2005b) show that the minimal number of singlets Alice and Bob need to share per copy of the initial state is given by the quantum conditional entropy

$$S(A|B) = S(\rho^{AB}) - S(\rho^{B}). \tag{4.21}$$

Since this quantity can be positive or negative, a positive value means that the process consumes singlets, while for a negative value singlets are gained.

In (Cavalcanti *et al.*, 2011) the authors argue that the total amount of entanglement consumed in quantum state merging is given by

$$\Gamma(A\rangle B) = E_f(\rho^{AB}) + S(A|B), \tag{4.22}$$

where E_f is the entanglement of formation defined in Section 3.4.2. In particular, the authors consider the scenario where Alice and Bob create many copies of a state with density operator $\rho^{AB} = \sum_i p_i |\psi_i\rangle\langle\psi_i|^{AB}$ by creating many copies of each pure state $|\psi_i\rangle^{AB}$ independently via local operations and classical communication. The minimal number of singlets which Alice and Bob need per copy of the mixed state is then given by $E_f(\rho^{AB})$ (Cavalcanti *et al.*, 2011). $\Gamma(A\rangle B)$ thus takes into account that Alice and Bob need a certain amount of entanglement to create the state ρ^{AB} before the state merging is performed. In their main result, the authors of (Cavalcanti *et al.*, 2011) show that the total amount of entanglement $\Gamma(A\rangle B)$ is equal to quantum discord between Alice's and Charlie's system:

$$\Gamma(A\rangle B) = D^{A|C}(\rho^{AC}). \tag{4.23}$$

This result can be proven using the Koashi-Winter relation given in Eq. (4.12) on page 20.

The role of quantum discord and general quantum correlations in other tasks like entanglement distribution and the quantum measurement process will be discussed in the following chapter.

5 Summary of results

In this chapter we summarize the main results of this thesis. In Section 5.1 we review two publications on quantum entanglement (Streltsov *et al.*, 2010, 2011c). In Section 5.2 we examine four further publications on quantum discord and general quantum correlations beyond entanglement (Streltsov *et al.*, 2011a,b, 2012a,b).

5.1 Quantum entanglement

Entanglement measures for general mixed states have been presented in Section 3.4.2. There, two distinct classes of entanglement measures were considered, namely *convex roof measures* on the one hand, and *distance-based measures* on the other hand. In this section we will show that some measures of entanglement belong to both classes at the same time, i.e., there exist distance-based measures which coincide with their convex roof (Streltsov *et al.*, 2010). This result can be used to construct algorithms for computing the geometric measure of entanglement in multipartite systems (Streltsov *et al.*, 2011c).

5.1.1 Linking a distance measure of entanglement to its convex roof

The existence of an entanglement measure which belongs to the class of distance-based and convex roof measures simultaneously has been studied in (Streltsov *et al.*, 2010). In particular, the *geometric measure of entanglement* is defined for pure states as (Shimony, 1995; Barnum and Linden, 2001; Wei and Goldbart, 2003)

$$E_G(|\psi\rangle) = \min_{|\phi\rangle\in\mathcal{S}}(1 - |\langle\psi|\phi\rangle|^2), \tag{5.1}$$

where the minimum is taken over all separable states $|\phi\rangle \in \mathcal{S}$. For mixed states, the geometric measure of entanglement was defined via the convex roof construction (Wei and Goldbart, 2003)

$$E_G(\rho) = \inf_{\{p_i,|\psi_i\rangle\}} \sum_i p_i E_G(|\psi_i\rangle), \tag{5.2}$$

where the infimum is taken over all decompositions $\{p_i, |\psi_i\rangle\}$ of the density operator ρ, see also Section 3.4.

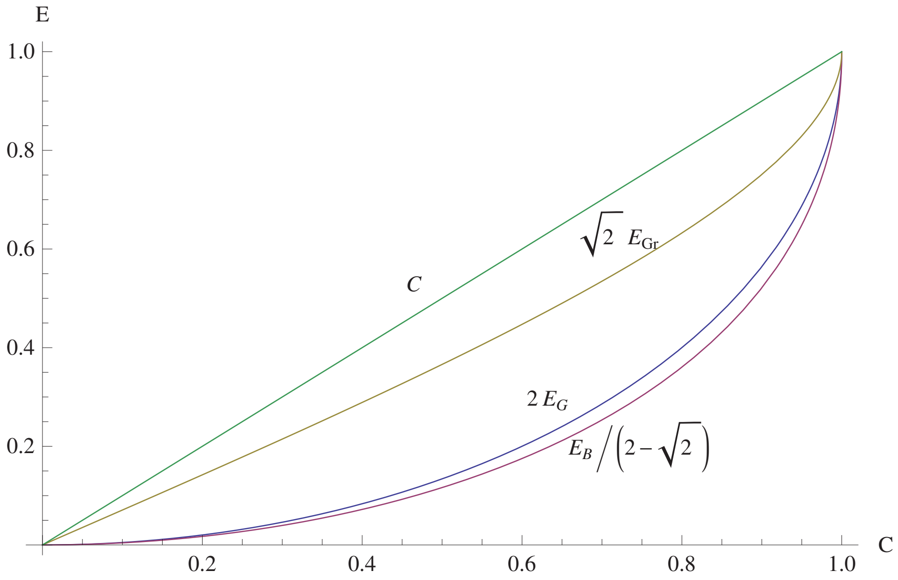

Figure 5.1: Plot of the geometric measure of entanglement E_G, Bures measure of entanglement E_B and Groverian measure of entanglement E_{Gr} as a function of the concurrence C for two-qubit states. All measures were renormalized such that they reach 1 for maximally entangled states. Figure and caption are taken from (Streltsov *et al.*, 2010).

The main result of (Streltsov *et al.*, 2010) is the finding that the geometric measure of entanglement as defined in Eq. (5.2) can also be regarded as a distace-based measure of entanglement, i.e.,

$$E_G(\rho) = \inf_{\sigma \in \mathcal{S}} D(\rho, \sigma), \tag{5.3}$$

where the distance D is given by $D(\rho, \sigma) = 1 - F(\rho, \sigma)$ with fidelity $F(\rho, \sigma) = \left(\mathrm{Tr}[\sqrt{\sqrt{\rho}\sigma\sqrt{\rho}}]\right)^2$, and the infimum is taken over the set of density operators $\mathcal{S}$ corresponding to separable states. Note that $D(\rho, \sigma) = 1 - F(\rho, \sigma)$ is not a faithful distance in the mathematical sense, since it does not satisfy the triangle inequality. We will discuss the meaning of this result in the following, and refer to (Streltsov *et al.*, 2010) for the proof.

The result presented above allows to relate the geometric measure of entanglement to other measures presented in the literature. One such measure is the Bures measure of entanglement defined in (Vedral *et al.*, 1997; Vedral and Plenio, 1998):

$$E_B(\rho) = \inf_{\sigma \in \mathcal{S}} (2 - 2\sqrt{F(\rho, \sigma)}). \tag{5.4}$$

Our main result in Eq. (5.3) reveals a simple connection between these two measures (Streltsov *et al.*, 2010):

$$E_B(\rho) = 2(1 - \sqrt{1 - E_G(\rho)}). \tag{5.5}$$

In particular, this result also implies a simple formula for the Bures measure of entanglement for all states of two qubits. This can be seen using the corresponding two-qubit formula for the geometric measure of entanglement given in (Wei and Goldbart, 2003):

$$E_G(\rho) = \frac{1}{2}(1 - \sqrt{1 - C(\rho)^2}). \tag{5.6}$$

Here, ρ is an arbitrary density operator corresponding to a two-qubit state, and C is the concurrence defined below Eq. (3.8) on page 14. Inserting this expression into Eq. (5.5) we find the corresponding formula for the Bures measure of entanglement given in (Streltsov *et al.*, 2010):

$$E_B(\rho) = 2 - 2\sqrt{\frac{1 + \sqrt{1 - C(\rho)^2}}{2}}. \tag{5.7}$$

For comparison, the geometric measure of entanglement and the Bures measure of entanglement are shown as a function of the concurrence in Fig. 5.1. Additionally, we also show the Groverian measure of entanglement defined in (Biham *et al.*, 2002; Shapira *et al.*, 2006) as

$$E_{Gr}(\rho) = \inf_{\sigma \in \mathcal{S}} \sqrt{1 - F(\rho, \sigma)}. \tag{5.8}$$

5.1.2 Simple algorithm for computing the geometric measure of entanglement

The results presented in the previous section can be used to build an algorithm for approximating the geometric measure of entanglement from above. This has been done in (Streltsov *et al.*, 2011c). For a given density operator ρ the algorithm iteratively computes a sequence of density operators σ_i corresponding to separable states such that

$$F(\rho, \sigma_i) \leq F(\rho, \sigma_{i+1}), \tag{5.9}$$

where F is the fidelity. Such a sequence can be computed in a simple way, by solving an eigenproblem and finding a singular value decomposition of a matrix (Streltsov *et al.*, 2011c). If the algorithm stops after n iterations, we take

$$\tilde{E}_G(\rho) = 1 - F(\rho, \sigma_n) \tag{5.10}$$

as an approximation of the geometric measure of entanglement from above, see (Streltsov *et al.*, 2011c) for details.

The algorithm was tested on different states, where the exact amount of the geometric measure of entanglement is known, and convergence into the exact value was always found within a reasonable precision (Streltsov *et al.*, 2011c). The algorithm was also applied to the isotropic XX model of three qubits in a constant magnetic field. The corresponding Hamiltonian is given by (Lieb *et al.*, 1961; Katsura, 1962)

$$H = \frac{B}{2}\sum_{i=1}^{3}\sigma_i^z + J\sum_{i=1}^{3}(\sigma_i^x\sigma_{i+1}^x + \sigma_i^y\sigma_{i+1}^y) \tag{5.11}$$

with coupling constant J, magnetic field B, and periodic boundary conditions $\sigma_4^x = \sigma_1^x$ and $\sigma_4^y = \sigma_1^y$. In thermal equilibrium the system is found in the mixed state with density operator $\rho = \frac{e^{-\frac{H}{kT}}}{Z}$ with $Z = \mathrm{Tr}[e^{-\frac{H}{kT}}]$. In (Streltsov *et al.*, 2011c) the Boltzmann constant was set to $k = 1$, and the coupling constant to $J = \frac{1}{2}$.

In Fig. 5.2 on the following page we show the approximated value of the geometric measure of entanglement $\tilde{E}_G$ as a function of the temperature T for four different values of the magnetic field B. We observe that the behavior of the system in the low temperature limit depends on the magnetic field. This behavior is explained in (Streltsov *et al.*, 2011c). In Fig. 5.3 on the next page we also show the approximated value $\tilde{E}_G$ as a function of the magnetic field B for three different temperatures T. In the limit $T \to 0$ the approximated value $\tilde{E}_G$ becomes a nonanalytic function of B for two different values of the magnetic field, namely for $B = 0$ and $B = 2J$, see (Streltsov *et al.*, 2011c) for details.

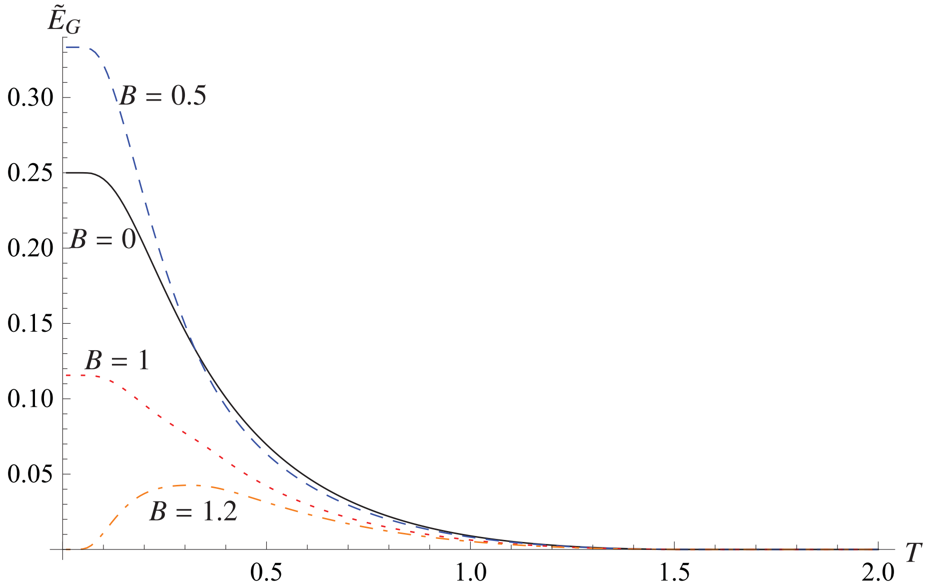

Figure 5.2: Approximation of the geometric measure of entanglement $\tilde{E}_G$ plotted as function of the temperature T for $\rho = \frac{e^{-\frac{H}{kT}}}{Z}$ with H given in Eq. (5.11). The parameter J is set to $\frac{1}{2}$, and $k = 1$. Figure and caption are taken from (Streltsov *et al.*, 2011c).

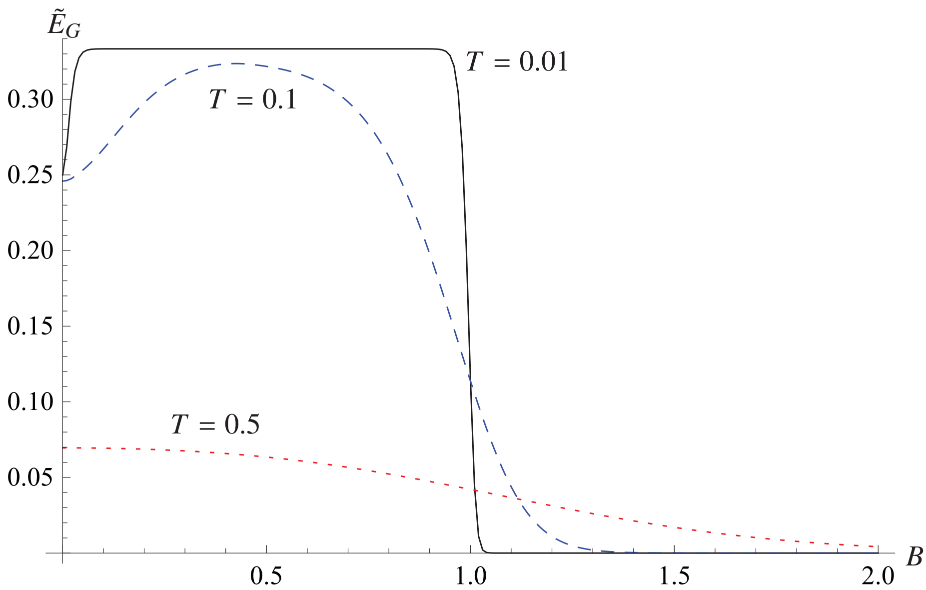

Figure 5.3: Approximation of the geometric measure of entanglement $\tilde{E}_G$ for fixed values of T plotted as function of the magnetic field B. The parameter J is set to $\frac{1}{2}$, and $k = 1$. Figure and caption are taken from (Streltsov *et al.*, 2011c).

5.2 Quantum correlations beyond entanglement

General measures of quantum correlations, like quantum discord and information deficit, have been presented in Chapter 4, where also basic properties of these measures were discussed. The role of quantum discord in two important tasks in quantum information theory was considered in Section 4.3: namely in the DQC1 algorithm, and in quantum state merging. In this section we will consider two other fundamental tasks where quantum correlations play an essential role. These tasks are the entanglement distribution (Streltsov *et al.*, 2012b), and the quantum measurement process (Streltsov *et al.*, 2011b). New important properties of general quantum correlations will also be discussed. These are the behavior of quantum correlations under local noise (Streltsov *et al.*, 2011a) and their monogamy (Streltsov *et al.*, 2012a).

5.2.1 Quantum cost for sending entanglement

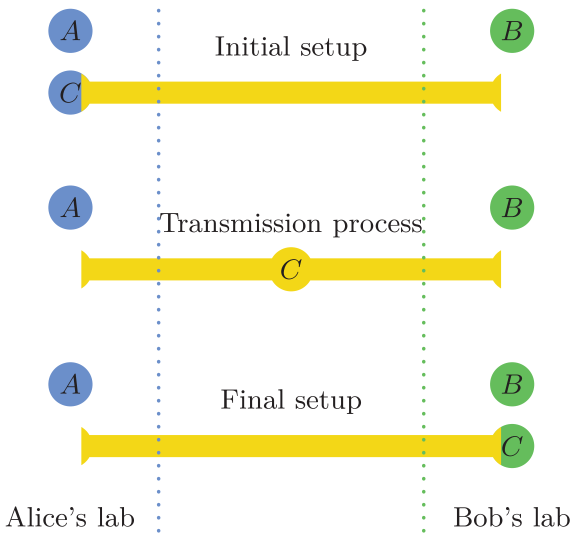

Figure 5.4: Entanglement distribution between Alice and Bob. Blue circles illustrate particles which belong to Alice, green circles belong to Bob. The upper figure shows the initial setup before the transmission: Alice holds the particles A and C, while Bob is in possession of the particle B. The middle figure shows the transmission process: Alice uses a quantum channel (yellow) to send C to Bob. The final situation is shown in the lower figure. Figure and caption are taken from (Streltsov *et al.*, 2012b).

The role of quantum correlations in the task of *entanglement distribution* was considered in (Streltsov *et al.*, 2012b). The setting is illustrated in Fig. 5.4: Alice is initially in possession of two particles, A and C, while Bob is in possession of one particle B (upper part of Fig. 5.4). If

Alice sends the particle C to Bob via a perfect quantum channel (middle part of Fig. 5.4), they end up in the final setup, where Bob is in possession of both particles B and C, while Alice is in possession of A (lower part of Fig. 5.4).

If the total state of Alice and Bob is described by the density operator $\rho = \rho^{ABC}$, then the initial amount of entanglement between Alice and Bob is given by $E^{AC|B} = E^{AC|B}(\rho)$, while the final amount of entanglement after sending the particle C is given by $E^{A|BC} = E^{A|BC}(\rho)$. As a measure of entanglement we use the relative entropy of entanglement. For two parties X and Y it was defined in Section 3.4.2 as the minimal relative entropy between a given density operator and the set of density operators $\mathcal{S}$ corresponding to separable states:

$$E^{X|Y}(\rho^{XY}) = \min_{\sigma^{XY}\in\mathcal{S}} S(\rho^{XY}\|\sigma^{XY}), \tag{5.12}$$

where $S(\rho\|\sigma)$ is the relative entropy between the density operators ρ and σ.

It is natural to assume that in order to distribute entanglement some amount of correlations has to be sent from Alice to Bob. This assumption was formulated in (Streltsov *et al.*, 2012b) as the following inequality:

$$Q^{AB|C} \geq E^{A|BC} - E^{AC|B}, \tag{5.13}$$

where $Q^{AB|C}$ denotes a yet undefined kind of correlations between the system AB and the particle C (Streltsov *et al.*, 2012b). Following (Streltsov *et al.*, 2012b), "this inequality quantifies the intuition, that entanglement distribution does not come for free, but always requires to invest some correlations". If Alice and Bob share some preestablished amount of entanglement $E^{AC|B}$, and wish to achieve a larger amount $E^{A|BC}$, the transmitted particle C should carry at least an amount of correlations given by the difference of final and initial entanglement (Streltsov *et al.*, 2012b). For this reason, the quantity Q can be regarded as the *cost* for the distribution of entanglement (Streltsov *et al.*, 2012b).

Surprisingly, the entanglement between AB and C does not play any role in this protocol (Streltsov *et al.*, 2012b). As was shown in (Cubitt *et al.*, 2003), this protocol can be implemented without any entanglement between the particle C and the rest of the system (Streltsov *et al.*, 2012b). This means that the quantity Q in Eq. (5.13) cannot be a measure of entanglement (Streltsov *et al.*, 2012b). However, in (Streltsov *et al.*, 2012b) we have shown that the inequality (5.13) is satisfied for the one-way information deficit. In Section 4.2.2 it was defined as the minimal relative entropy between a given density operator and the set of density operators corresponding to quantum-classical states. Here we use an alternative expression (Modi *et al.*, 2012)

$$\Delta^{X|Y}(\rho^{XY}) = \min_{\{\Pi_i^Y\}} S(\rho^{XY}\| \sum_i \Pi_i^Y \rho^{XY} \Pi_i^Y), \tag{5.14}$$

where the minimum is taken over sets of measurement operators $\left\{\Pi_i^Y\right\}$ corresponding to a local von Neumann measurement on subsystem Y.

The one-way information deficit quantifies the cost for entanglement distribution in the sense discussed above (Streltsov *et al.*, 2012b):

$$\Delta^{AB|C} \geq E^{A|BC} - E^{AC|B}, \tag{5.15}$$

”thus revealing the fundamental role of quantum correlations as a resource for the distribution of entanglement” (Streltsov *et al.*, 2012b). Our main result in inequality (5.15) also holds in a more general case, where the relative entropy in both equations (5.12) and (5.14) is replaced by a general distance D which does not increase under quantum operations, and satisfies the triangle inequality (Streltsov *et al.*, 2012b). In the following we will briefly discuss the meaning and implications of this result, and refer to (Streltsov *et al.*, 2012b) for the proofs.

In the protocol considered so far one particle was sent from Alice to Bob. However, our results can be generalized to the most general distribution protocol, where Alice and Bob may send n particles between each other, and also apply local operations and classical communication. The amount of entanglement distributed in this way cannot be larger than the total cost in the protocol (Streltsov *et al.*, 2012b):

$$E_{\mathrm{final}} - E_{\mathrm{initial}} \leq \sum_{i=1}^{n} \Delta_i, \tag{5.16}$$

where E_{initial} and E_{final} is the amount of entanglement between Alice and Bob before and after the protocol, and Δ_i is the amount of quantum correlations between the remaining system and the sent particle in the i-th application of the quantum channel (Streltsov *et al.*, 2012b). This result can be used to find the cheapest way to distribute entanglement, i.e., where the inequality (5.16) becomes equality. On the one hand, this can be achieved by sending entanglement directly, where Alice locally prepares a pure state $|\psi\rangle^{AC}$ with entanglement $E^{A|C}$, and sends the particle C to Bob. However, this is not the only possibility. As is shown in (Streltsov *et al.*, 2012b), the inequality (5.16) can also be satisfied without sending entanglement, leading us to the following conclusion:

> *“If one considers entanglement to be an expensive resource, one may thus be able to distribute entanglement in a ’cheaper’ way by sending quantum correlations without entanglement.”* (Streltsov *et al.*, 2012b)

Similar results were found independently in (Chuan *et al.*, 2012).

5.2.2 Linking quantum discord to entanglement in a measurement

The role of quantum correlations in the quantum measurement process was studied in (Streltsov *et al.*, 2011b). Any von Neumann measurement on a system S with density operator ρ^S can be described by coupling the system S to the measurement apparatus M in a pure initial state $|0\rangle^M$. The joint initial state of the measurement apparatus and the system is then described by the density operator

$$\rho_1 = |0\rangle\langle 0|^M \otimes \rho^S. \tag{5.17}$$

In the measurement process, a unitary is applied on the joint state, leading to the final density operator (Schlosshauer, 2005)

$$\rho_2 = U\rho_1 U^\dagger. \tag{5.18}$$

A simple example, considered in (Streltsov *et al.*, 2011b), is a von Neumann measurement in the eigenbasis $\{|i\rangle^S\}$ of the mixed state $\rho^S = \sum_i p_i |i\rangle\langle i|^S$ with eigenvalues p_i. After the application of the unitary, the final density operator is given by $\rho_2 = \sum_i p_i |i\rangle\langle i|^M \otimes |i\rangle\langle i|^S$. In this case the final state is separable, i.e., no entanglement between the measurement apparatus M and the system S was created in the measurement process (Streltsov *et al.*, 2011b).

As is shown in (Streltsov *et al.*, 2011b), the situation changes completely if we consider *partial von Neumann measurements*. These are measurements which are restricted to a part of the system. In particular, the system S is now divided into two subsystems A and B. In (Streltsov *et al.*, 2011b) we only consider von Neumann measurements on the subsystem A, and we say that a unitary U realizes a von Neumann measurement with measurement operators $\{\Pi_i^A\}$ on the subsystem A, if for any density operator ρ^{AB} holds:

$$\mathrm{Tr}_M[U(|0\rangle\langle 0|^M \otimes \rho^{AB})U^\dagger] = \sum_i \Pi_i^A \rho^{AB} \Pi_i^A. \tag{5.19}$$

The entanglement between the apparatus M and the total system AB in the final state represented by the density operator $\rho_2 = U(|0\rangle\langle 0|^M \otimes \rho^{AB})U^\dagger$ is called *entanglement created in the von Neumann measurement* $\{\Pi_i^A\}$ *on* A (Streltsov *et al.*, 2011b).

Since entanglement is considered to be an expensive resource, we are interested in measurement processes which create as little entanglement as possible. The minimal amount of entanglement, minimized over all von Neumann measurements on A, is called E_{meas}, and it depends on the entanglement measure used (Streltsov *et al.*, 2011b). In (Streltsov *et al.*, 2011b) we use the distillable entanglement E_d, and thus E_{meas} is defined as

$$E_{\mathrm{meas}}(\rho^{AB}) = \min_U E_d^{M|AB}\{U(|0\rangle\langle 0|^M \otimes \rho^{AB})U^\dagger\}, \tag{5.20}$$

where the minimization is done over all unitaries U which realize some von Neumann measurement on A. The main result is the relation between E_{meas} and the one-way information deficit, stated in Theorem 1 in (Streltsov *et al.*, 2011b):

> *"The minimal distillable entanglement created in a von Neumann measurement on A is equal to the one-way information deficit:"*
>
> $$E_{\mathrm{meas}}(\rho^{AB}) = \Delta^{B|A}(\rho^{AB}). \tag{5.21}$$

This result is illustrated in the upper part of Fig. 5.5, where the one-way information deficit is denoted by $\Delta^{\rightarrow} := \Delta^{B|A}$. In the following we will discuss the implications of this result. The proof can be found in (Streltsov *et al.*, 2011b).

Our main result in Eq. (5.21) allows to define a new class of quantum-correlation measures by varying the measure of entanglement E. In this way, we introduce the generalized one-way information deficit as follows (Streltsov *et al.*, 2011b):

$$\Delta_E^{B|A}(\rho^{AB}) = \min_U E^{M|AB}\{U(|0\rangle\langle 0|^M \otimes \rho^{AB})U^\dagger\}, \tag{5.22}$$

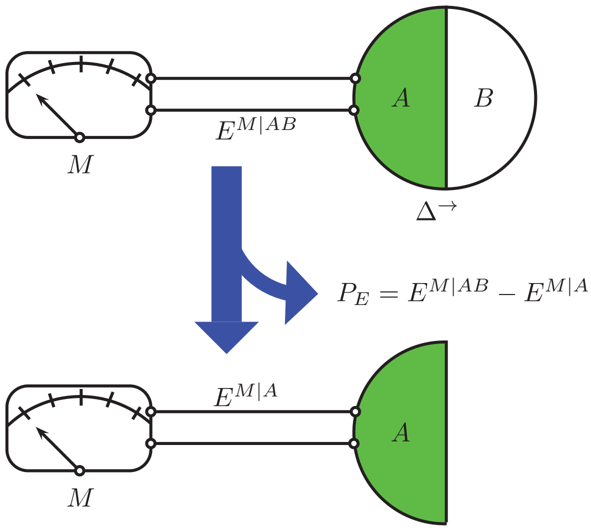

Figure 5.5: A measurement apparatus M is used for a von Neumann measurement on A (green colored area), which is part of the total quantum system AB. The measurement implies a unitary evolution on the system MA, which can create entanglement $E^{M|AB}$ between the apparatus and the system. The minimal amount of distillable entanglement created in this way is equal to the one-way information deficit $\Delta^{\rightarrow} := \Delta^{B|A}$ between B and A. The partial entanglement $P_E = E^{M|AB} - E^{M|A}$ quantifies the part of entanglement which is lost when ignoring B. The minimal partial distillable entanglement is equal to the quantum discord between B and A, see main text for details. Figure and caption are taken from (Streltsov *et al.*, 2011b).

where the minimum is taken over all unitaries U which realize a von Neumann measurement on A. The generalized one-way information deficit is zero if and only if the state of the system AB is classical-quantum, i.e., if the density operator has the form $\rho_{\mathrm{cq}} = \sum_i p_i \left|i\right\rangle\left\langle i\right|^A \otimes \rho_i^B$. This holds for any measure of entanglement E which is zero on separable states only (Streltsov *et al.*, 2011b).

The approach presented so far can also be applied to the quantum discord defined in Section 4.2.1. This is done by introducing the *partial entanglement* (Streltsov *et al.*, 2011b)

$$P_E(\rho) = E^{M|AB}(\rho) - E^{M|A}(\rho^{MA}). \tag{5.23}$$

As noted in (Streltsov *et al.*, 2011b), the partial entanglement "quantifies the part of entanglement which is lost when the subsystem B is ignored". This is illustrated in the lower part of Fig. 5.5. As is also shown in (Streltsov *et al.*, 2011b), the minimal distillable partial entanglement created in a von Neumann measurement on A is equal to the quantum discord:

$$\delta^{B|A}(\rho^{AB}) = \min_U P_{E_d}\{U(\left|0\right\rangle\left\langle 0\right|^M \otimes \rho^{AB})U^\dagger\}, \tag{5.24}$$

where the minimum is taken over all unitaries U which realize a von Neumann measurement on A. The proof can be found in (Streltsov *et al.*, 2011b).

The relation between entanglement and the generalized one-way information deficit in Eq. (5.22) can be used to study the properties of general quantum correlations. In particular, it allows to define a class of quantum operations which do not increase the generalized one-way information deficit. As we show in (Streltsov *et al.*, 2011b), any such measure of quantum correlations does not increase under local operations on the subsystem B, denoted by Λ_B:

$$\Delta_E^{B|A}(\Lambda_B(\rho^{AB})) \leq \Delta_E^{B|A}(\rho^{AB}). \tag{5.25}$$

This inequality follows from the fact that the corresponding measure of entanglement $E^{M|AB}$ does not increase under Λ_B (Streltsov *et al.*, 2011b). In the same way, the correspondence between quantum discord and partial entanglement in Eq. (5.24) is used in (Streltsov *et al.*, 2011b) to show that the quantum discord does not increase under local operations on the subsystem B: $\delta^{B|A}(\Lambda_B(\rho^{AB})) \leq \delta^{B|A}(\rho^{AB})$. Similar results were found independently in (Piani *et al.*, 2011), see also (Modi *et al.*, 2012) for discussion and comparison of both approaches.

5.2.3 Behavior of quantum correlations under local noise

The behavior of quantum correlations under the action of local noisy channels has been investigated in (Streltsov *et al.*, 2011a). Noisy *quantum channels* are equivalent to quantum operations introduced in Section 2.2. The action of a noisy quantum channel can be described by a linear map Λ taking a density operator ρ onto a new density operator (Nielsen and Chuang, 2000, p. 360ff.)

$$\Lambda(\rho) = \sum_i E_i \rho E_i^\dagger, \tag{5.26}$$

where E_i are Kraus operators satisfying the completeness equation $\sum_i E_i^\dagger E_i = \mathbb{1}$. For composite quantum systems consisting of two subsystems, Alice and Bob, local noise on Alice's subsystem does not affect the subsystem of Bob. The corresponding Kraus operators have the form $E_i = E_i^A \otimes \mathbb{1}_B$.

As a simple example, given in (Streltsov *et al.*, 2011a), consider the classically correlated state of two qubits represented by the density operator

$$\rho_{\mathrm{cc}} = \frac{1}{2}\left|0\right\rangle\left\langle 0\right|^A \otimes \left|0\right\rangle\left\langle 0\right|^B + \frac{1}{2}\left|1\right\rangle\left\langle 1\right|^A \otimes \left|1\right\rangle\left\langle 1\right|^B . \tag{5.27}$$

As was shown in (Streltsov *et al.*, 2011a), using a local channel on qubit A only, it is possible to create a quantum correlated state with the density operator

$$\rho = \frac{1}{2}\left|0\right\rangle\left\langle 0\right|^A \otimes \left|0\right\rangle\left\langle 0\right|^B + \frac{1}{2}\left|+\right\rangle\left\langle +\right|^A \otimes \left|1\right\rangle\left\langle 1\right|^B , \tag{5.28}$$

where $\left|+\right\rangle^A = \frac{1}{\sqrt{2}}(\left|0\right\rangle^A + \left|1\right\rangle^A)$. This transformation is achieved by a local quantum channel $\Lambda_A(\rho)$ with two Kraus operators $E_1^A = \left|0\right\rangle\left\langle 0\right|^A$ and $E_2^A = \left|+\right\rangle\left\langle 1\right|^A$ acting on qubit A only (Streltsov *et al.*, 2011a). This example demonstrates that local noise can create quantum correlations from an initially classically correlated state (Streltsov *et al.*, 2011a).

The main reason for this phenomenon lies in the action of the local channel onto the maximally mixed state, represented by the density operator $\frac{1}{2}\mathbb{1}_A$ (Streltsov *et al.*, 2011a). In particular, $\Lambda_A\left(\frac{1}{2}\mathbb{1}_A\right) = \frac{1}{2}\left|0\right\rangle\left\langle 0\right|^A + \frac{1}{2}\left|+\right\rangle\left\langle +\right|^A \neq \frac{1}{2}\mathbb{1}_A$. This property is known as nonunitality: "a single-qubit quantum channel Λ is called *unital* if and only if it maps the maximally mixed state onto itself: $\Lambda\left(\frac{1}{2}\mathbb{1}\right) = \frac{1}{2}\mathbb{1}$" (Streltsov *et al.*, 2011a), see also Fig. 5.6. In the following we will also need another important type of channels, which we called *semiclassical* in (Streltsov *et al.*, 2011a). A semiclassical channel Λ_{sc} maps all density operators ρ onto density operators $\Lambda_{sc}(\rho)$ which are diagonal in the same basis[1]:

$$\Lambda_{sc}(\rho) = \sum_k p_k(\rho)\left|k\right\rangle\left\langle k\right| . \tag{5.29}$$

Following (Streltsov *et al.*, 2011a), "the non-negative probabilities $p_k(\rho)$ can, in general, depend on the input state ρ, while the orthogonal states $\left|k\right\rangle$ are independent of ρ". Our main result is given in Theorem 1 in (Streltsov *et al.*, 2011a):

> *"A local quantum channel acting on a single qubit can create quantum correlations in a multiqubit system if and only if it is neither semiclassical nor unital."*

In the following we will discuss the meaning and implications of this result. The proof can be found in (Streltsov *et al.*, 2011a).

[1]Channels of this type were also considered in (Holevo, 1998; Horodecki *et al.*, 2003; Piani *et al.*, 2008), where they were called quantum-classical channels or measurement maps.

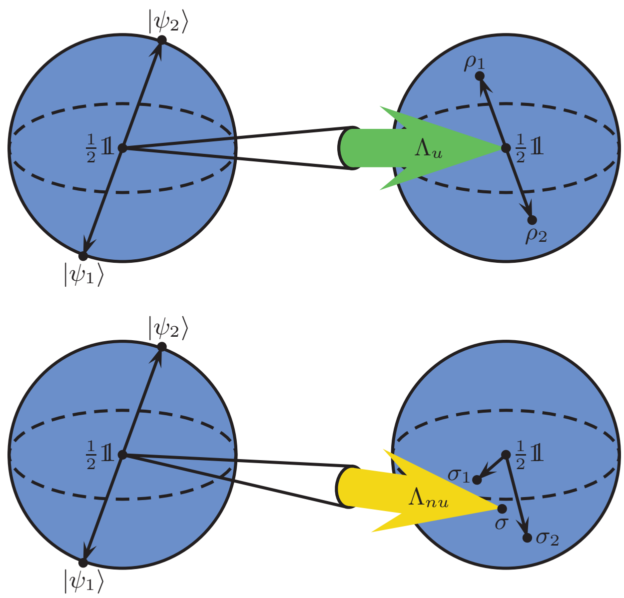

Figure 5.6: Quantum channels on a single qubit: The upper figure shows a unital quantum channel Λ_u (green arrow) which maps the maximally mixed state onto itself: $\Lambda_u\left(\frac{1}{2}\mathbb{1}\right) = \frac{1}{2}\mathbb{1}$. Two orthogonal states $|\psi_1\rangle$ and $|\psi_2\rangle$ with collinear Bloch vectors are mapped onto the density operators $\rho_1 = \Lambda_u(|\psi_1\rangle\langle\psi_1|)$ and $\rho_2 = \Lambda_u(|\psi_2\rangle\langle\psi_2|)$ with collinear Bloch vectors. The lower figure shows a nonunital quantum channel Λ_{nu} (yellow arrow) which maps the maximally mixed state onto the density operator $\sigma = \Lambda_{nu}\left(\frac{1}{2}\mathbb{1}\right) \neq \frac{1}{2}\mathbb{1}$. The Bloch vectors of $\sigma_1 = \Lambda_{nu}(|\psi_1\rangle\langle\psi_1|)$ and $\sigma_2 = \Lambda_{nu}(|\psi_2\rangle\langle\psi_2|)$ add up to twice the nonzero Bloch vector of σ. Figure and caption are taken from (Streltsov *et al.*, 2011a).

Our main result in (Streltsov *et al.*, 2011a) allows to show that a very general class of measures for quantum correlations does not increase under local unital and local semiclassical channels in multiqubit systems. In (Streltsov *et al.*, 2011a) we consider distance-based measures of quantum correlations Q_D, which are defined via the minimal distance D between the given density operator ρ and the set of density operators CC corresponding to classically correlated states:

$$Q_D(\rho) = \min_{\sigma \in CC} D(\rho, \sigma), \tag{5.30}$$

see also Section 4.2.2. As is shown in (Streltsov *et al.*, 2011a), all such distance-based measures do not increase under local unital channels Λ_{lu} and local semiclassical channels Λ_{lsc} in multiqubit systems if the distance D does not increase under any quantum channel, i.e.,

$$Q_D(\Lambda_{lu}(\rho)) \leq Q_D(\rho), \qquad Q_D(\Lambda_{lsc}(\rho)) \leq Q_D(\rho), \tag{5.31}$$

if $D(\Lambda(\rho), \Lambda(\sigma)) \leq D(\rho, \sigma)$ holds for any quantum channel Λ.

One example for such a measure is the *geometric measure of quantumness* which was defined in (Streltsov *et al.*, 2011a) as

$$Q_G(\rho) = \min_{\sigma \in CC}(1 - F(\rho, \sigma)) \tag{5.32}$$

with the fidelity $F(\rho, \sigma) = (\mathrm{Tr}[\sqrt{\sqrt{\rho}\sigma\sqrt{\rho}}])^2$. Using the fact that the fidelity does not decrease on quantum channels (Nielsen and Chuang, 2000, p. 414), we showed in (Streltsov *et al.*, 2011a) that the geometric measure of quantumness does not increase under local unital and local semiclassical channels in multiqubit systems. In (Streltsov *et al.*, 2011a) we also used the quantum relative entropy $S(\rho||\sigma)$, which is also nonincreasing on quantum channels. It follows that the resulting measure of quantum correlations $Q_R(\rho) = \min_{\sigma \in CC} S(\rho||\sigma)$ does not increase under local unital and local semiclassical channels in multiqubit systems (Streltsov *et al.*, 2011a). This measure was defined in (Piani *et al.*, 2011) as the relative entropy of quantumness, see also Section 4.2.2. Note that the relative entropy $S(\rho||\sigma)$ and the quantity $1 - F(\rho, \sigma)$ used in the definition of the geometric measure of quantumness do not satisfy the triangle inequality, and thus they are no distances in the mathematical sense.

Finally, we show in (Streltsov *et al.*, 2011a) that for higher-dimensional systems quantum correlations can be created even by local unital channels. In particular, this is demonstrated for the *phase-damping channel*, which is a model for decoherence in a quantum system (Streltsov *et al.*, 2011a):

> *"Under decoherence the quantum state* $\rho = \sum_{i,j} \rho_{ij} |i\rangle \langle j|$ *is transformed to the state*
>
> $$\Lambda(\rho) = \sum_i \rho_{ii} |i\rangle \langle i| + (1 - p) \sum_{i \neq j} \rho_{ij} |i\rangle \langle j| \tag{5.33}$$
>
> *with the damping parameter* $0 \leq p \leq 1$*. Since* Λ *is unital, it is not possible to create quantum correlations with local phase damping in a multiqubit system. Surprisingly, this is not true if the local systems are not qubits: Qubits are special."*

In particular, we prove in (Streltsov *et al.*, 2011a) that local decoherence can create quantum correlations if the corresponding local system is a qutrit, i.e., has dimension three.

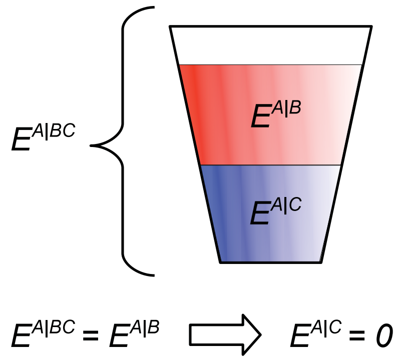

Figure 5.7: Entanglement is monogamous: for a fixed amount of entanglement between A and BC, the more entanglement exists between A and B, the less can exist between A and C. Quantitatively this is expressed using the monogamy relation, see Eq. (5.34) in the main text. In particular, the latter implies—for a monogamous measure of entanglement E—that $E^{A|C} = 0$ if $E^{A|BC} = E^{A|B}$. In (Streltsov *et al.*, 2012a) we show that the monogamy relation does not hold in general for any quantum correlation measure beyond entanglement, i.e., for any measure that does not vanish on separable states. Figure and caption are taken from (Streltsov *et al.*, 2012a).

5.2.4 Are general quantum correlations monogamous?

Monogamy of quantum correlations beyond entanglement has been investigated in (Streltsov *et al.*, 2012a). In general, a bipartite measure of correlations Q satisfies monogamy if (Coffman *et al.*, 2000)

$$Q^{A|BC}(\rho^{ABC}) \geq Q^{A|B}(\rho^{AB}) + Q^{A|C}(\rho^{AC}) \tag{5.34}$$

holds for all density operators ρ^{ABC}. For entanglement the concept of monogamy is illustrated in Fig. 5.7.

For entanglement the question of monogamy has been extensively studied in the literature. In particular, it was shown in (Coffman *et al.*, 2000) that for pure states of three qubits the squared concurrence defined below Eq. (3.8) on page 14 is monogamous. This result has been extended to an arbitrary number of qubits in (Osborne and Verstraete, 2006). The existence of a measure of entanglement that is monogamous in general, i.e., for three arbitrary systems A, B and C was shown in (Koashi and Winter, 2004). The authors showed that a certain measure of entanglement known as squashed entanglement satisfies Eq. (5.34) for all density operators ρ^{ABC}. However, other entanglement measures, such as the entanglement of formation, do not satisfy the monogamy relation (Coffman *et al.*, 2000).

In (Streltsov *et al.*, 2012a) we raised the question of whether monogamy can extend to quantum correlations beyond entanglement:

> *"Does there exist a measure of correlations Q that obeys the monogamy relation and is nonzero on a separable state?"* (Streltsov *et al.*, 2012a)

We gave a complete answer to this question in (Streltsov *et al.*, 2012a) by proving that all measures that are nonvanishing on at least some separable states and that respect some basic properties are not monogamous in general. These basic properties of the correlation measure Q are the following (Streltsov *et al.*, 2012a):

1. positivity:
$$Q^{A|B}(\rho^{AB}) \geq 0; \tag{5.35}$$

2. invariance under local unitaries $U_A \otimes V_B$:
$$Q^{A|B}(\rho^{AB}) = Q^{A|B}(U_A \otimes V_B \rho^{AB} U_A^\dagger \otimes V_B^\dagger); \tag{5.36}$$

3. no increase upon attaching a local pure ancilla:
$$Q^{A|B}(\rho^{AB}) \geq Q^{A|BC}(\rho^{AB} \otimes |0\rangle\langle 0|^C). \tag{5.37}$$

As mentioned in (Streltsov *et al.*, 2012a), "these properties are valid for several measures of correlations known in the literature, including all entanglement measures. In particular, positivity and invariance under local unitaries are standard requirements." The third property in Eq. (5.37) is satisfied for quantum discord, and all measures of quantum correlations which are defined as the minimal distance to the set of classically correlated states, as long as the distance does not change upon attaching an ancilla: $D(\rho, \sigma) = D(\rho \otimes |0\rangle\langle 0|, \sigma \otimes |0\rangle\langle 0|)$ (Streltsov *et al.*, 2012a). The same arguments apply to measures that are defined via the minimal distance to the set of quantum-classical or classical-quantum states, or via measurements on local subsystems (Streltsov *et al.*, 2012a).

The main result of (Streltsov *et al.*, 2012a) is the finding that any measure of quantum correlations Q which respects Eqs. (5.35)–(5.37) and is also monogamous according to Eq. (5.34) must vanish on all separable states, see Theorem 1 in (Streltsov *et al.*, 2012a). We will discuss the meaning and implications of this result in the following, and refer to (Streltsov *et al.*, 2012a) for the proof. As pointed out in (Streltsov *et al.*, 2012a), the power of this result lies in its generality. "Under very weak assumptions, it rules out the existence of monogamous correlations beyond entanglement" (Streltsov *et al.*, 2012a). Moreover, this result is strong enough to show the violation of monogamy even in three-qubit systems: "The measure Q violates monogamy [in a three-qubit system] if it is nonzero on some separable two-qubit state of rank two. This is the case for quantum discord and any related measures of quantum correlations" (Streltsov *et al.*, 2012a).

The results presented so far can also be applied to the geometric measure of discord D_G defined in Eq. (4.17) on page 22, i.e., the geometric measure of discord is not monogamous. On the other hand, this measure respects monogamy on pure states of three qubits in the following sense (Streltsov *et al.*, 2012a):

$$D_G^{AB|C}(|\psi\rangle\langle\psi|^{ABC}) \geq D_G^{A|C}(\rho^{AC}) + D_G^{B|C}(\rho^{BC}), \tag{5.38}$$

where $|\psi\rangle^{ABC}$ is an arbitrary pure state of three qubits, and the reduced density operators are given by $\rho^{AC} = \mathrm{Tr}_B[|\psi\rangle\langle\psi|^{ABC}]$ and $\rho^{BC} = \mathrm{Tr}_A[|\psi\rangle\langle\psi|^{ABC}]$. For the proof we refer to (Streltsov *et al.*, 2012a), where this result is stated in Theorem 3. The meaning of this result was also pointed out in (Streltsov *et al.*, 2012a): "Even though quantum correlations beyond entanglement cannot be monogamous in general, Theorem 3 demonstrates that for pure states of three qubits, monogamy of the geometric measure of discord is still preserved. To the best of our knowledge, this is the first instance of a measure of quantum correlations beyond entanglement that satisfies a restricted monogamy inequality."

6 Outlook

Several results presented in this thesis have attracted considerable attention, and many publications are based on the ideas presented here. As an example we mention (Modi *et al.*, 2012, Section VIII B), where the authors review our results on the behavior of quantum correlations under local noise, see Section 5.2.3 of this work. Extension of these results to higher-dimensional systems has been proposed in (Hu *et al.*, 2012). The power of local channels for producing quantum correlations has been investigated recently in (Abad *et al.*, 2012).

A great amount of interest has also been devoted to the question of monogamy of general quantum correlations presented in Section 5.2.4 of this work. A detailed review of these results can also be found in (Modi *et al.*, 2012, Section III D 6). As was pointed out in (Streltsov *et al.*, 2012a), several previous publications showed that quantum discord violates monogamy by finding explicit examples of states for which the monogamy inequality does not hold (Giorgi, 2011; Prabhu *et al.*, 2012a,b; Sudha *et al.*, 2012; Allegra *et al.*, 2011; Ren and Fan, 2011). It was also stated in (Streltsov *et al.*, 2012a) that "those examples, however, do not exclude the possibility that other measures of quantum correlations, akin to the quantum discord, could exist that do satisfy a monogamy inequality". The results presented in (Streltsov *et al.*, 2012a) close this gap and put the question of monogamy for general quantum correlations to rest.

Our results on the role of quantum correlations in the measurement process presented in Section 5.2.2 were also used as a basis for several publications. In particular, the results of Section 5.2.2 can be extended to the geometric measure of entanglement using the new expression for the geometric measure of entanglement presented in Section 5.1.1. This connection was already pointed out by us in (Streltsov *et al.*, 2011b), and was treated in detail later in (Coles, 2012).

Finally, we recall one of our most important results presented in Section 5.2.1. It was the finding that the distribution of entanglement always requires the transmission of quantum correlations beyond entanglement, thus providing "a fundamental connection between quantum entanglement on one side and quantum correlations on the other side" (Streltsov *et al.*, 2012b). However, the inverse of this statement does not hold: the presence of quantum correlations alone does not guarantee that entanglement can be successfully distributed. As a simple example consider a fully separable state with the density operator

$$\rho^{ABC} = \sum_i p_i \rho_i^A \otimes \rho_i^B \otimes \rho_i^C. \tag{6.1}$$

Clearly, such a state cannot be used for entanglement distribution, since sending the particle C from Alice to Bob will not create any entanglement. However, the state still can have quantum correlations between AB and C.

It is thus an open question, under which circumstances two parties can successfully use quantum correlations beyond entanglement for entanglement distribution. A possible future research direction could arise from the question whether quantum correlations can be “activated” into an entanglement distribution protocol. This question is also interesting in the light of the finding that quantum correlations can be created by local noise, see Section 5.2.3. Starting from this result, one might be tempted to ask whether noise can be useful for entanglement distribution. Moreover, the results presented in Section 5.2.1 might also be used to find new protocols for entanglement distribution. We expect that such protocols, where entanglement is distributed by sending quantum correlations without entanglement, have several desirable properties. In particular, they could show a higher noise-robustness compared to the simple procedure where entanglement is sent directly.

7 List of main results

- The geometric measure of entanglement belongs to two classes of entanglement measures simultaneously: it is a convex roof and a distance-based measure of entanglement. This result can be used to build an algorithm for approximating the geometric measure of entanglement from above.

- The distribution of any finite amount of entanglement always requires the transmission of quantum correlations beyond entanglement. The amount of transmitted quantum correlations cannot be smaller than the amount of the distributed entanglement. This result is valid for a very general class of entanglement and quantum correlation measures, and also for an arbitrary distribution protocol.

- Any von Neumann measurement on a part of a composite quantum system unavoidably creates entanglement between the measurement apparatus and the total system whenever the total system has nonzero quantum discord. The minimal amount of the distillable entanglement created in this way is equal to the one-way information deficit.

- Local noise can create quantum correlations. For multiqubit systems we give a full characterization of local noisy channels with this property: a local noisy channel can create quantum correlations if and only if it is neither unital nor semiclassical. We also show that a very general class of quantum correlation measures does not increase under local unital and local semiclassical channels.

- Under very general assumptions we show that quantum correlations beyond entanglement cannot be monogamous. Entanglement is the only kind of quantum correlations which can be monogamous. This result puts the question about monogamy of general quantum correlations to rest.

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New Journal of Physics
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Linking a distance measure of entanglement to its convex roof

Alexander Streltsov, Hermann Kampermann and Dagmar Bruß
Heinrich-Heine-Universität Düsseldorf, Institut für Theoretische Physik III, D-40225 Düsseldorf, Germany
E-mail: streltsov@thphy.uni-duesseldorf.de, kampermann@thphy.uni-duesseldorf.de and bruss@thphy.uni-duesseldorf.de

New Journal of Physics **12** (2010) 123004 (19pp)
Received 23 June 2010
Published 6 December 2010
Online at http://www.njp.org/
doi:10.1088/1367-2630/12/12/123004

Abstract. An important problem in quantum information theory is the quantification of entanglement in multipartite mixed quantum states. In this work, a connection between the geometric measure of entanglement and a distance measure of entanglement is established. We present a new expression for the geometric measure of entanglement in terms of the maximal fidelity with a separable state. A direct application of this result provides a closed expression for the Bures measure of entanglementof two qubits. We also prove that the number of elements in an optimal decomposition w.r.t. the geometric measure of entanglement is bounded from above by the Caratheodory bound, and we find necessary conditions for the structure of an optimal decomposition.

Contents

1. Introduction

Entanglement [1] is one of the most fascinating features of quantum mechanics, and allows a new view on information processing. In spite of the central role of entanglement there does not yet exist a complete theory for its quantification. Various entanglement measures have been suggested—for an overview see [2, 3].

A composite pure quantum state $|\psi\rangle$ is called entangled iff it cannot be written as a product state. A composite mixed quantum state ρ on a Hilbert space $\mathcal{H} = \otimes_{j=1}^{n}\mathcal{H}_j$ is called entangled iff it cannot be written in the form [2, 4]

$$\rho = \sum_i p_i \left(\otimes_{j=1}^{n} |\psi_i^{(j)}\rangle\psi_i^{(j)}|\right) \tag{1}$$

with $p_i > 0$, $\sum_i p_i = 1$, and where $n \geqslant 2$ and $|\psi_i^{(j)}\rangle \in \mathcal{H}_j$.

The degree of entanglement can be captured in a function $E(\rho)$ that should fulfil at least the following criteria [2]:

- $E(\rho) \geqslant 0$ and equality holds iff ρ is separable[1],
- E cannot increase under local operations and classical communication (LOCC), i.e. $E(\Lambda(\rho)) \leqslant E(\rho)$ for any LOCC map Λ.

[1] Note that the distillable entanglement E_D does not satisfy this criterion, i.e. it can be zero on entangled states. However it is also accepted as a measure of entanglement [2].

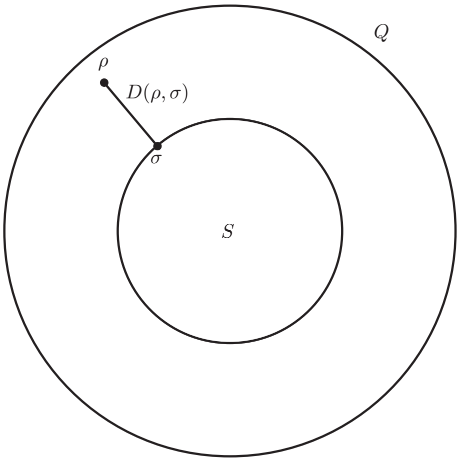

Figure 1. S denotes the set of separable states within the set of all quantum states Q. The state σ is the closest separable state to ρ, w.r.t. the distance D.

These criteria are satisfied by all measures of entanglement presented in this paper. One possibility to define an entanglement measure for a mixed quantum state ρ is via its *distance* to the set of separable states [5]; for an illustration see figure 1. Another possibility to define an entanglement measure for a mixed quantum state ρ is the *convex roof* extension, in which the entanglement is quantified by the weighted sum of the entanglement measure of the pure states in a given decomposition of ρ, minimized over all possible decompositions. There is no *a priori* reason why these two types of entanglement measures should be related. In this paper, we will establish a link between them, by showing the equality between the convex roof extension of the geometric measure of entanglement for pure states and the corresponding distance measure based on the fidelity with the closest separable state. Using this result, we will also study the properties of the optimal decompositions of the given state ρ and its closest separable state.

Our paper is organized as follows: in section 2, we provide the definitions of the used entanglement measures. In section 3, we derive the main result of this paper, namely the equality between the convex roof extension of the geometric measure of entanglement and the fidelity-based distance measure. In section 4, we study the simplest composite quantum system, namely two qubits, give an analytical expression for the Bures measure of entanglement and consider other measures that are based on the geometric measure of entanglement. In section 5, we characterize the optimal decomposition of ρ (i.e. the one that reaches the minimum in the convex roof construction) from knowledge of the closest separable state and vice versa. Finally, in section 6, we derive a necessary criterion that the states in an optimal decomposition have to fulfil. We conclude in section 7.

2. Definitions

Two classes of entanglement measures are considered in this paper. The first class consists of measures based on a distance [5, 6],

$$E_D(\rho) = \inf_{\sigma \in S} D(\rho, \sigma), \tag{2}$$

where $D(\rho,\sigma)$ is the 'distance' between ρ and σ and S is the set of separable states. This concept is illustrated in figure 1. Following [2], we do not require a distance to be a metric. In this paper, we will consider for example the Bures measure of entanglement [6]

$$E_{\mathrm{B}}(\rho) = \min_{\sigma\in S}(2-2\sqrt{F(\rho,\sigma)}), \tag{3}$$

where $F(\rho,\sigma) = \left(\mathrm{Tr}\left[\sqrt{\sqrt{\rho}\sigma\sqrt{\rho}}\right]\right)^2$ is Uhlmann's fidelity [7]. A very similar measure is the Groverian measure of entanglement [8, 9], defined as

$$E_{\mathrm{Gr}}(\rho) = \min_{\sigma\in S}\sqrt{1-F(\rho,\sigma)}. \tag{4}$$

As it can be expressed as a simple function of E_{B}, we will not consider it explicitly. Another important representative of the first class is the relative entropy of entanglement defined as [6]

$$E_{\mathrm{R}}(\rho) = \min_{\sigma\in S} S(\rho\|\sigma), \tag{5}$$

where $S(\rho\|\sigma)$ is the relative entropy,

$$S(\rho\|\sigma) = \mathrm{Tr}\left[\rho\log_2\rho\right] - \mathrm{Tr}\left[\rho\log_2\sigma\right]. \tag{6}$$

The second class of entanglement measures consists of convex roof measures [10]

$$E(\rho) = \min\sum_i p_i E(|\psi_i\rangle), \tag{7}$$

where $\sum_i p_i = 1$, $p_i \geqslant 0$, and the minimum is taken over all pure state decompositions of $\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$. An important example of the second class is the geometric measure of entanglement E_{G}, defined as follows [11]:

$$E_{\mathrm{G}}(|\psi\rangle) = 1 - \max_{|\phi\rangle\in S}|\langle\phi|\psi\rangle|^2, \tag{8}$$

$$E_{\mathrm{G}}(\rho) = \min\sum_i p_i E_{\mathrm{G}}(|\psi_i\rangle), \tag{9}$$

where the minimum is taken over all pure state decompositions of ρ. Entanglement measures of this form were considered earlier in [12, 13]. Another important representative of the second class for bipartite states ρ^{AB} is the entanglement of formation E_{F}, which is for pure states $\rho = |\psi\rangle\langle\psi|$ defined as the von Neumann entropy of the reduced density matrix,

$$E_{\mathrm{F}}(|\psi\rangle) = -\mathrm{Tr}\left[\rho^A\log_2\rho^A\right], \tag{10}$$

where $\rho^A = \mathrm{Tr}_{\mathrm{B}}[|\psi\rangle\langle\psi|]$. For mixed states this measure is again defined via the convex roof construction [14]:

$$E_{\mathrm{F}}(\rho) = \min_{\{p_i,|\psi_i\rangle\}}\sum_i p_i E_{\mathrm{F}}(|\psi_i\rangle). \tag{11}$$

For two-qubit states analytic formulae for E_{F} and E_{G} are known; both are simple functions of the concurrence [11, 15].

Remember that the concurrence for a two-qubit state ρ is given by [15]

$$C(\rho) = \max\{\xi_1-\xi_2-\xi_3-\xi_4, 0\}, \tag{12}$$

where ξ_i, with $i\in\{1,2,3,4\}$, are the square roots of the eigenvalues of $\rho\cdot\tilde{\rho}$ in decreasing order, and $\tilde{\rho}$ is defined as $\tilde{\rho} = (\sigma_y\otimes\sigma_y)\rho^*(\sigma_y\otimes\sigma_y)$.

The entanglement of formation for a two-qubit state ρ as a function of the concurrence is expressed as [15]

$$E_{\mathrm{F}}(\rho) = h(\tfrac{1}{2} + \tfrac{1}{2}\sqrt{1 - C(\rho)^2}), \tag{13}$$

where $h(x) = -x\log_2 x - (1-x)\log_2(1-x)$ is the Shannon entropy. The geometric measure of entanglement for a two-qubit state ρ as a function of the concurrence was shown in [11] to be

$$E_{\mathrm{G}}(\rho) = \tfrac{1}{2}(1 - \sqrt{1 - C(\rho)^2}). \tag{14}$$

This formula was already found in [16] in a different context. For bipartite states, it is furthermore known that [6]

$$E_{\mathrm{F}}(\rho) \geqslant E_{\mathrm{R}}(\rho), \tag{15}$$

where for bipartite pure states the equal sign holds [6].

The geometric measure of entanglement plays an important role in the research on fundamental properties of quantum systems. Recently it has been used to show that most quantum states are too entangled to be used for quantum computation [17]. In [18] the authors have shown how a lower bound on the geometric measure of entanglement can be estimated in experiments. A connection to Bell inequalities for graph states has also been reported [19].

3. Geometric measure of entanglement for mixed states

In this section, we will show the main result of our paper: the geometric measure of entanglement, defined via the convex roof, see equation (9), is equal to a distance-based alternative.

We introduce the *fidelity of separability*

$$F_s(\rho) = \max_{\sigma \in S} F(\rho, \sigma), \tag{16}$$

where the maximum is taken over all separable states of the form (1).

Theorem 1. *For a multipartite mixed state ρ on a finite dimensional Hilbert space $\mathcal{H} = \otimes_{j=1}^{n} \mathcal{H}_j$ the following equality holds:*

$$F_s(\rho) = \max_{\{p_i, |\psi_i\rangle\}} \sum_i p_i F_s(|\psi_i\rangle), \tag{17}$$

where the maximization is done over all pure state decompositions of $\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$.

Proof. Remember that according to Uhlmann's theorem [20, p 411],

$$F(\rho, \sigma) = \max_{|\phi\rangle} |\langle\psi|\phi\rangle|^2 \tag{18}$$

holds for two arbitrary states ρ and σ, where $|\psi\rangle$ is a purification of ρ and the maximization is done over all purifications of σ, which are denoted by $|\phi\rangle$.

We start the proof with equation (16). In order to find $F_s(\rho)$, we have to maximize $|\langle\psi|\phi\rangle|^2$ over all purifications $|\phi\rangle$ of all separable states $\sigma = \sum_j q_j |\phi_j\rangle\langle\phi_j|$, where all $|\phi_j\rangle$ are separable.

The purifications of ρ and σ can in general be written as

$$|\psi'\rangle = \sum_i \sqrt{p_i'}\, |\psi_i'\rangle \otimes |i\rangle, \tag{19}$$

$$\left|\phi'\right\rangle = \sum_j \sqrt{q_j}\,\left|\phi_j\right\rangle \otimes U^\dagger\,|j\rangle\,, \tag{20}$$

where $\{p_i', |\psi_i'\rangle\}$ is a fixed decomposition of ρ, $\langle k|l\rangle = \delta_{kl}$ and U is a unitary on the ancillary Hilbert space spanned by the states $\{|i\rangle\}$. To see whether all purifications of a separable state $\sigma = \sum_j q_j|\phi_j\rangle\langle\phi_j|$ are of the form given by $|\phi'\rangle$, we start with an arbitrary purification $|\phi''\rangle = \sum_k \sqrt{r_k}\,|\alpha_k\rangle \otimes |k\rangle$, such that $\sigma = \sum_k r_k\,|\alpha_k\rangle\,\langle\alpha_k|$ and $\langle k|l\rangle = \delta_{k,l}$. Further the following holds $\sqrt{r_k}\,|\alpha_k\rangle = \sum_j u_{kj}\sqrt{q_j}|\phi_j\rangle$, with u_{kj} being elements of a unitary matrix [21]. Using the last relation we get $|\phi''\rangle = \sum_j \sqrt{q_j}|\phi_j\rangle \otimes |j'\rangle$, with $|j'\rangle = \sum_k u_{kj}\,|k\rangle$. Thus we brought an arbitrary purification of σ to the form given by $|\phi'\rangle$.

In order to find $F_s(\rho)$ in the above parametrization we have to maximize the overlap $|\langle\psi'|\phi'\rangle|^2$ over all unitaries U, all probability distributions $\{q_i\}$ and all sets of separable states $\{|\phi_i\rangle\}$.

We will now show that we can also achieve $F_s(\rho)$ by maximizing the overlap $|\langle\psi|\phi\rangle|^2$ of the purifications

$$|\psi\rangle = \sum_i \sqrt{p_i}\,|\psi_i\rangle \otimes |i\rangle\,, \tag{21}$$

$$|\phi\rangle = \sum_j \sqrt{q_j}\,\left|\phi_j\right\rangle \otimes |j\rangle\,, \tag{22}$$

where now the maximization has to be done over all decompositions $\{p_i, |\psi_i\rangle\}$ of the given state ρ, all probability distributions $\{q_i\}$ and all sets of separable states $\{|\phi_i\rangle\}$. To see how this works we write the matrix U in its elements, $U = \sum_{kl} u_{kl}\,|k\rangle\,\langle l|$, and apply it in the overlap $|\langle\psi'|\phi'\rangle|^2$, thus noting that the action of the unitary is equivalent to a transformation of the set of unnormalized states $\{\sqrt{p_i'}|\psi_i'\rangle\}$ into the new set $\{\sqrt{p_i}|\psi_i\rangle\}$. The connection between the two sets is given by the unitary: $\sqrt{p_i}|\psi_i\rangle = \sum_j u_{ij}\sqrt{p_j'}|\psi_j'\rangle$, which is a transformation between two decompositions of the state ρ, see also [20, p 103f]. The advantage of this parametrization is that now both purifications have the same orthogonal states on the ancillary Hilbert space.

We now do the maximization of the overlap

$$|\langle\psi|\phi\rangle| = \left|\sum_i \sqrt{q_i}\sqrt{p_i}\,\langle\psi_i|\phi_i\rangle\right| \tag{23}$$

starting with the separable states $\{|\phi_i\rangle\}$. The optimal states can be chosen such that all terms $\langle\psi_i|\phi_i\rangle$ are real, positive and equal to $\sqrt{F_s\,(|\psi_i\rangle)} = \max_{|\phi\rangle\in S}|\langle\psi_i|\phi\rangle|$; it is obvious that this choice is optimal. We also used the fact that for pure states $|\psi\rangle$ it is enough to maximize over pure separable states: $F_s(|\psi\rangle) = \max_{|\phi\rangle\in S}|\langle\psi|\phi\rangle|^2$. To see this, note that $F(|\psi\rangle\,\langle\psi|\,,\sigma) = \langle\psi|\sigma|\psi\rangle$. Suppose now the closest separable state to $|\psi\rangle$ is the mixed state σ with the separable decomposition $\sigma = \sum_j q_j|\phi_j\rangle\langle\phi_j|$, all $|\phi_j\rangle$ being separable. Without loss of generality let $|\langle\psi|\phi_1\rangle| \geqslant |\langle\psi|\phi_j\rangle|$ be true for all j. Then the following holds: $F\,(|\psi\rangle\,\langle\psi|\,,\sigma) = \langle\psi|\sigma|\psi\rangle = \sum_j q_j|\langle\psi|\phi_j\rangle|^2 \leqslant \sum_j q_j\,|\langle\psi|\phi_1\rangle|^2 = |\langle\psi|\phi_1\rangle|^2$, and thus $|\phi_1\rangle$ is a closest separable state to $|\psi\rangle$.

The maximization over $\{|\phi_i\rangle\}$ gives us

$$\max_{\{|\phi_j\rangle\}}|\langle\psi|\phi\rangle| = \sum_i \sqrt{q_i}\sqrt{p_i}\sqrt{F_s\,(|\psi_i\rangle)}. \tag{24}$$

Now we do the optimization over q_i. Using Lagrange multipliers we obtain

$$\sqrt{q_i} = \frac{\sqrt{p_i}\sqrt{F_s\left(|\psi_i\rangle\right)}}{\sqrt{\sum_k p_k F_s\left(|\psi_k\rangle\right)}}, \tag{25}$$

with the result

$$\max_{\{q_j,|\phi_j\rangle\}} |\langle\psi|\phi\rangle|^2 = \sum_i p_i F_s\left(|\psi_i\rangle\right). \tag{26}$$

It is easy to understand that this choice of $\{q_i\}$ is optimal when one interprets the right-hand side of equation (24) as a scalar product between a vector with entries $(\sqrt{p_1}\sqrt{F_s\left(|\psi_1\rangle\right)}, \sqrt{p_2}\sqrt{F_s\left(|\psi_2\rangle\right)}, \ldots)$ and a vector with entries $(\sqrt{q_1}, \sqrt{q_2}, \ldots)$. The scalar product of two vectors with given length is maximal when they are parallel.

In the last step, we do the maximization over all decompositions $\{p_i, |\psi_i\rangle\}$ of the given state ρ which leads to the end of the proof, namely

$$F_s\left(\rho\right) = \max |\langle\psi|\phi\rangle|^2 = \max_{\{p_i,|\psi_i\rangle\}} \sum_i p_i F_s\left(|\psi_i\rangle\right). \tag{27}$$

□

We can generalize theorem 1 for arbitrary convex sets; the result can be found in appendix A. Using theorem 1 it follows immediately that the geometric measure of entanglement is not only a convex roof measure, but also a distance-based measure of entanglement:

Proposition 1. *For a multipartite mixed state ρ on a finite dimensional Hilbert space $\mathcal{H} = \otimes_{j=1}^{n}\mathcal{H}_j$ the following equality holds:*

$$E_{\mathrm{G}}\left(\rho\right) = 1 - \max_{\sigma\in S} F(\rho, \sigma). \tag{28}$$

Proposition 1 establishes a connection between E_{G} and distance-based measures such as the Bures measure E_{B} and Groverian measure E_{Gr}. All of them are simple functions of each other.

In [22] the authors found the following connection between E_{R} and E_{G} for pure states:

$$E_{\mathrm{R}}\left(|\psi\rangle\right) \geqslant -\log_2(1 - E_{\mathrm{G}}\left(|\psi\rangle\right)). \tag{29}$$

This inequality can be generalized to mixed states as follows:

$$E_{\mathrm{R}}\left(\rho\right) \geqslant \max\{0, -\log_2(1 - E_{\mathrm{G}}\left(\rho\right)) - S\left(\rho\right)\}, \tag{30}$$

where $S(\rho) = -\mathrm{Tr}[\rho \log_2 \rho]$ is the von Neumann entropy of the state. Inequality (30) is a direct consequence of the following proposition.

Proposition 2. *For two arbitrary quantum states ρ and σ holds*

$$S\left(\rho||\sigma\right) \geqslant \mathrm{Tr}\left[\rho \log_2 \rho\right] - \log_2 F(\rho, \sigma). \tag{31}$$

Proof. With $\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$ we will estimate $-\mathrm{Tr}[\rho \log_2 \sigma]$ from below:

$$-\mathrm{Tr}\left[\rho \log_2 \sigma\right] = -\sum_i p_i \langle\psi_i| \log_2 \sigma |\psi_i\rangle \tag{32}$$

$$\geqslant -\sum_i p_i \log_2 \langle\psi_i|\sigma|\psi_i\rangle. \tag{33}$$

Here we used concavity of the log function

$$\log_2 \langle\psi_i|\sigma|\psi_i\rangle \geqslant \langle\psi_i|\log_2 \sigma|\psi_i\rangle. \tag{34}$$

Using concavity again we obtain $\sum_i p_i \log_2 \langle\psi_i|\sigma|\psi_i\rangle \leqslant \log_2 \sum_i p_i \langle\psi_i|\sigma|\psi_i\rangle$ and thus

$$-\mathrm{Tr}\left[\rho \log_2 \sigma\right] \geqslant -\log_2 \sum_i p_i \langle\psi_i|\sigma|\psi_i\rangle \tag{35}$$

$$= -\log_2 \mathrm{Tr}\,[\rho\sigma]\,. \tag{36}$$

The fidelity can be bounded from below as follows:

$$F(\rho,\sigma) = \left(\mathrm{Tr}\left[\sqrt{\sqrt{\rho}\sigma\sqrt{\rho}}\right]\right)^2 = \left(\sum_i \lambda_i\right)^2 \tag{37}$$

$$\geqslant \sum_i \lambda_i^2 = \mathrm{Tr}\left[\sqrt{\rho}\sigma\sqrt{\rho}\right] = \mathrm{Tr}\,[\rho\sigma]\,, \tag{38}$$

where λ_i are the eigenvalues of the positive operator $\sqrt{\sqrt{\rho}\sigma\sqrt{\rho}}$. □

Inequality (30) becomes trivial for states with high entropy. As a nontrivial example we consider the two-qubit state

$$\rho = p|\psi\rangle\langle\psi| + (1-p)|01\rangle\langle 01|\,, \tag{39}$$

with $|\psi\rangle = \sqrt{a}\,|01\rangle + \sqrt{1-a}\,|10\rangle$. This state was called the generalized Vedral–Plenio state in [23], where the authors showed that the closest separable state σ w.r.t. the relative entropy of entanglement is given by

$$\sigma = (1-p+pa)\,|01\rangle\langle 01| + p\,(1-a)\,|10\rangle\langle 10|\,. \tag{40}$$

In figures 2 and 3, we show the plot of E_{F} (dotted curve), E_{R} (solid curve) and $\mathcal{E} = \max\{0, -\log_2(1-E_{\mathrm{G}}(\rho)) - S(\rho)\}$ (dashed curve) as a function of a for $p = \frac{99}{100}$ and $p = \frac{9}{10}$, respectively. It can be seen that $\mathcal{E}$ drops quickly with increasing entropy of the state and thus is nontrivial only for states close to pure states with high entanglement.

In [24, 25], the authors gave lower bounds for the relative entropy of entanglement in terms of the von Neumann entropies of the reduced states, which provide better lower bounds for E_{R} than (30). Thus, the inequality (30) should be seen as a connection between the two entanglement measures E_{R} and E_{G}, and not as an improved lower bound for E_{R}.

4. Entanglement measures for two qubits

4.1. Bures measure of entanglement

We can use proposition 1 to evaluate entanglement measures for two qubit states. From [11, 16] we know the geometric measure for two-qubit states as a function of the concurrence, see equation (14). Using this together with equation (28), we find the fidelity of separability as a function of the concurrence:

$$F_{\mathrm{s}}(\rho) = \max_{\sigma\in S} F(\rho,\sigma) = \frac{1}{2}\left(1+\sqrt{1-C(\rho)^2}\right). \tag{41}$$

Now we are able to give an expression for the Bures measure of entanglement for two-qubit states, remember its definition in equation (3).

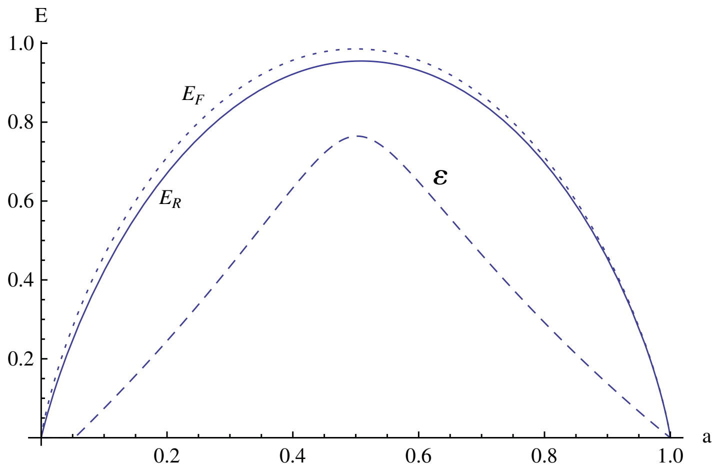

Figure 2. Entanglement of formation E_{F} (dotted curve), relative entropy of entanglement E_{R} (solid curve) and $\mathcal{E} = \max\{0, -\log_2(1 - E_{\mathrm{G}}(\rho)) - S(\rho)\}$ (dashed curve) of the state $\rho = p\,|\psi\rangle\langle\psi| + (1-p)\,|01\rangle\langle 01|$ with $|\psi\rangle = \sqrt{a}\,|01\rangle + \sqrt{1-a}\,|10\rangle$ for $p = \frac{99}{100}$ as a function of a.

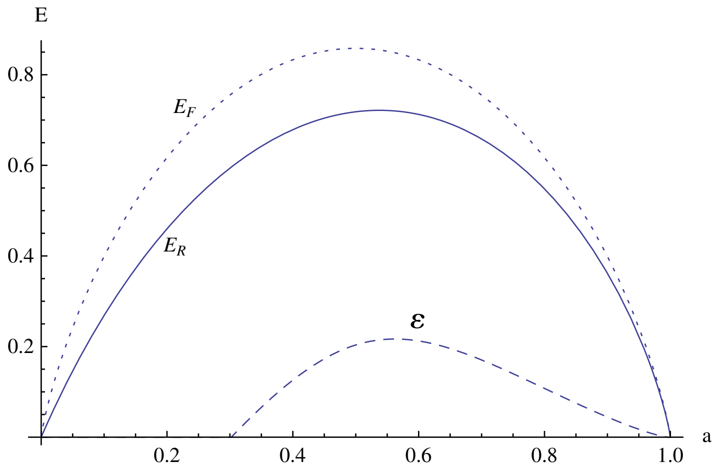

Figure 3. Entanglement of formation E_{F} (dotted curve), relative entropy of entanglement E_{R} (solid curve) and $\mathcal{E} = \max\{0, -\log_2(1 - E_G(\rho)) - S(\rho)\}$ (dashed curve) of the state $\rho = p\,|\psi\rangle\langle\psi| + (1-p)\,|01\rangle\langle 01|$ with $|\psi\rangle = \sqrt{a}\,|01\rangle + \sqrt{1-a}\,|10\rangle$ for $p = \frac{9}{10}$ as a function of a.

Proposition 3. *For any two-qubit state ρ the Bures measure of entanglement is given by*

$$E_{\mathrm{B}}(\rho) = 2 - 2\sqrt{\frac{1 + \sqrt{1 - C(\rho)^2}}{2}}. \tag{42}$$

Note that for a maximally entangled state, $E_{\mathrm{G}} = \frac{1}{2}$ and $E_{\mathrm{B}} = 2 - \sqrt{2}$. In order to compare these measures we renormalize them such that each of them becomes equal to 1 for maximally entangled states. We show the result in figure 4. There we also plot the Groverian measure of entanglement, see equation (4).

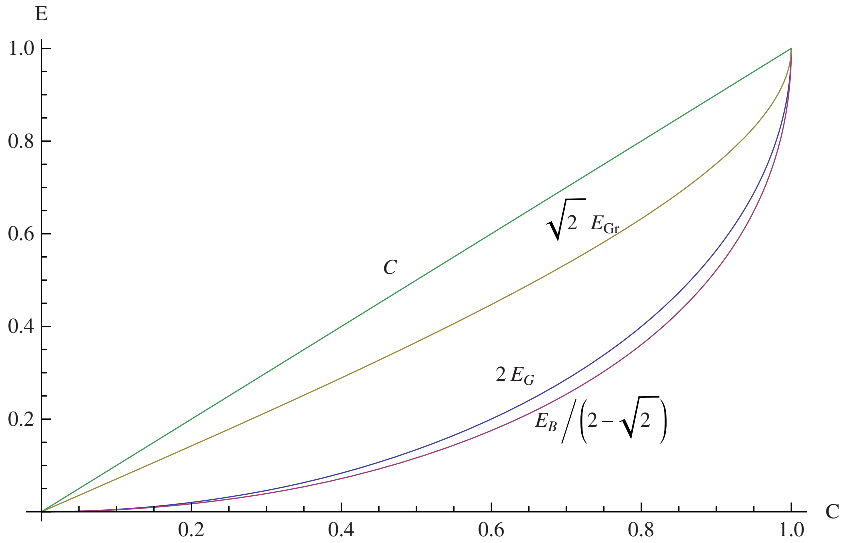

Figure 4. Plot of the geometric measure of entanglement E_{G}, Bures measure of entanglement E_{B} and Groverian measure of entanglement E_{Gr} as a function of the concurrence C for two qubit states. All measures were renormalised such that they reach 1 for maximally entangled states.

4.2. Measures induced by the geometric measure of entanglement

We consider now any generalized measure of entanglement for two-qubit states ρ which can be written as a function of the geometric measure of entanglement:

$$E_f(\rho) = f(E_{\mathrm{G}}(\rho)). \tag{43}$$

Proposition 4. *Let $f(x)$ be any convex function that is non-negative for $x \geqslant 0$ and obeys $f(0) = 0$. Then for two qubits $E_f(\rho) = f(E_{\mathrm{G}}(\rho))$ is equal to its convex roof, that is,*

$$E_f(\rho) = \min \sum_i p_i E_f(|\psi_i\rangle) = f\left(\frac{1}{2}\left(1 - \sqrt{1 - C(\rho)^2}\right)\right), \tag{44}$$

where the minimization is done over all pure state decompositions of ρ.

Proof. From [11] we know that the geometric measure of entanglement is a convex non-negative function of the concurrence, see also (14) and figure 4. As shown in [11], from convexity follows that E_{G} and E_{F} have identical optimal decompositions, and every state in this optimal decomposition has the same concurrence. This observation led directly to expression (14) for E_{G} of two qubit states.

As f is convex, E_f also is a convex function of the concurrence. To see this we note that convexity of E_{G} implies

$$E_{\mathrm{G}}\left(\sum_i p_i C_i\right) \leqslant \sum_i p_i E_{\mathrm{G}}(C_i), \tag{45}$$

where we defined $E_G(C) = \frac{1}{2}(1 - \sqrt{1 - C^2})$. As $f(x)$ is convex, non-negative and $f(0) = 0$, it also must be monotonically increasing for $x \geqslant 0$. Thus we have

$$f\left(E_G\left(\sum_i p_i C_i\right)\right) \leqslant f\left(\sum_i p_i E_G(C_i)\right). \tag{46}$$

Now we can use convexity of f to obtain

$$f\left(E_G\left(\sum_i p_i C_i\right)\right) \leqslant \sum_i p_i f(E_G(C_i)). \tag{47}$$

Defining $E_f(C) = f(E_G(C)) = f(\frac{1}{2}(1 - \sqrt{1 - C^2}))$ the inequality above becomes

$$E_f\left(\sum_i p_i C_i\right) \leq \sum_i p_i E_f(C_i). \tag{48}$$

This proves that $E_f(C)$ is a convex function of the concurrence. Using the same argumentation as was used in [11] to prove expression (14) we see that (44) must hold. □

As an example consider the Bures measure of entanglement, which can be written as $E_B(\rho) = E_f(\rho)$ with the convex function $f = 2 - 2\sqrt{1 - E_G(\rho)}$. Using proposition 4, we see that for two qubits the Bures measure of entanglement is equal to its convex roof.

However, this might not be the case for a general higher-dimensional state ρ. To see this assume that $E_B(\rho)$ is equal to $\min \sum_i p_i E_B(|\psi_i\rangle)$. This means that $\sqrt{F_s(\rho)}$ is equal to $\max \sum_i p_i \sqrt{F_s(|\psi_i\rangle)}$. On the other hand, from theorem 1 we know that

$$F_s(\rho) = \max \sum_i p_i F_s(|\psi_i\rangle), \tag{49}$$

and using monotonicity and concavity of the square root, we find

$$\sqrt{F_s(\rho)} = \max \sqrt{\sum_i p_i F_s(|\psi_i\rangle)} \geqslant \max \sum_i p_i \sqrt{F_s(|\psi_i\rangle)}. \tag{50}$$

The Bures measure of entanglement is equal to its convex roof if and only if the inequality (50) becomes an equality for all states ρ.

Finally we note that any entanglement measure E_h defined as $E_h(\rho) = \min_{\sigma \in S} h(F(\rho, \sigma))$ with a monotonically decreasing non-negative function h, $h(1) = 0$, becomes $E_h(\rho) = h(F_s(\rho))$, and can be evaluated exactly for two qubits using proposition 1. An example of such a measure is the Bures measure of entanglement.

5. Optimal decompositions w.r.t. geometric measure of entanglement and consequences for closest separable states

Let ρ be an n-partite quantum state acting on a finite-dimensional Hilbert space $\mathcal{H} = \otimes_{i=1}^n \mathcal{H}_i$ of dimension d. A decomposition of a mixed state ρ is a set $\{p_i, |\psi_i\rangle\}$ with $p_i > 0$, $\sum_i p_i = 1$ and $\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$. Throughout this paper, we will call a decomposition optimal if it minimizes the geometric measure of entanglement, i.e. if $E_G(\rho) = \sum_i p_i E_G(|\psi_i\rangle)$. A separable state σ is a closest separable state to ρ if $E_G(\rho) = 1 - F(\rho, \sigma)$. In the following, we will show how to find an optimal decomposition of ρ, given a closest separable state.

5.1. Equivalence between closest separable states and optimal decompositions

In the maximization of $F(\rho,\sigma)$, we can restrict ourselves to separable states σ acting on the same Hilbert space $\mathcal{H}$. To see this, note that this is obviously true for pure states, as we can always find a pure separable state $|\phi\rangle \in \mathcal{H}$ such that $|\langle\psi|\phi\rangle|^2$ is maximal. (Extra dimensions cannot increase the overlap with the original state.) Let now $\sigma = \sum_i q_i \,|\phi_i\rangle\,\langle\phi_i|$ be the closest separable state with purification $|\phi\rangle$ such that $F_s(\rho) = |\langle\psi|\phi\rangle|^2$, where $|\psi\rangle$ is a purification of ρ. We can again write the purifications as

$$|\psi\rangle = \sum_i \sqrt{p_i}\,|\psi_i\rangle|i\rangle, \tag{51}$$

$$|\phi\rangle = \sum_j \sqrt{q_j}|\phi_j\rangle\,|j\rangle, \tag{52}$$

with separable pure states $|\phi_j\rangle$ such that $\sqrt{F_s\left(|\psi_i\rangle\right)} = \langle\psi_i|\phi_i\rangle$. As the states $|\phi_j\rangle$ are elements of $\mathcal{H}$, the reduced state $\sigma = \mathrm{Tr}_\mathrm{a}[|\phi\rangle\,\langle\phi|]$ is a bounded operator acting on the same Hilbert space $\mathcal{H}$, Tr_a denotes partial trace over the ancillary Hilbert space spanned by the orthonormal basis $\{|i\rangle\}$.

Now we are in a position to prove the following result:

Proposition 5. *Let ρ be an n-partite quantum state acting on $\mathcal{H} = \otimes_{i=1}^n \mathcal{H}_i$. The separable state $\sigma = \sum_{j=1}^s q_j|\phi_j\rangle\langle\phi_j|$ with $s \geqslant d$ separable pure states $|\phi_j\rangle$ and $\sum_{j=1}^s q_j = 1$, $q_i \geqslant 0$, is the closest separable state if and only if there exists an optimal decomposition $\{p_i, |\psi_i\rangle\}_{i=1}^s$ with $s \geqslant d$ elements such that the following holds: $\sqrt{F_s\left(|\psi_i\rangle\right)} = \langle\psi_i|\phi_i\rangle$ and $q_i = \frac{p_i F_s(|\psi_i\rangle)}{\sum_k p_k F_s(|\psi_k\rangle)}$.*

Proof. In the following, $\{|i\rangle\}$ denotes a basis on the ancillary Hilbert space $\mathcal{H}_\mathrm{a}$. The closest separable state $\sigma = \sum_{j=1}^s q_j|\phi_j\rangle\langle\phi_j|$ can be purified by

$$|\phi\rangle = \sum_{j=1}^s \sqrt{q_j}|\phi_j\rangle\,|j\rangle. \tag{53}$$

We write a purification of the state ρ as

$$|\psi\rangle = \sum_{i=1}^s \sqrt{\lambda_i}\,|\lambda_i\rangle\, U\,|i\rangle, \tag{54}$$

where λ_i are the eigenvalues and $|\lambda_i\rangle$ are the corresponding eigenstates of ρ, with $\lambda_i = 0$ for $i \geqslant d$, and U is a unitary acting on the ancillary Hilbert space $\mathcal{H}_\mathrm{a}$. According to Uhlmann's theorem [7, 20] it holds

$$|\langle\psi|\phi\rangle|^2 \leqslant F\left(\rho,\sigma\right) = F_s\left(\rho\right). \tag{55}$$

In the following, let U be a unitary such that equality is achieved in (55); its existence is assured by Uhlmann's theorem. Writing $U = \sum_{k,l=1}^s u_{kl}|k\rangle\langle l|$ in (54), we obtain

$$|\psi\rangle = \sum_{k,l=1}^s u_{kl}\sqrt{\lambda_l}\,|\lambda_l\rangle\,|k\rangle = \sum_{k=1}^s \sqrt{p_k}\,|\psi_k\rangle\,|k\rangle \tag{56}$$

with $\sqrt{p_k}\,|\psi_k\rangle = \sum_{l=1}^s u_{kl}\sqrt{\lambda_l}\,|\lambda_l\rangle$. Note that $\{p_k, |\psi_k\rangle\}_{k=1}^s$ is a decomposition of ρ.

We will now show that $\{p_k, |\psi_k\rangle\}_{k=1}^s$ is an optimal decomposition by showing that $|\langle\psi|\phi\rangle|^2 = \sum_i p_i F_s(|\psi_i\rangle)$. As we chose the purifications such that $|\langle\psi|\phi\rangle|^2 = F_s(\rho)$, this will complete the proof. Computing the overlap $|\langle\psi|\phi\rangle|^2$ using (53) and (56) we obtain

$$|\langle\psi|\phi\rangle|^2 = \left|\sum_i \sqrt{p_i q_i}\,\langle\psi_i|\phi_i\rangle\right|^2 . \tag{57}$$

As in the proof of theorem 1, maximality of (57) implies that $|\langle\psi_i|\phi_i\rangle| = \sqrt{F_s(|\psi_i\rangle)}$ and $q_i = \frac{p_i F_s(|\psi_i\rangle)}{\sum_k p_k F_s(|\psi_k\rangle)}$. Then we immediately see that $\{p_k, |\psi_k\rangle\}_{k=1}^s$ is optimal, because $F_s(\rho) = |\langle\psi|\phi\rangle|^2 = \sum_{i=1}^s p_i F_s(|\psi_i\rangle)$, which is exactly the optimality condition.

So far, we proved the existence of an optimal decomposition $\{p_i, |\psi_i\rangle\}$ with the property $\sqrt{F_s(|\psi_i\rangle)} = \langle\psi_i|\phi_i\rangle$ starting from the existence of the closest separable state $\sigma = \sum_{j=1}^s q_j |\phi_j\rangle\langle\phi_j|$. Now we will prove the inverse direction. Given an optimal decomposition $\{p_i, |\psi_i\rangle\}_{i=1}^s$, we will find the closest separable state. We again define the purifications of ρ and σ as

$$|\psi\rangle = \sum_{i=1}^s \sqrt{p_i}\,|\psi_i\rangle \otimes |i\rangle, \tag{58}$$

$$|\phi\rangle = \sum_{j=1}^s \sqrt{q_j}\,|\phi_j\rangle \otimes |j\rangle, \tag{59}$$

where we define the states $|\phi_j\rangle$ to be separable and to have maximal overlap with $|\psi_j\rangle$, i.e. $\langle\psi_j|\phi_j\rangle = \sqrt{F_s(|\psi_j\rangle)}$. The real numbers q_j are defined as follows: $q_j = \frac{p_j F_s(|\psi_j\rangle)}{\sum_k p_k F_s(|\psi_k\rangle)}$. Now we note that $|\langle\psi|\phi\rangle|^2 = F_s(\rho)$ because the decomposition $\{p_i, |\psi_i\rangle\}$ was defined to be optimal. Thus, we see that there exists no purification $|\phi'\rangle$ such that $|\langle\psi|\phi'\rangle| > |\langle\psi|\phi\rangle|$. Together with Uhlmann's theorem this implies that $F(\rho, \sigma) = F_s(\rho)$. □

5.2. Caratheodory bound

Now we are in a position to show that the number of elements in an optimal decomposition (w.r.t. the geometric measure of entanglement) is bounded from above by the Caratheodory bound.

Corollary 1. *For any state ρ acting on a Hilbert space of dimension d there always exists an optimal (w.r.t. the geometric measure of entanglement) decomposition $\{p_i, |\psi_i\rangle\}_{i=1}^s$ such that $s \leqslant d^2$.*

Proof. Let σ be the closest separable state. From Caratheodory's theorem [6, 26] follows that σ can be written as a convex combination of $s \leqslant d^2$ pure separable states. According to proposition 5 the state σ can be used to find an optimal decomposition with s elements. □

6. Structure of optimal decomposition w.r.t. geometric measure of entanglement

In this section, we will show that the optimal decomposition of ρ w.r.t. the geometric measure of entanglement has a certain symmetric structure.

6.1. *n-partite states*

First, we derive the structure of an optimal decomposition $\{p_i, |\psi_i\rangle\}$ for a general n-partite state.

Proposition 6. *Every optimal decomposition* $\{p_i, |\psi_i\rangle\}_{i=1}^s$ *must have the following structure,*

$$\sqrt{F_s(|\psi_k\rangle)}\,\langle\psi_i|\phi_k\rangle = \sqrt{F_s(|\psi_i\rangle)}\,\langle\phi_i|\psi_k\rangle \tag{60}$$

for all $1 \leqslant i, k \leqslant s$. *Here the states* $|\phi_i\rangle$ *are separable and have the property* $\langle\phi_i|\psi_i\rangle = \sqrt{F_s(|\psi_i\rangle)}$.

Equation (60) represents a nonlinear system of equations. Finding all solutions of it is equivalent to computing the optimal decomposition of ρ. For pure states our result reduces to the nonlinear eigenproblem given in equations (5*a*) and (5*b*) in [11].

Proof. Let the states $|i\rangle$ denote an orthonormal basis on the ancillary Hilbert space $\mathcal{H}_\text{a}$. Let $|\psi\rangle = \sum_i \sqrt{p_i}\,|\psi_i\rangle\,|i\rangle$ and $|\phi\rangle = \sum_j \sqrt{q_j}|\phi_j\rangle\,|j\rangle$ be purifications of ρ and σ, respectively, such that $\{p_i, |\psi_i\rangle\}$ is an optimal decomposition of ρ, $\langle\psi_i|\phi_i\rangle = \sqrt{F_s(|\psi_i\rangle)}$ and $q_i = \frac{p_i F_s(|\psi_i\rangle)}{\sum_k p_k F_s(|\psi_k\rangle)}$. This implies that

$$F_s(\rho) = |\langle\psi|\phi\rangle|^2 = \sum_i |\langle\psi|\,(|\phi_i\rangle \otimes |i\rangle)|^2 \,. \tag{61}$$

Optimality implies that $|\langle\psi|\phi\rangle|^2$ is stationary under unitaries acting on the ancillary Hilbert space $\mathcal{H}_\text{a}$ (for stationarity under unitaries acting on the original space see subsection 6.5), that is,

$$\frac{\mathrm{d}}{\mathrm{d}t}|\langle\psi|\mathrm{e}^{\mathrm{i}tH_\text{a}}|\phi\rangle|^2_{t=0} = 0 \tag{62}$$

for any Hermitian $H_\text{a} = H_\text{a}^\dagger$ acting on $\mathcal{H}_\text{a}$ and the derivative is taken at $t = 0$. Using (61) we can write

$$|\langle\psi|\mathrm{e}^{\mathrm{i}tH_\text{a}}|\phi\rangle|^2 = \sum_k |\langle\psi|\,(|\phi_k\rangle\,\mathrm{e}^{\mathrm{i}tH_\text{a}}\,|k\rangle)|^2. \tag{63}$$

The derivative at $t = 0$ becomes

$$\frac{\mathrm{d}}{\mathrm{d}t}|\langle\psi|\mathrm{e}^{\mathrm{i}tH_\text{a}}|\phi\rangle|^2_{t=0} = \mathrm{Tr}_\text{a}\left[H_\text{a}\cdot\mathrm{Tr}_{\bar{\text{a}}}\left[\sum_k\left(A_k + A_k^\dagger\right)\right]\right] \tag{64}$$

with $A_k = \mathrm{i}(|\phi_k\rangle\langle\phi_k| \otimes |k\rangle\langle k|)\,|\psi\rangle\langle\psi|$ and $\mathrm{Tr}_{\bar{\text{a}}}$ means partial trace over all parts except for the ancillary space $\mathcal{H}_\text{a}$. Using $(\langle\phi_k|\langle k|)|\psi\rangle = \sqrt{p_k}\sqrt{F_s(|\psi_k\rangle)}$, we can write A_k as

$$A_k = \mathrm{i}\sqrt{p_k F_s(|\psi_k\rangle)}\,|\phi_k\rangle|k\rangle\langle\psi|\,. \tag{65}$$

Expression (64) has to be zero for all Hermitians H_a, which can only be true if $\mathrm{Tr}_{\bar{\text{a}}}[\sum_k (A_k + A_k^\dagger)] = 0$, which is equivalent to

$$\sum_k \mathrm{Tr}_{\bar{\text{a}}}\left[\sqrt{p_k F_s(|\psi_k\rangle)}\,|\phi_k\rangle\,|k\rangle\,\langle\psi|\right] = \sum_k \mathrm{Tr}_{\bar{\text{a}}}\left[\sqrt{p_k F_s(|\psi_k\rangle)}\,|\psi\rangle\,\langle k|\,\langle\phi_k|\right]. \tag{66}$$

With $|\psi\rangle = \sum_i \sqrt{p_i}\,|\psi_i\rangle\,|i\rangle$ we obtain

$$\sum_{i,k}\sqrt{p_k p_i F_s(|\psi_k\rangle)}\,\langle\psi_i|\phi_k\rangle\,|k\rangle\,\langle i| = \sum_{i,k}\sqrt{p_i p_k F_s(|\psi_k\rangle)}\,\langle\phi_k|\psi_i\rangle\,|i\rangle\,\langle k|\,. \tag{67}$$

Using orthogonality of $\{|i\rangle\}$ completes the proof. □

6.2. Bipartite states

Let us illustrate the structure of an optimal decomposition with the example of bipartite states. We consider expression (60) for a bipartite mixed state ρ with optimal decomposition $\{p_i, |\psi_i\rangle\}$. In this case it is possible to write the Schmidt decomposition of the pure states $|\psi_i\rangle$ as follows:

$$|\psi_i\rangle = \sum_j \lambda_{i,j}|j_i^{(1)}\rangle|j_i^{(2)}\rangle \tag{68}$$

with $\sum_j \lambda_{i,j}^2 = 1$, and the Schmidt coefficients are in decreasing order, i.e. $\lambda_{i,1} \geqslant \lambda_{i,2} \geqslant \cdots > 0$. The separable states $|\phi_i\rangle$ that have the highest overlap with $|\psi_i\rangle$ are given by

$$|\phi_i\rangle = |1_i^{(1)}\rangle|1_i^{(2)}\rangle,$$

and $\sqrt{F_s\left(|\psi_i\rangle\right)} = \lambda_{i,1}$. With this in mind, expression (60) reduces to

$$\lambda_{k,1}\langle\psi_i|1_k^{(1)}\rangle|1_k^{(2)}\rangle = \lambda_{i,1}\langle 1_i^{(1)}|\langle 1_i^{(2)}|\psi_k\rangle \tag{69}$$

for all i, k.

6.3. Qubit–qudit states

Let now the first system be a qubit, that is, $d_1 = 2$. In this case, we can set $\lambda_{k,1} = \cos\alpha_k$ and $\lambda_{k,2} = \sin\alpha_k$, with $\cos\alpha_k \geqslant \sin\alpha_k$. With $|\psi_k\rangle = \cos\alpha_k\,|11\rangle + \sin\alpha_k\,|22\rangle$, we get from equation (69)

$$\cos\alpha_k \sin\alpha_i(\langle 2_i^{(1)}|1_k^{(1)}\rangle\langle 2_i^{(2)}|1_k^{(2)}\rangle) = \cos\alpha_i \sin\alpha_k(\langle 1_i^{(1)}|2_k^{(1)}\rangle\langle 1_i^{(2)}|2_k^{(2)}\rangle). \tag{70}$$

Noting that $|\langle 2_i^{(1)}|1_k^{(1)}\rangle| = |\langle 1_i^{(1)}|2_k^{(1)}\rangle|$ it follows that

$$\frac{\tan\alpha_i}{\tan\alpha_k} = \left|\frac{\langle 1_i^{(2)}|2_k^{(2)}\rangle}{\langle 2_i^{(2)}|1_k^{(2)}\rangle}\right|. \tag{71}$$

It is interesting to mention that in the case $d_2 = 2$, we can simplify (71) to $\tan\alpha_i = \tan\alpha_k$. This means that in the optimal decomposition $\{p_i, |\psi_i\rangle\}$ of a two-qubit state all states $|\psi_i\rangle$ have the same Schmidt coefficients, a result already known from [15].

6.4. Nonoptimal stationary decompositions

Note that expression (60) is necessary, but not sufficient for a decomposition to be optimal. To prove this we will give two nonoptimal decompositions that satisfy (60).

6.4.1. Bell diagonal states. Consider the state

$$\rho = \tfrac{1}{2}\,|\psi^+\rangle\,\langle\psi^+| + \tfrac{1}{2}\,|\phi^+\rangle\,\langle\phi^+|\,, \tag{72}$$

with $|\psi^+\rangle = \frac{1}{\sqrt{2}}\,(|01\rangle + |10\rangle)$ and $|\phi^+\rangle = \frac{1}{\sqrt{2}}\,(|00\rangle + |11\rangle)$. It is well known that the state (72) is separable, and thus the decomposition into Bell states cannot be optimal. On the other hand, it is easy to see that this decomposition satisfies (60).

6.4.2. Separable states. Now we will give a more complicated example. We call a decomposition $\{p_i, |\psi_i\rangle\}_{i=1}^s$ s-optimal if for a given number of terms s there is no decomposition

$\{q_i, |\phi_i\rangle\}_{i=1}^s$ such that $\sum_{i=1}^s q_i E_G(|\phi_i\rangle) < \sum_{i=1}^s p_i E_G|\psi_i\rangle$. It is known [2] that there exist separable states ρ of dimension d with the property that any d-optimal decomposition is not separable and thus not optimal. Let $\{p_i, |\psi_i\rangle\}_{i=1}^d$ be a d-optimal decomposition of such a state ρ.

We write a purification of ρ as $|\psi\rangle = \sum_{i=1}^d \sqrt{p_i}\,|\psi_i\rangle|i\rangle$. Further, we define separable states $|\phi_i\rangle$ such that $\langle\psi_i|\phi_i\rangle = \sqrt{F_s(|\psi_i\rangle)}$, $q_i = \frac{p_i F_s(|\psi_i\rangle)}{\sum_k p_k F_s(|\psi_k\rangle)}$ and $|\phi\rangle = \sum_{j=1}^d \sqrt{q_j}\,|\phi_j\rangle\,|j\rangle$. Then it holds

$$|\langle\psi|\phi\rangle|^2 = \sum_{i=1}^d p_i F_s(|\psi_i\rangle)^2 . \tag{73}$$

From d-optimality of $|\langle\psi|\phi\rangle|^2$ it follows that for all Hermitian matrices acting on a d-dimensional Hilbert space $\mathcal{H}_a$

$$\frac{\mathrm{d}}{\mathrm{d}t}|\langle\psi|\mathrm{e}^{\mathrm{i}tH_a}|\phi\rangle|^2_{t=0} = 0 \tag{74}$$

holds. We will now show that $\frac{\mathrm{d}}{\mathrm{d}t}|\langle\psi|\mathrm{e}^{\mathrm{i}tH_a}|\phi\rangle|^2_{t=0} = 0$ also holds for $\dim(\mathcal{H}_a) \geqslant d$. This means that adding more dimensions to the ancillary Hilbert space will not help. Performing the same calculation as in the proof of proposition 6 we obtain

$$\frac{\mathrm{d}}{\mathrm{d}t}|\langle\psi|\mathrm{e}^{\mathrm{i}tH_a}|\phi\rangle|^2_{t=0} = \mathrm{Tr}_a\left[H_a \cdot \mathrm{Tr}_{\bar{a}}\left[\sum_{k=1}^{d(\mathcal{H}_a)}\left(A_k + A_k^\dagger\right)\right]\right] \tag{75}$$

with $A_k = \mathrm{i}\sqrt{p_k F_s(|\psi_k\rangle)}\,|\phi_k\rangle|k\rangle\langle\psi|$. Note that A_k is non-zero only for $k \leqslant d$, because $p_k = 0$ otherwise. Thus, we can restrict ourselves to $k \leqslant d$ in the calculation, which is equivalent to setting $\dim(\mathcal{H}_a) = d$. Then (74) implies $\mathrm{Tr}_{\bar{a}}[\sum_{k=1}^{d(\mathcal{H}_a)}(A_k + A_k^\dagger)] = 0$ and it follows that (74) holds for arbitrary $d(\mathcal{H}_a) \geqslant d$.

6.5. Stationarity on the original subspace

In proposition 6, we used the argument that in the optimal case $|\langle\psi|\phi\rangle|^2$ has to be stationary under unitaries acting on the ancillary Hilbert space $\mathcal{H}_a$. In (61), we could rewrite this expression as

$$F_s(\rho) = |\langle\psi|\phi\rangle|^2 = \sum_i |\langle\psi|\phi_i\rangle|i\rangle|^2 ,$$

where all $|\phi_i\rangle$ are separable. We can also demand $\sum_i |\langle\psi|\phi_i\rangle\,|i\rangle|^2$ to be stationary under (separable) unitaries acting on the original Hilbert space of the states $|\phi_i\rangle$. From this procedure we will gain stationary equations describing the states $|\phi_i\rangle$. However, we already know that in the optimal case we can choose $|\phi_i\rangle$ to be the closest separable state to $|\psi_i\rangle$, that is, $\langle\psi_i|\phi_i\rangle = \sqrt{F_s(|\psi_i\rangle)}$, such that this method does not give new results.

7. Concluding remarks

We have shown in this paper that the geometric measure of entanglement belongs to two classes of entanglement measures. Namely it is a convex roof measure and also a distance measure of entanglement. As an application we gave a closed formula for the Bures measure of entanglement for two qubits. We also note that the revised geometric measure of entanglement defined in [27] is equal to the original geometric measure of entanglement.

We furthermore proved that the problems of finding a closest separable state and finding an optimal decomposition are equivalent. We used this insight to bound the number of elements in an optimal decomposition (w.r.t. the geometric measure of entanglement). It turns out that the bound is exactly given by the Caratheodory bound.

Finally, we obtained stationary equations that ensure optimality of a decomposition. For the case of two qubits these equations lead to the known fact that each constituting state of an optimal decomposition has equal concurrence. Our equations hold for any dimension. However, they are only necessary, not sufficient for a decomposition to be optimal. Given an arbitrary decomposition, they provide a simple test whether the decomposition may be optimal.

Acknowledgments

We acknowledge discussions with M Plenio. AS thanks C Gogolin, H Hinrichsen and P Janotta. This work was partially supported by Deutsche Forschungsgemeinschaft.

Appendix A. Geometric measure of a convex set

In theorem 1 we stated that if S is the set of separable states it holds

$$F_s(\rho) = \max \sum_i p_i F_s(|\psi_i\rangle), \tag{A.1}$$

where F_s is the maximal fidelity between ρ and the set of separable states: $F_s(\rho) = \max_{\sigma\in S} F(\rho,\sigma)$ and the maximization is done over all pure state decompositions of ρ. In the following, we will generalize this result to arbitrary convex sets.

Let X be a set of states $\{\sigma_k\}$ and C be a set containing all convex combinations of the elements of X, these are states σ such that it holds

$$\sigma = \sum_k q_k \sigma_k \tag{A.2}$$

with $q_k \geqslant 0$, $\sum_k q_k = 1$. We define the quantities $F_X(\rho)$ and $F_C(\rho)$ to be the maximal fidelity between ρ and an element of X and C, respectively,

$$F_X(\rho) = \max_{\sigma\in X} F(\rho,\sigma), \tag{A.3}$$

$$F_C(\rho) = \max_{\sigma\in C} F(\rho,\sigma). \tag{A.4}$$

Theorem 2. *For an arbitrary quantum state ρ and a convex set of states C it holds*

$$F_C(\rho) = \max_{\rho=\sum_k p_k\rho_k} \sum_i p_i F_X(\rho_i), \tag{A.5}$$

where the maximization is done over all decompositions of $\rho = \sum_i p_i\rho_i$, $p_i \geqslant 0$.

Proof. The proof is a modification of the proof of theorem 1. According to Uhlmann's theorem [20, p 411] it holds

$$F(\rho,\sigma) = \max_{|\phi\rangle} |\langle\psi|\phi\rangle|^2, \tag{A.6}$$

where $|\psi\rangle$ is a purification of ρ and the maximization is done over all purifications of σ denoted by $|\phi\rangle$.

In order to find $F_C(\rho)$ we have to maximize $|\langle\psi|\phi\rangle|^2$ over purifications $|\phi\rangle$ of all states of the form $\sigma = \sum_k q_k\sigma_k$, $\sigma_k \in X$. Using similar arguments as in the proof of the theorem 1, we see that the purifications can always be written as

$$|\psi\rangle = \sum_i \sqrt{p_i}\left(\sum_j \sqrt{p_{i,j}}|\psi_{i,j}\rangle \otimes |i, j\rangle\right), \tag{A.7}$$

$$|\phi\rangle = \sum_k \sqrt{q_k}\left(\sum_l \sqrt{q_{k,l}}|\phi_{k,l}\rangle \otimes |k, l\rangle\right), \tag{A.8}$$

with $\langle i, j|k, l\rangle = \delta_{ik}\delta_{jl}$. In the maximization of $|\langle\psi|\phi\rangle|^2$ we are free to choose the states $|\phi_{k,l}\rangle$ under the restriction that $\sum_l \sqrt{q_{k,l}}|\phi_{k,l}\rangle \otimes |k, l\rangle$ purifies $\sigma_k \in X$, the probabilities $q_k > 0$ are restricted only by $\sum_k q_k = 1$. We are also free to choose $\{|\psi_{i,j}\rangle\}$, $\{p_i\}$ and $\{p_{i,j}\}$ under the restriction $\rho = \sum_{i,j} p_i p_{ij}|\psi_{i,j}\rangle\langle\psi_{i,j}|$. With this in mind we obtain

$$|\langle\psi|\phi\rangle| = \left|\sum_{i,k} \sqrt{p_i q_k} a_{i,k}\right|, \tag{A.9}$$

with $a_{i,k}$ being the product of the purifications of ρ_i and σ_k:

$$a_{i,k} = \left(\sum_j \sqrt{p_{i,j}}\langle\psi_{i,j}| \otimes \langle i, j|\right)\left(\sum_l \sqrt{q_{k,l}}|\phi_{k,l}\rangle \otimes |k, l\rangle\right).$$

Now we optimize over $\{q_{k,l}, |\phi_{k,l}\rangle\}$ with the result

$$a_{i,k} = \sqrt{F_X(\rho_i)}\delta_{ik} \tag{A.10}$$

and thus

$$\max_{\{q_{k,l},|\phi_{k,l}\rangle\}} |\langle\psi|\phi\rangle| = \sum_i \sqrt{q_i p_i}\sqrt{F_X(\rho_i)}. \tag{A.11}$$

Now we do the optimization over q_i. Using Lagrange multipliers we obtain

$$\sqrt{q_i} = \frac{\sqrt{p_i}\sqrt{F_X(\rho_i)}}{\sqrt{\sum_k p_k F_X(\rho_k)}}, \tag{A.12}$$

with the result

$$\max_{\{q_j,q_{k,l},|\phi_{k,l}\rangle\}} |\langle\psi|\phi\rangle|^2 = \sum_i p_i F_X(\rho_i). \tag{A.13}$$

In the last step we do the maximization over all decompositions $\{p_i, \rho_i\}$ of the given state ρ, which leads to the final result

$$F_C(\rho) = \max |\langle\psi|\phi\rangle|^2 = \max \sum_i p_i F_X(\rho_i). \tag{A.14}$$

□

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(Streltsov *et al.*, 2010) New J. Phys. **12**, 123004.

Journal: New Journal of Physics
Impact Factor 2011: 4,177
Contribution: first author, scientific work and preparation of the manuscript, 90%

Behavior of Quantum Correlations under Local Noise

Alexander Streltsov,* Hermann Kampermann, and Dagmar Bruß

Heinrich-Heine-Universität Düsseldorf, Institut für Theoretische Physik III, D-40225 Düsseldorf, Germany

(Received 10 June 2011; published 17 October 2011)

We characterize the behavior of quantum correlations under the influence of local noisy channels. Intuition suggests that such noise should be detrimental for quantumness. When considering qubit systems, we show for which channels this is indeed the case: The amount of quantum correlations can only decrease under the action of unital channels. However, nonunital channels (e.g., such as dissipation) can create quantum correlations for some initially classical states. Furthermore, for higher-dimensional systems even unital channels may increase the amount of quantum correlations. Thus, counterintuitively, local decoherence can generate quantum correlations.

DOI: 10.1103/PhysRevLett.107.170502 PACS numbers: 03.67.Hk, 05.40.Ca

Composite quantum states often reveal puzzling features of nature. Recently, much interest [1] has been devoted to the study of quantum correlations that may arise without entanglement: Here, the quantumness of a composite system manifests itself even in a separable state. The fact that such quantum correlations are present [2] in an algorithm for mixed state quantum computing [3] has stimulated intensive investigations into measures for quantum correlations [4–13] and their properties and interpretations [14–28]. Experimental detection of quantum correlations beyond entanglement is also receiving more and more attention [29]. Some studies of the dynamics of quantum correlations have been presented in Refs. [30–34]. The importance of quantum correlations beyond entanglement is also highlighted by the task of efficiently locking classical correlations in quantum states [35]. There, two parties can arbitrarily increase their classical correlations by sending only one classical bit. The fact that no entanglement is needed in this process leads to the conclusion that other types of correlations are responsible for this phenomenon. Understanding fundamental properties of such correlations is the aim of this Letter.

An appeal of mixed state quantum computation lies in the possibility to be run in a noisy environment: Pure entangled states are typically fragile, and the resource of entanglement is easily destroyed by noise. For an open system the transition from entangled to separable states is only a matter of time—as the volume of the set of separable states is nonzero [36], typically it takes a finite time for entanglement to disappear under noise such as dissipation or decoherence [37].

Mixed state quantum computation as suggested in Ref. [3] already uses separable states, so it is natural to assume that it can be run also in a noisy environment. However, in order to verify or falsify this conjecture, one has to study the behavior of quantum correlations under noisy channels (described by trace-preserving completely positive maps). Here we consider only local noisy channels—as correlated channels may also preserve entanglement (with or even without some degradation, depending on the amount of correlation); see, e.g., [38]. The goal of this Letter is to answer such questions as the following: Which types of noisy channels decrease the amount of quantum correlations? Are there any noisy channels that might even increase the amount of quantum correlations? How does dissipation influence quantum correlations, and how are they affected by decoherence? We point out that our answers to these questions also apply to the situation where one actively performs local operations on a composite quantum system, e.g., with the aim of creating or preserving quantum correlations.

In general, a bipartite quantum state is called fully classically correlated [39] if it can be written in the form [6,7]

$$\rho_{cc} = \sum_{i,j} p_{ij} |i^A\rangle\langle i^A| \otimes |j^B\rangle\langle j^B|, \quad (1)$$

where $\{|i^A\rangle\}$ and $\{|j^B\rangle\}$ are sets of orthogonal states of party A and B, respectively, with non-negative probabilities p_{ij} that add up to 1. If a state cannot be written as in Eq. (1), it is called quantum correlated. These definitions can be extended to any number of parties [13].

As a simple example, consider the classically correlated state of two qubits $\rho_{cc} = \frac{1}{2}|0^A\rangle\langle 0^A| \otimes |0^B\rangle\langle 0^B| + \frac{1}{2}|1^A\rangle \times \langle 1^A| \otimes |1^B\rangle\langle 1^B|$. By using a local channel on qubit A only, it is possible to create the quantum correlated state

$$\rho = \tfrac{1}{2}|0^A\rangle\langle 0^A| \otimes |0^B\rangle\langle 0^B| + \tfrac{1}{2}|+^A\rangle\langle +^A| \otimes |1^B\rangle\langle 1^B| \quad (2)$$

with $|+^A\rangle = (1/\sqrt{2})(|0\rangle + |1\rangle)$. The quantum channel that achieves this transformation can be formally written as the completely positive trace-preserving map

$$\rho = \Lambda_A(\rho_{cc}) = E_1 \rho E_1^\dagger + E_2 \rho E_2^\dagger \quad (3)$$

with local Kraus operators $E_1 = |0^A\rangle\langle 0^A|$ and $E_2 = |+^A\rangle\langle 1^A|$ acting only on qubit A. The state in Eq. (2) is not of the form (1); i.e., it is quantum correlated.

As will become clear below in this Letter, one reason why the local quantum channel in Eq. (3) is able to create quantum correlations lies in its action on the maximally mixed state $\frac{1}{2}\mathbb{1}_A$. Observe that $\Lambda_A(\frac{1}{2}\mathbb{1}_A) = \frac{1}{2}|0^A\rangle \times \langle 0^A| + \frac{1}{2}|+^A\rangle\langle +^A| \neq \frac{1}{2}\mathbb{1}_A$. This property is also known as nonunitality. A single-qubit quantum channel Λ is called unital if and only if it maps the maximally mixed state onto itself: $\Lambda(\frac{1}{2}\mathbb{1}) = \frac{1}{2}\mathbb{1}$; see also Fig. 1. We will turn this observation into Theorem 1 by showing that nonunitality is one property which enables a local channel to create quantum correlations in a multiqubit system. In Theorem 2, we will show that, on the other hand, local unital quantum channels cannot increase quantum correlations in a multiqubit system. However, this statement does not hold for higher dimensions.

Before presenting the main result of this Letter, we introduce the semiclassical channel $\Lambda_{\rm sc}$. It maps all input states ρ onto states $\Lambda_{\rm sc}(\rho)$ which are diagonal in the same basis: $\Lambda_{\rm sc}(\rho) = \sum_k p_k(\rho)|k\rangle\langle k|$. The non-negative probabilities $p_k(\rho)$ can, in general, depend on the input state ρ, while the orthogonal states $|k\rangle$ are independent of ρ. Such a channel is, e.g., realized by complete decoherence, after which only the diagonal elements of a density matrix may be nonzero. Channels of this form were also considered in Ref. [40], where they were called measurement maps. We are now in the position to prove the following theorem.

Theorem 1.—A local quantum channel acting on a single qubit can create quantum correlations in a multiqubit system if and only if it is neither semiclassical nor unital.

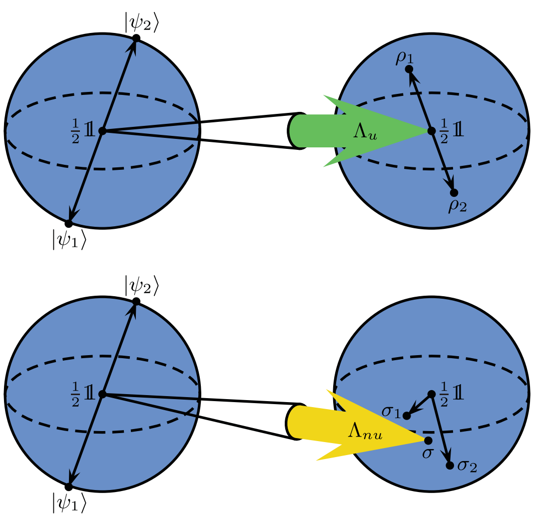

FIG. 1 (color online). Quantum channels on a single qubit: The upper figure shows a unital quantum channel Λ_u (green arrow) which maps the maximally mixed state $\frac{1}{2}\mathbb{1}$ onto itself: $\Lambda_u(\frac{1}{2}\mathbb{1}) = \frac{1}{2}\mathbb{1}$. Two orthogonal states $|\psi_1\rangle$ and $|\psi_2\rangle$ with collinear Bloch vectors are mapped onto the states $\rho_1 = \Lambda_u(|\psi_1\rangle\langle\psi_1|)$ and $\rho_2 = \Lambda_u(|\psi_2\rangle\langle\psi_2|)$ with collinear Bloch vectors. The lower figure shows a nonunital quantum channel Λ_{nu} (yellow arrow) which maps the maximally mixed state onto the state $\sigma = \Lambda_{nu}(\frac{1}{2}\mathbb{1}) \neq \frac{1}{2}\mathbb{1}$. The Bloch vectors of $\sigma_1 = \Lambda_{nu}(|\psi_1\rangle \times \langle\psi_1|)$ and $\sigma_2 = \Lambda_{nu}(|\psi_2\rangle\langle\psi_2|)$ add up to twice the nonzero Bloch vector of σ; see the main text.

Proof.—For simplicity, we restrict ourselves to two qubits only. A generalization to an arbitrary number of qubits is straightforward. The action of a local semiclassical channel $\Lambda_{\rm sc}^A$ on the classically correlated state (1) is, due to linearity, $\Lambda_{\rm sc}^A(\rho_{cc}) = \sum_{i,j} p_{ij}\Lambda_{\rm sc}^A(|i^A\rangle\langle i^A|) \otimes |j^B\rangle\langle j^B|$. The definition of a semiclassical channel directly implies that $\Lambda_{\rm sc}^A(\rho_{cc})$ is classically correlated.

Now we will show that a local unital channel never creates quantum correlations in a multiqubit system. A local unital channel Λ_u^A on the qubit A takes a classically correlated state to the state $\Lambda_u^A(\rho_{cc}) = \sum_{i,j} p_{ij}\Lambda_u^A(|i^A\rangle \times \langle i^A|) \otimes |j^B\rangle\langle j^B|$. The action of the unital channel on the pure state $|i^A\rangle\langle i^A|$ can be studied by using the Bloch representation: $|0^A\rangle\langle 0^A| = \frac{1}{2}(\mathbb{1}_A + \sum_i r_i\sigma_i^A)$, where σ_i^A are the Pauli operators with $i \in \{x, y, z\}$ and $|1^A\rangle\langle 1^A| = \frac{1}{2}(\mathbb{1}_A - \sum_i r_i\sigma_i^A)$. Using linearity and unitality of Λ_u^A, we see that the state $|0^A\rangle\langle 0^A|$ is mapped onto the state $\rho_0^A = \Lambda_u^A(|0^A\rangle\langle 0^A|) = \frac{1}{2}[\mathbb{1}_A + \sum_i r_i\Lambda_u^A(\sigma_i^A)]$. The same procedure for $|1^A\rangle\langle 1^A|$ results in $\rho_1^A = \Lambda_u^A(|1^A\rangle\langle 1^A|) = \frac{1}{2}[\mathbb{1}_A - \sum_i r_i\Lambda_u^A(\sigma_i^A)]$. Note that the Bloch vectors of the states ρ_0^A and ρ_1^A point into opposite directions; see Fig. 1 for illustration. States with this property can be diagonalized in the same basis. This implies that it is possible to write the state $\Lambda_u^A(\rho_{cc})$ in the form (1). Thus we proved that local unital quantum channels cannot create quantum correlations in a classically correlated multiqubit state.

In the following, we will complete the proof of Theorem 1 by showing that any local quantum channel Λ_{nu}^A that is neither unital nor semiclassical can create quantum correlations. By definition, Λ_{nu}^A maps the maximally mixed state $\frac{1}{2}\mathbb{1}_A$ onto some state that is not maximally mixed: $\Lambda_{nu}^A(\frac{1}{2}\mathbb{1}_A) = \frac{1}{2}(\mathbb{1}_A + \sum_i s_i\sigma_i^A)$, with $\sum_i s_i^2 \neq 0$. Since we demand that the quantum channel is not semiclassical, there exists a state ρ^A such that $\Lambda_{nu}^A(\rho^A)$ is not diagonal in the eigenbasis of $\Lambda_{nu}^A(\frac{1}{2}\mathbb{1}_A)$. Again we consider the Bloch representation $\Lambda_{nu}^A(\rho^A) = \frac{1}{2}(\mathbb{1}_A + \sum_j r_j\sigma_j^A)$ and note that the two Bloch vectors $\mathbf{r}$ and $\mathbf{s}$ are linearly independent. Otherwise, the states $\Lambda_{nu}^A(\rho^A)$ and $\Lambda_{nu}^A(\frac{1}{2}\mathbb{1}_A)$ could be diagonalized in the same basis, which is in contradiction to the definition of ρ^A. We can write the state as $\rho^A = \frac{1}{2}(\mathbb{1}_A + \sum_i v_i\sigma_i^A)$. Consider now the classically correlated state $\rho_{cc} = \frac{1}{2}\rho^A \otimes |0^B\rangle\langle 0^B| + \frac{1}{2}\tau^A \otimes |1^B\rangle\langle 1^B|$ with $\tau^A = \frac{1}{2}(\mathbb{1}_A - \sum_i v_i\sigma_i^A)$. We define the vector $\mathbf{w}$ such that the equality $\Lambda_{nu}(\sum_i v_i\sigma_i^A) = \sum_i w_i\sigma_i^A$ with $\sum_i w_i^2 \neq 0$ is satisfied. This is always possible, since Λ_{nu}^A is trace-preserving. The action of the channel onto the two states ρ^A and τ^A is as follows: $\Lambda_{nu}^A(\rho^A) = \frac{1}{2}[\mathbb{1}_A + \sum_i(s_i + w_i)\sigma_i^A]$ and $\Lambda_{nu}^A(\tau^A) = \frac{1}{2}[\mathbb{1}_A + \sum_i(s_i - w_i)\sigma_i^A]$. As noted above, the two Bloch vectors $\mathbf{s}$ and $\mathbf{r} = \mathbf{s} + \mathbf{w}$ are linearly independent. The same must hold for the vectors $\mathbf{s} + \mathbf{w}$ and $\mathbf{s} - \mathbf{w}$. This implies that the two states $\Lambda_{nu}^A(\rho^A)$ and $\Lambda_{nu}^A(\tau^A)$ are not diagonal in the same basis. This completes the proof. ■

So far, we have seen that local unital and local semiclassical channels acting on a single qubit cannot create quantum correlations from a classically correlated multiqubit state. These results hold independently of the chosen measure for quantum correlations. In the following, we will go one step further by showing that these local channels never increase a very general class of measures for quantum correlations in multiqubit systems. We consider distance-based measures of quantum correlations Q_D, which are defined via the minimal distance D to the set of the classically correlated states CC [8,9]: $Q_D = \min_{\sigma\in CC} D(\rho, \sigma)$, where D does not necessarily have to be a distance in the mathematical sense. The statement mentioned above will be shown to hold for all distance measures D with the property of being nonincreasing under any quantum channel Λ, i.e., $D(\Lambda(\rho), \Lambda(\sigma)) \leq D(\rho, \sigma)$. This property is also frequently used for defining entanglement measures [41,42].

Theorem 2.—Quantum correlations in multiqubit systems, quantified by a distance-based measure Q_D, do not increase under local unital channels Λ_{lu} and local semiclassical channels Λ_{lsc}:

$$Q_D(\Lambda_{\mathrm{lu}}(\rho)) \leq Q_D(\rho), \tag{4}$$

$$Q_D(\Lambda_{\mathrm{lsc}}(\rho)) \leq Q_D(\rho). \tag{5}$$

Proof.—Let ξ be the classically correlated state which minimizes the distance, i.e., $Q_D(\rho) = D(\rho, \xi)$. Using the property of the distance to be nonincreasing under quantum channels, we obtain $Q_D(\rho) = D(\rho, \xi) \geq D(\Lambda_{\mathrm{lu}}(\rho), \Lambda_{\mathrm{lu}}(\xi))$ and $Q_D(\rho) = D(\rho, \xi) \geq D(\Lambda_{\mathrm{lsc}}(\rho), \Lambda_{\mathrm{lsc}}(\xi))$. Now we use Theorem 1 noting that local unital channels Λ_{lu} and local semiclassical channels Λ_{lsc} map the classically correlated multiqubit state ξ onto another classically correlated state $\Lambda(\xi)$ which is not necessarily the one that minimizes the distance to $\Lambda(\rho)$. This observation finishes the proof. ■

One example for a measure that satisfies the properties (4) and (5)—and thus Theorem 2 holds—is the geometric measure of quantumness, which we define as

$$Q_G(\rho) = \min_{\sigma\in CC}[1 - F(\rho, \sigma)] \tag{6}$$

with the fidelity $F(\rho, \sigma) = (\mathrm{Tr}[\sqrt{\sqrt{\rho}\sigma\sqrt{\rho}}])^2$. Using the fact that the fidelity is nondecreasing on quantum channels together with Theorem 2, we see that the geometric measure of quantumness does not increase under local unital channels and local semiclassical channels in multiqubit systems. Alternatively, we can use the quantum relative entropy $S(\rho||\sigma) = -\mathrm{Tr}[\rho \log_2\sigma] + \mathrm{Tr}[\rho\log_2\rho]$, which is also nonincreasing on quantum channels [41,42]. From Theorem 2 follows that the resulting measure of quantum correlations $Q_S = \min_{\sigma\in CC} S(\rho||\sigma)$ does not increase under local unital and local semiclassical channels in multiqubit systems. Q_S was also studied in Ref. [13], where it was called relative entropy of quantumness.

So far, we have considered states consisting of an arbitrary number of qubits. We have shown that local unital and local semiclassical channels acting on a single qubit never increase quantum correlations as defined by a distance-based measure Q_D, where the minimization is done over all classically correlated multiqubit states. On the other hand, any local channel which is nonunital and not semiclassical can, in principle, create quantum correlations, independently of the considered measure, out of a classically correlated state. An example for such a channel is the amplitude damping channel as a model for dissipation. Thus, dissipation can increase quantum correlations.

At the present stage, it is natural to ask the question, for what kind of input states this behavior can or cannot be observed in general. The following theorem shows that pure states are special.

Theorem 3.—The geometric measure of quantumness of multipartite systems with arbitrary dimension cannot increase under any local quantum channel, if the initial state is pure:

$$Q_G(\Lambda_l(|\psi\rangle\langle\psi|)) \leq Q_G(|\psi\rangle\langle\psi|), \tag{7}$$

where Λ_l is an arbitrary local quantum channel.

Proof.—Let $\xi \in CC$ be defined such that $Q_G(|\psi\rangle \times \langle\psi|) = 1 - F(|\psi\rangle\langle\psi|, \xi)$. Using the properties of the fidelity F, we see that ξ can be chosen to be a pure product state $\xi = |\phi\rangle\langle\phi|$. Moreover, $1 - F$ does not increase under the action of any quantum channel, i.e., $1 - F(|\psi\rangle \times \langle\psi|, |\phi\rangle\langle\phi|) \geq 1 - F(\Lambda_l(|\psi\rangle\langle\psi|), \Lambda_l(|\phi\rangle\langle\phi|))$. Since $|\phi\rangle$ is a product state, $\Lambda_l(|\phi\rangle\langle\phi|)$ is also a product state. This observation completes the proof. ■

So far, we have shown that quantum correlations in multiqubit systems cannot increase under local unital quantum channels. A prominent example for a unital channel is the phase-damping channel, which is a model for decoherence in a quantum system. Under decoherence the quantum state $\rho = \sum_{i,j}\rho_{ij}|i\rangle\langle j|$ is transformed to the state

$$\Lambda(\rho) = \sum_i \rho_{ii}|i\rangle\langle i| + (1 - p)\sum_{i\neq j}\rho_{ij}|i\rangle\langle j| \tag{8}$$

with the damping parameter $0 \leq p \leq 1$. Since Λ is unital, it is not possible to create quantum correlations with local phase damping in a multiqubit system. Surprisingly, this is not true if the local systems are not qubits: Qubits are special. This can be demonstrated via the classically correlated state as input: $\rho_{cc} = \frac{1}{2}|\psi^A\rangle\langle\psi^A| \otimes |0^B\rangle \times \langle 0^B| + \frac{1}{2}|\phi^A\rangle\langle\phi^A| \otimes |1^B\rangle\langle 1^B|$ with the orthogonal single-qutrit states $|\psi^A\rangle = (1/\sqrt{3})(-|0^A\rangle + |1^A\rangle + |2^A\rangle)$ and $|\phi^A\rangle = \frac{1}{\sqrt{2}}(|0^A\rangle + |1^A\rangle)$. We will show that a local phase-damping channel Λ_A acting on subsystem A generates quantum correlations. We consider the action of the channel (8) with the damping parameter $p = \frac{1}{2}$ on the state ρ_{cc}: $\Lambda_A(\rho_{cc}) = \frac{1}{2}\sum_{i=1}^3 \lambda_i|\psi_i^A\rangle\langle\psi_i^A| \otimes |0^B\rangle\langle 0^B| + \frac{1}{2}\sum_{j=1}^3 \mu_j|\phi_j^A\rangle\langle\phi_j^A| \otimes |1^B\rangle\langle 1^B|$, where the states $\{|\psi_i^A\rangle\}$ are the eigenstates of $\Lambda_A(|\psi^A\rangle\langle\psi^A|)$ with the corresponding eigenvalues λ_i. Similarly, the states $\{|\phi_j^A\rangle\}$ are eigenstates of $\Lambda_A(|\phi^A\rangle\langle\phi^A|)$ with the eigenvalues μ_j. One can see as follows that the state $\Lambda_A(\rho_{cc})$ is quantum correlated: The eigenvalues of $\Lambda_A(|\psi^A\rangle\langle\psi^A|)$ are given by $\lambda_1 = \frac{2}{3}$ and $\lambda_2 = \lambda_3 = \frac{1}{6}$. The eigenstate to the largest eigenvalue λ_1 is given by $|\psi_1^A\rangle = |\psi^A\rangle$. It is easy to check that $|\psi_1^A\rangle$ is not an eigenstate of $\Lambda_A(|\phi^A\rangle\langle\phi^A|)$, and therefore the state $\Lambda_A(\rho_{cc})$ is not classically correlated. Thus we proved that it is possible to create quantum correlations with a local phase-damping channel, i.e., via local decoherence.

In conclusion, we have investigated the effect of local noisy channels (i.e., trace-preserving completely positive maps) on quantum correlations. While entanglement can never increase under such local channels, quantum correlations without entanglement may or may not increase, depending on the type of channel and the type of input state. For multiqubit systems, we fully answer the question which local channels can increase quantum correlations: Unital and semiclassical local channels cannot enhance quantum correlations, while nonunital and nonsemiclassical local channels (e.g., dissipation, corresponding to amplitude damping) can increase quantum correlations. Surprisingly, for higher-dimensional systems, even unital channels such as decoherence, corresponding to phase damping, can generate quantum correlations from an initially classically correlated state. However, quantum correlations as quantified by the geometric measure of quantumness can become larger under local channels only when the initial state is mixed. Thus, we have shed some light on the behavior of quantum correlated states in a noisy environment.

We also mention the connection of our approach to the quantum discord; see [4] for a definition. A quantum state has zero quantum discord if it can be written in the classical-quantum form $\rho_{cq} = \sum_i p_i |i^A\rangle\langle i^A| \otimes \rho_i^B$. Note that Theorem 1 also holds in this case, if the subsystem A is a qubit. Moreover, Theorems 2 and 3 also hold if the corresponding measure is defined via the minimal distance to the set of classical-quantum states. The proofs follow the same lines as above.

We acknowledge partial financial support by Deutsche Forschungsgemeinschaft (DFG) and by the ELES foundation.

Note added.—While finishing this Letter, we became aware of two related works. In Ref. [43], the authors show that the quantum discord can increase under a local amplitude damping channel. The dynamics of quantum correlations in a spin chain under the action of local noise is studied in Ref. [44].

*streltsov@thphy.uni-duesseldorf.de

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[39] A given state is classically correlated, i.e., of the form (1), if and only if it has zero quantum discord [4] with respect to all bipartitions. A necessary and sufficient condition for nonzero quantum discord was proposed in Ref. [9]. This condition can be easily extended to the concept of quantum correlations.

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(Streltsov *et al.*, 2011a) Phys. Rev. Lett. **107**, 170502.

Journal: Physical Review Letters
Impact Factor 2011: 7,37
Contribution: first author, scientific work and preparation of the manuscript, 90%

Linking Quantum Discord to Entanglement in a Measurement

Alexander Streltsov,* Hermann Kampermann, and Dagmar Bruß
Heinrich-Heine-Universität Düsseldorf, Institut für Theoretische Physik III, D-40225 Düsseldorf, Germany
(Received 22 December 2010; revised manuscript received 4 March 2011; published 22 April 2011)

We show that a von Neumann measurement on a part of a composite quantum system unavoidably creates distillable entanglement between the measurement apparatus and the system if the state has nonzero quantum discord. The minimal distillable entanglement is equal to the one-way information deficit. The quantum discord is shown to be equal to the minimal partial distillable entanglement that is the part of entanglement which is lost, when we ignore the subsystem which is not measured. We then show that any entanglement measure corresponds to some measure of quantum correlations. This powerful correspondence also yields necessary properties for quantum correlations. We generalize the results to multipartite measurements on a part of the system and on the total system.

DOI: 10.1103/PhysRevLett.106.160401 PACS numbers: 03.65.Ta, 03.67.Mn

Quantum entanglement is by far the most famous and best studied kind of quantum correlation [1]. One reason for this situation is the fact that entanglement plays an important role in quantum computation [2]. It was even believed that entanglement is the reason why a quantum computer can perform efficiently on some problems which cannot be solved efficiently on a classical computer. The situation started to change after a computational model was presented which is referred to as "the power of one qubit" with the acronym DQC1 [3,4]. Here, using a mixed separable state allows for efficient computation of the trace of any n-qubit unitary matrix. This problem is believed to be not solvable efficiently on a classical computer [4,5]. The fact that no entanglement is present in this model was one of the main reasons why new types of quantum correlations were studied during the past few years [6–9]. One of the measures of quantum correlations, the quantum discord [6], was considered to be the figure of merit for this model of quantum computation [10].

In this Letter, we introduce an alternative approach to quantum correlations via an interpretation of a measurement. In order to perform a von Neumann measurement on a system S in the quantum state ρ^S, correlations between the system and the measurement apparatus M must be created. As a simple example we consider a von Neumann measurement in the eigenbasis $\{|i^S\rangle\}$ of the mixed state $\rho^S = \sum_i p_i|i^S\rangle\langle i^S|$ with the eigenvalues p_i. Correlations between the measurement apparatus M and the system are found in the final state of the total system $\rho_{\rm final} = \sum_i p_i|i^M\rangle\langle i^M| \otimes |i^S\rangle\langle i^S|$, where $|i^M\rangle$ are orthogonal states of the measurement apparatus M. In this state $\rho_{\rm final}$ the correlations between M and the system S are purely classical, and no entanglement is created. The situation changes completely if we consider partial von Neumann measurements; that is, they are restricted to a part of the system. In our main result in Theorem 1 we will show that in this case creation of entanglement is usually unavoidable. We use this result to show the close connection of our approach to the one-way information deficit [8] before we extend our ideas to the quantum discord [6] in Theorem 2 and following.

If we consider bipartite quantum states ρ^{AB}, and von Neumann measurements on A with a complete set of orthogonal rank one projectors $\Pi_i^A = |i^A\rangle\langle i^A|$, $\sum_i \Pi_i^A = \mathbb{1}_A$, then the quantum discord is defined as [6]

$$\delta^{\rightarrow}(\rho^{AB}) = S(\rho^A) - S(\rho^{AB}) + \min_{\{\Pi_i^A\}} \sum_i p_i S(\rho_i), \quad (1)$$

with $p_i = {\rm Tr}[\Pi_i^A \rho^{AB} \Pi_i^A]$ being the probability of the outcome i, and $\rho_i = \Pi_i^A \rho^{AB} \Pi_i^A / p_i$ being the corresponding state after the measurement. The quantum discord is nonnegative and zero if and only if the state ρ^{AB} has the form $\rho^{AB} = \sum_i p_i |i^A\rangle\langle i^A| \otimes \rho_i^B$ with orthogonal states $|i^A\rangle$. Recently an interpretation of the quantum discord was found using a connection to extended state merging [11,12]. Another interpretation was given earlier in [13].

A closely related quantity is the one-way information deficit [8,14]. For a bipartite state ρ^{AB} it is defined as the minimal increase of entropy after a von Neumann measurement on A:

$$\Delta^{\rightarrow}(\rho^{AB}) = \min_{\{\Pi_i^A\}} S\Big(\sum_i \Pi_i^A \rho^{AB} \Pi_i^A\Big) - S(\rho^{AB}), \quad (2)$$

where the minimum is taken over $\{\Pi_i^A\}$ as defined above Eq. (1). The one-way information deficit is non-negative and zero only on states with zero quantum discord. It can be interpreted as the amount of information in the state ρ^{AB}, which cannot be localized via a classical communication channel from A to B [14].

Given a bipartite quantum state ρ^{AB}, we recall that a partial von Neumann measurement on A can be described by coupling the system in the state ρ^{AB} to the measurement apparatus M in a pure initial state $|0^M\rangle$, $\rho_1 = |0^M\rangle\langle 0^M| \otimes \rho^{AB}$, and applying a unitary on the total state [15], $\rho_2 = U\rho_1 U^\dagger$. This situation is illustrated in Fig. 1. As we will consider only measurements on the subsystem

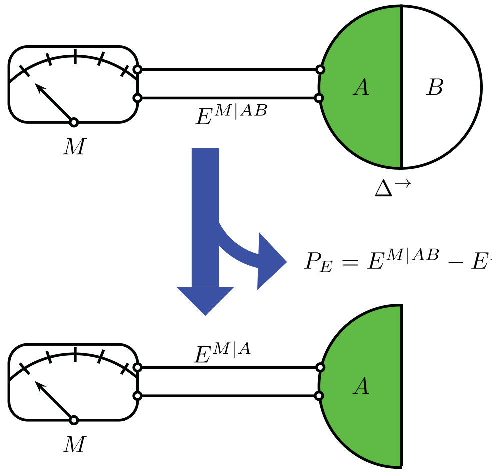

FIG. 1 (color online). A measurement apparatus M is used for a von Neumann measurement on A (green colored area), which is part of the total quantum system AB. The measurement implies a unitary evolution on the system MA, which can create entanglement $E^{M|AB}$ between the apparatus and the system. The partial entanglement $P_E = E^{M|AB} - E^{M|A}$ quantifies the part of entanglement which is lost when ignoring B.

A, the corresponding unitary U has the form $U = U_{MA} \otimes \mathbb{1}_B$. In the following, we will say that a unitary U realizes a von Neumann measurement $\{\Pi_i^A\}$ on A, if for any quantum state ρ^{AB} holds: $\mathrm{Tr}_M[U(|0^M\rangle\langle 0^M| \otimes \rho^{AB})U^\dagger] = \sum_i \Pi_i^A \rho^{AB} \Pi_i^A$. The measurement outcome is then obtained by measuring the apparatus M in its eigenbasis.

The entanglement between the apparatus M and the system AB in the state ρ_2 will be called entanglement created in the von Neumann measurement $\{\Pi_i^A\}$ on A. Given a state ρ^{AB}, we want to quantify the minimal entanglement created in a von Neumann measurement on A, minimized over all complete sets of rank one projectors $\{\Pi_i^A\}$. The minimal amount will be called E_{meas}, and it will depend on the entanglement measure used. In the following, the entanglement measure of interest will be the distillable entanglement E_D, which is defined in [16,17]. Thus, we define E_{meas} as follows: $E_{\mathrm{meas}}(\rho^{AB}) = \min_U E_D^{M|AB}(U\rho_1 U^\dagger)$, where the minimization is done over all unitaries which realize some von Neumann measurement on A. Recalling the definition of the one-way information deficit in (2), we present one of our main results.

Theorem 1. If a bipartite state ρ^{AB} has nonzero quantum discord $\delta^{\rightarrow}(\rho^{AB}) > 0$, any von Neumann measurement on A creates distillable entanglement between the measurement apparatus and the total system AB. The minimal distillable entanglement created in a von Neumann measurement on A is equal to the one-way information deficit: $E_{\mathrm{meas}}(\rho^{AB}) = \Delta^{\rightarrow}(\rho^{AB})$.

Proof.—As pointed out in [18], the unitary U must act on states of the form $|0^M\rangle \otimes |i^A\rangle$ as follows: $U(|0^M\rangle \otimes |i^A\rangle) = |i^M\rangle \otimes |i^A\rangle$, where $\{|i^A\rangle\}$ is the measurement basis, and $|i^M\rangle$ are orthogonal states of the measurement apparatus. In general we can always write $\rho^{AB} = \sum_{i,j} |i^A\rangle\langle j^A| \otimes O_{ij}^B$ with O_{ij}^B being operators on the Hilbert space $\mathcal{H}_B$. After the action of the unitary the state becomes $\rho_2 = \sum_{i,j} |i^M\rangle \times \langle j^M| \otimes |i^A\rangle\langle j^A| \otimes O_{ij}^B$. From [19] we know that the distillable entanglement is bounded from below as $E_D^{M|AB}(\rho_2) \geq S(\rho_2^{AB}) - S(\rho_2)$ with $\rho_2^{AB} = \mathrm{Tr}_M[\rho_2]$, and the von Neumann entropy $S(\rho) = -\mathrm{Tr}[\rho \log_2 \rho]$. We mention that the same inequality holds for the relative entropy of entanglement defined in [20] as $E_R = \min_{\sigma \in S} S(\rho || \sigma)$ with the quantum relative entropy $S(\rho \| \sigma) = -\mathrm{Tr}[\rho \log_2 \sigma] + \mathrm{Tr}[\rho \log_2 \rho]$; see [21] for details. Noting that $\rho_2^{AB} = \sum_i \Pi_i^A \rho^{AB} \Pi_i^A$ and $S(\rho_2) = S(\rho_1) = S(\rho^{AB})$ we see $E_D^{M|AB}(\rho_2) \geq S(\sum_i \Pi_i^A \rho^{AB} \Pi_i^A) - S(\rho^{AB})$. On the other hand, we know that E_R is an upper bound on the distillable entanglement [22]. Consider the state $\sigma = \sum_i \Pi_i^M \rho_2 \Pi_i^M$, which is separable with respect to the bipartition $M|AB$. From the definition of the relative entropy of entanglement follows: $E_R^{M|AB}(\rho_2) \leq S(\rho_2 \| \sigma)$. It can be seen by inspection that $S(\rho_2 \| \sigma) = S(\sum_i \Pi_i^A \rho^{AB} \Pi_i^A) - S(\rho^{AB})$. Thus we proved that $E_D^{M|AB}(\rho_2) = S(\sum_i \Pi_i^A \rho^{AB} \Pi_i^A) - S(\rho^{AB})$ holds for any measurement basis $\{|i^A\rangle\}$. If we minimize this equation over all von Neumann measurements on A, we get the desired result. ■

Note that from the above proof we conclude that $\min_U E_D^{M|AB}(U\rho_1 U^\dagger) = \min_U E_R^{M|AB}(U\rho_1 U^\dagger)$, and thus there does not exist bound entanglement in a partial measurement.

The approach presented so far can also be applied to any other measure of entanglement E, which satisfies the basic axiom to be nonincreasing under local operations and classical communication (LOCC) [20]. In this way we introduce the generalized one-way information deficit as follows:

$$\Delta_E^{\rightarrow}(\rho^{AB}) = \min_U E^{M|AB}(U\rho_1 U^\dagger), \tag{3}$$

where U realizes a von Neumann measurement on A and $\rho_1 = |0^M\rangle\langle 0^M| \otimes \rho^{AB}$. Using Theorem 1 it is easy to see that the generalized one-way information deficit is zero if and only if the state ρ^{AB} has zero quantum discord. This holds if E is zero on separable states only.

In the same way as different measures of entanglement capture different aspects of entanglement, the correspondence (3) can be used to capture different aspects of quantum correlations. Let us demonstrate this by using the geometric measure of entanglement E_G [23] on the right-hand side of (3). As the corresponding measure of quantum correlations, we obtain $\Delta_{E_G}^{\rightarrow}(\rho^{AB}) = \min_{\delta^{\rightarrow}(\sigma^{AB})=0}\{1 - F(\rho^{AB}, \sigma^{AB})\}$ with the fidelity $F(\rho, \sigma) = (\mathrm{Tr}[\sqrt{\sqrt{\rho}\sigma\sqrt{\rho}}])^2$ [24]. The minimization is done over all states σ^{AB} with zero quantum discord. Thus, this measure captures the geometric aspect of quantum correlations, similarly to the geometric measure of discord presented in [9].

The correspondence (3) also implies that certain properties of entanglement measures are transferred to corresponding properties of quantum correlation measures. This will be demonstrated in the following by finding a class of quantum operations which do not increase $\Delta_E^{\rightarrow}$. This class cannot be equal to the class of LOCC, since $\Delta_E^{\rightarrow}$ can increase under local operations on A. This can be seen by considering the classically correlated state $\rho_{cc} = \frac{1}{2}|0^A\rangle\langle 0^A| \otimes |0^B\rangle\langle 0^B| + \frac{1}{2}|1^A\rangle\langle 1^A| \otimes |1^B\rangle\langle 1^B|$ with $\Delta_E^{\rightarrow}(\rho_{cc}) = 0$. Using only local operations on A it is possible to create states with nonzero deficit $\Delta_E^{\rightarrow}$. Demanding that the subsystem A is unchanged, we are left with quantum operations on B only. In the following we will show that $\Delta_E^{\rightarrow}$ does not increase under arbitrary quantum operations on B, denoted by Λ_B:

$$\Delta_E^{\rightarrow}(\Lambda_B(\rho^{AB})) \leq \Delta_E^{\rightarrow}(\rho^{AB}). \tag{4}$$

Inequality (4) is seen to be true by noting that the entanglement $E^{M|AB}$ does not increase under Λ_B, as it does not increase under LOCC.

We can go one step further by noting that the distillable entanglement is also nonincreasing on average under stochastic LOCC. This captures the idea that two parties cannot share more entanglement on average, if they perform local generalized measurements on their subsystems and communicate the outcomes classically; see [17] for more details. Defining the global Kraus operators describing some LOCC protocol by $\{V_i\}$ with $\sum_i V_i^\dagger V_i = \mathbb{1}$, the probability of the outcome i is given by $q_i = \mathrm{Tr}[V_i \rho V_i^\dagger]$, and the state after the measurement with the outcome i is given by $\sigma_i = V_i \rho V_i^\dagger / q_i$. Then for the distillable entanglement [25] and the relative entropy of entanglement holds [26]

$$\sum_i q_i E(\sigma_i) \leq E(\rho). \tag{5}$$

Inequality (5) implies that the corresponding quantity $\Delta_E^{\rightarrow}$ satisfies the related property

$$\sum_i q_i \Delta_E^{\rightarrow}(\sigma_i^{AB}) \leq \Delta_E^{\rightarrow}(\rho^{AB}), \tag{6}$$

where q_i, σ_i^{AB} are defined as above Eq. (5), and now $\{V_i\}$ are Kraus operators describing a local quantum operation on B. Inequality (6) is seen to be true by using (5) in the definition (3).

In the following we will include the quantum discord $\delta^{\rightarrow}$ into our approach. We call the non-negative quantity

$$P_E(\rho) = E^{M|AB}(\rho) - E^{M|A}(\rho^{MA}) \tag{7}$$

the partial entanglement. It quantifies the part of entanglement which is lost when the subsystem B is ignored; see also Fig. 1. The following theorem establishes a connection between the partial entanglement and the quantum discord.

Theorem 2. The quantum discord of a bipartite state ρ^{AB} is equal to the minimal partial distillable entanglement in a von Neumann measurement on A: $\delta^{\rightarrow}(\rho^{AB}) = \min_U P_{E_D}(U\rho_1 U^\dagger)$. The minimization is done over all unitaries U which realize a von Neumann measurement on A, and $\rho_1 = |0^M\rangle\langle 0^M| \otimes \rho^{AB}$.

Proof.—We note that for any state ρ^{AB} the quantum discord can be written as $\delta^{\rightarrow}(\rho^{AB}) = S(\rho^A) - S(\rho^{AB}) + \min_{\{\Pi_i^A\}}\{S(\sum_i \Pi_i^A \rho^{AB} \Pi_i^A) - S(\sum_i \Pi_i^A \rho^A \Pi_i^A)\}$ with the minimization over all von Neumann measurements on A. To see this we start with the definition of the discord in (1). Then it is sufficient to show that for $p_i = \mathrm{Tr}[\Pi_i^A \rho^{AB} \Pi_i^A]$ and $\rho_i = \Pi_i^A \rho^{AB} \Pi_i^A / p_i$ holds $\sum_i p_i S(\rho_i) = S(\sum_i \Pi_i^A \rho^{AB} \Pi_i^A) - S(\sum_i \Pi_i^A \rho^A \Pi_i^A)$, which can be seen by inspection using the fact that $\{p_i\}$ are eigenvalues of $\sum_i \Pi_i^A \rho^A \Pi_i^A$. Using the same arguments as in the proof of Theorem 1 the desired result follows. ■

Using Theorem 2 we will show that the properties (4) and (6) are also satisfied by the quantum discord. Inequality (4) can be seen to be true by noting that E_D does not increase under LOCC and that Λ_B does not change the state $\mathrm{Tr}_B[U\rho_1 U^\dagger]$. To see that (6) also holds for the quantum discord note that, using the same arguments as in the proof of Theorem 1, we can replace the distillable entanglement E_D by the relative entropy of entanglement E_R in Theorem 2 without changing the statement. Because of convexity of E_R [26], the entanglement $E_R^{M|A}$ is nondecreasing on average under quantum operations on B: $\sum_i q_i E_R^{M|A}(\sigma_i^{MA}) \geq E_R^{M|A}(\rho^{MA})$. This implies that the partial entanglement $P_{E_R}(\rho) = E_R^{M|AB}(\rho) - E_R^{M|A}(\rho^{MA})$ is nonincreasing on average under quantum operations on B. Using this result we see that (6) also holds for the quantum discord.

Theorem 2 allows us to generalize the quantum discord to arbitrary measures of entanglement E in the same way as it was done for the one-way information deficit in (3):

$$\delta_E^{\rightarrow}(\rho^{AB}) = \min_U P_E(U\rho_1 U^\dagger). \tag{8}$$

Using the same arguments as above Eq. (8) we see that the generalized quantum discord $\delta_E^{\rightarrow}$ satisfies the properties (4) and (6) for all measures of entanglement E which are convex and obey (5).

So far we have only considered von Neumann measurements. In the following we will show that our approach is also valid with an alternative definition of the quantum discord [11,12,27]: $\delta_{\mathrm{POVM}}^{\rightarrow}(\rho^{AB}) = S(\rho^A) - S(\rho^{AB}) + \min_{\{M_i^A\}} \sum_i p_i S(\rho_i^B)$, with $\{M_i^A\}$ being a positive operator-valued measure (POVM) on A, $p_i = \mathrm{Tr}[M_i^A \rho^{AB}]$ and $\rho_i^B = \mathrm{Tr}_A[M_i^A \rho^{AB}]/p_i$. The minimization over POVMs can be replaced by a minimization over orthogonal projectors of rank one $\{\Pi_i^{A'}\}$ on an extended Hilbert space $\mathcal{H}_{A'}$ with $\dim\mathcal{H}_{A'} \geq \dim\mathcal{H}_A$ [28]. With this observation we see that all results presented for the quantum discord also hold for the alternative definition of the quantum discord.

In the following we will generalize our approach to multipartite von Neumann measurements on A.

We split the system A into n subsystems: $A = \cup_{i=1}^{n} A_i$. A von Neumann measurement Λ will be called n-partite, if it can be expressed as a sequence of von Neumann measurements Λ_i on each subsystem A_i: $\Lambda(\rho) = \Lambda_1(\ldots\Lambda_n(\rho))$. Now we can introduce the n-partite one-way information deficit $\Delta_n^{\rightarrow}$ and the n-partite quantum discord $\delta_n^{\rightarrow}$ as follows:

$$\Delta_n^{\rightarrow}(\rho^{AB}) = \min_{\Lambda} S(\Lambda(\rho^{AB})) - S(\rho^{AB}), \tag{9}$$

$$\delta_n^{\rightarrow}(\rho^{AB}) = \min_{\Lambda}\{S(\Lambda(\rho^{AB})) - S(\Lambda(\rho^{A}))\} - S(\rho^{AB}) + S(\rho^{A}). \tag{10}$$

Using the same arguments as in the proof of Theorems 1 and 2, we see that $\Delta_n^{\rightarrow}$ quantifies the minimal distillable entanglement between M and AB created in an n-partite von Neumann measurement on A. $\delta_n^{\rightarrow}$ can be interpreted as the corresponding minimal partial distillable entanglement P_{E_D}. We also note that this generalization includes n-partite von Neumann measurements on the total system. This can be achieved by defining A to be the total system. Since $\delta_n^{\rightarrow} = 0$ in this case, the only nontrivial quantity is the generalized information deficit $\Delta_n^{\rightarrow}$. A different approach to extend the quantum discord to multipartite settings was introduced in [29].

In this work we showed that the one-way information deficit is equal to the minimal distillable entanglement between the measurement apparatus M and the system AB which has to be created in a von Neumann measurement on A. The quantum discord is equal to the corresponding minimal partial distillable entanglement. Our approach can also be applied to any other measure of entanglement, thus defining a class of quantum correlation measures. This correspondence allows us to translate certain properties of entanglement measures to corresponding properties of quantum correlation measures. It may lead to a better understanding of the quantum discord and related measures of quantum correlations, since it allows us to use the great variety of powerful tools developed for quantum entanglement. We found a class of quantum operations which do not increase the generalized versions of the one-way information deficit and the quantum discord. We also generalized our results to multipartite settings.

We thank Sevag Gharibian for interesting discussions and an anonymous referee for constructive suggestions. We acknowledge partial financial support by Deutsche Forschungsgemeinschaft.

Note added.—Recently an alternative approach to connect the entanglement to quantum correlation measures was presented in [30]. There the authors show that nonclassical correlations in a multipartite state can be used to create entanglement in an activation protocol.

*streltsov@thphy.uni-duesseldorf.de

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(Streltsov *et al.*, 2011b) Phys. Rev. Lett. **106**, 160401.

Journal: Physical Review Letters
Impact Factor 2011: 7,37
Contribution: first author, scientific work and preparation of the manuscript, 90%

Simple algorithm for computing the geometric measure of entanglement

Alexander Streltsov,* Hermann Kampermann, and Dagmar Bruß
Heinrich-Heine-Universität Düsseldorf, Institut für Theoretische Physik III, D-40225 Düsseldorf, Germany
(Received 6 April 2011; published 18 August 2011)

We present an easy implementable algorithm for approximating the geometric measure of entanglement from above. The algorithm can be applied to any multipartite mixed state. It involves only the solution of an eigenproblem and finding a singular value decomposition; no further numerical techniques are needed. To provide examples, the algorithm was applied to the isotropic states of three qubits and the three-qubit XX model with external magnetic field.

DOI: 10.1103/PhysRevA.84.022323 PACS number(s): 03.67.Mn

I. INTRODUCTION

Quantum entanglement as a fascinating nonclassical feature has attracted attention since the early days of quantum theory [1,2]. In the last decades its importance for quantum information theory has been recognized, since entanglement plays a crucial role in almost every quantum computational task [3].

A bipartite pure state is said to be entangled if it cannot be written in the product form,

$$\left|\psi_{\text{sep}}^{AB}\right\rangle = |\psi^A\rangle \otimes |\psi^B\rangle. \tag{1}$$

States which are not entangled are called separable. In general, the number of parties is $n \geqslant 2$, and fully separable pure states become

$$|\psi_{\text{sep}}\rangle = \otimes_{i=1}^{n} |\psi^{(i)}\rangle. \tag{2}$$

The theory of entanglement has also been extended to the case where the quantum state is not pure [4,5]. Then a mixed state ρ_{sep} is called separable, if it can be written as a convex combination of separable pure states,

$$\rho_{\text{sep}} = \sum_i p_i \otimes_{j=1}^{n} \left|\psi_i^{(j)}\right\rangle\left\langle\psi_i^{(j)}\right|, \tag{3}$$

with non-negative probabilities p_i, $\sum_i p_i = 1$. Quantification of entanglement is one of the main research areas in quantum information theory [5]. For bipartite pure states, the entanglement is usually quantified using the von Neumann entropy of the reduced state,

$$E(|\psi^{AB}\rangle) = -\text{Tr}[\rho^A \log_2 \rho^A], \tag{4}$$

where $\rho^A = \text{Tr}_B[|\psi^{AB}\rangle\langle\psi^{AB}|]$. For multipartite systems and mixed states many different measures of entanglement were proposed [5,6]. In general, a measure of entanglement is any continuous function E on the space of mixed states ρ which satisfies at least the following properties [5]:

(i) E is non-negative and zero if and only if the state is separable;

(ii) E does not increase under local operations and classical communication:

$$E(\Lambda(\rho)) \leqslant E(\rho),$$

where Λ is any local operations and classical communication operation.

For bipartite mixed states, an important measure of entanglement is the entanglement of formation E_f. For pure states it is defined as the von Neumann entropy of the reduced state as given in (4). The extension to mixed states is done via the convex roof construction [7,8],

$$E_f(\rho) = \min \sum_i p_i E(|\psi_i\rangle), \tag{5}$$

where the minimum is taken over all pure state decompositions of ρ.

In this paper we consider the geometric measure of entanglement. For pure states it is defined as follows [9]:

$$E_G(|\psi\rangle) = 1 - \max_{|\phi\rangle \in S} |\langle\psi|\phi\rangle|^2, \tag{6}$$

where the maximization is done over the set of separable states S. For mixed states ρ the geometric measure of entanglement was originally defined via the convex roof construction, in the same way as was done for the entanglement of formation [9]:

$$E_G(\rho) = \min \sum_i p_i E_G(|\psi_i\rangle) \tag{7}$$

with minimization over all pure state decompositions of ρ. Similar measures of entanglement were also considered earlier in [10,11].

If ρ is a two-qubit state, general expressions for E_f and E_G are known [9,12,13]:

$$E_f(\rho) = h\left(\tfrac{1}{2} + \tfrac{1}{2}\sqrt{1 - C(\rho)^2}\right), \tag{8}$$

$$E_G(\rho) = \tfrac{1}{2}\left(1 - \sqrt{1 - C(\rho)^2}\right). \tag{9}$$

The concurrence $C(\rho)$ is given by

$$C(\rho) = \max\{0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4\}, \tag{10}$$

where λ_i are the square roots of the eigenvalues of $\rho \cdot \tilde{\rho}$ in decreasing order, and $\tilde{\rho}$ is defined as $\tilde{\rho} = (\sigma_y \otimes \sigma_y) \rho^\star (\sigma_y \otimes \sigma_y)$.

For most quantum states no exact expression for any measure of entanglement is known, and thus numerical algorithms must be used. One of the first algorithms computing entanglement has been presented in [14]. There the entanglement of formation was approximated using a random walk algorithm on the space of the decompositions of the given

*streltsov@thphy.uni-duesseldorf.de

mixed state. A much faster algorithm for the entanglement of formation was presented in [15]. This algorithm made use of the conjugate gradient method. In [16] the authors extended and improved the algorithm. The authors also applied the algorithm to the convex roof extension of the multipartite Meyer-Wallach measure [17]. We also note that the geometric measure of entanglement for some bound entangled states was computed numerically in Ref. [18].

In this paper we present an algorithm for the geometric measure of entanglement. The algorithm is easy to implement, since every step is either the solution of an eigenproblem or finding a singular value decomposition of a matrix, and no further numerical techniques are needed.

This paper is organized as follows. In Sec. II we present the algorithm for pure and mixed states. We also discuss its properties and convergence. In Sec. III we test our algorithm on bipartite and multipartite mixed states with the known value of the geometric measure of entanglement. Further, we compute an approximation of the geometric measure of entanglement for the isotropic states of three qubits, and the three-qubit XX model with a constant magnetic field. We conclude in Sec. IV.

II. ALGORITHM

Before we present our algorithm for general multipartite states, we begin with bipartite and multipartite pure states.

A. Pure states

1. Bipartite states

For bipartite pure states $|\psi\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_2$ the geometric measure of entanglement is given by [10]

$$E_G(|\psi\rangle) = 1 - \lambda_{\max}^2, \tag{11}$$

where $\lambda_{\max}$ is the largest Schmidt coefficient of $|\psi\rangle$. Note that $\lambda_{\max}^2$ is also the maximal eigenvalue of $\mathrm{Tr}_1[|\psi\rangle\langle\psi|]$ and $\mathrm{Tr}_2[|\psi\rangle\langle\psi|]$. Further, let $|\phi_1\rangle \in \mathcal{H}_1$ and $|\phi_2\rangle \in \mathcal{H}_2$ be the eigenstate corresponding to the maximal eigenvalue of $\mathrm{Tr}_2[|\psi\rangle\langle\psi|]$ and $\mathrm{Tr}_1[|\psi\rangle\langle\psi|]$ respectively. Then the state $|\phi\rangle = |\phi_1\rangle \otimes |\phi_2\rangle$ is a closest separable state to $|\psi\rangle$.

2. Multipartite states

If we consider pure states $|\psi\rangle$ on an n-partite Hilbert space $\mathcal{H} \in \otimes_{i=1}^n \mathcal{H}_i$ with $n > 2$, the geometric measure of entanglement is only known for a few special cases [9,19]. In Refs. [20,21] the authors presented an algorithm for an approximation of E_G for pure states. For simplicity we discuss the algorithm from [20,21] for a pure state of three qubits, a generalization to arbitrary systems is done at the end of this section.

Let $|\psi\rangle$ be the given state of three qubits. The algorithm starts with a random product state $|\phi_0\rangle = |0_0^{(1)}\rangle|0_0^{(2)}\rangle|0_0^{(3)}\rangle$ of three qubits, where the lower index will be used for counting the steps of the algorithm and the upper index denotes the "number" of the qubit. Now we consider $|\tilde{\psi}\rangle = (\langle 0_0^{(2)}|\langle 0_0^{(3)}|)|\psi\rangle$, which is a pure un-normalized state on the space of the first qubit. If we want to maximize the overlap $|\langle\phi_0|\psi\rangle|$ for fixed states $|0_0^{(2)}\rangle$ and $|0_0^{(3)}\rangle$, we have to replace $|0_0^{(1)}\rangle$ with the state $|0_1^{(1)}\rangle = \frac{1}{\sqrt{\langle\tilde{\psi}|\tilde{\psi}\rangle}}|\tilde{\psi}\rangle$. The procedure is repeated for the second qubit, starting in the product state $|0_1^{(1)}\rangle|0_0^{(2)}\rangle|0_0^{(3)}\rangle$ and resulting in the state $|0_1^{(1)}\rangle|0_1^{(2)}\rangle|0_0^{(3)}\rangle$. Finally, the same maximization is done for the third qubit with the final state $|\phi_1\rangle = |0_1^{(1)}\rangle|0_1^{(2)}\rangle|0_1^{(3)}\rangle$. In the same way we define the product state $|\phi_n\rangle = |0_n^{(1)}\rangle|0_n^{(2)}\rangle|0_n^{(3)}\rangle$ to be the result of n iterations of the algorithm. In the following we prove some properties of the algorithm.

Proposition 1. Let $|000\rangle = \lim_{n\to\infty}|\phi_n\rangle$ be the product state after an infinite number of steps of the algorithm, giving

$$\langle 100|\psi\rangle = \langle 010|\psi\rangle = \langle 001|\psi\rangle = 0. \tag{12}$$

Proof. If $\langle 100|\psi\rangle \neq 0$, then there exists a product state of the form $|\phi\rangle = |\phi^{(1)}\rangle|00\rangle$ such that $|\langle\phi|\psi\rangle| > |\langle 000|\psi\rangle|$. This means that $|000\rangle \neq \lim_{n\to\infty}|\phi_n\rangle$, which is a contradiction to the definition of $|000\rangle$. Using the same argument it can be seen that $\langle 010|\psi\rangle = \langle 001|\psi\rangle = 0$ also holds. ■

From Proposition 1 we see that the state $|\psi\rangle$ can be written as follows:

$$|\psi\rangle = \lambda_1|000\rangle + \lambda_2|110\rangle + \lambda_3|101\rangle + \lambda_4|011\rangle + \lambda_5|111\rangle, \tag{13}$$

where four of the coefficients λ_i can be chosen real and non-negative, and $\sum_i |\lambda_i|^2 = 1$. The form (13) is also known as *generalized Schmidt decomposition* [22,23]. For a general multipartite pure state $|\psi\rangle$ it is defined [23] as an expansion in the product basis $\{|\psi_{i_1}^{(1)}\rangle\cdots|\psi_{i_n}^{(n)}\rangle\}$,

$$|\psi\rangle = \sum_{i_1,\ldots,i_n} c_{i_1,\ldots,i_n}\left|\psi_{i_1}^{(1)}\right\rangle\cdots\left|\psi_{i_n}^{(n)}\right\rangle, \tag{14}$$

where the coefficients $c_{i_1,\ldots,i_n}$ have the property $c_{jii,\ldots,i} = c_{iji,\ldots,i} = \cdots = c_{ii,\ldots,ij} = 0$ if $1 \leqslant i < j \leqslant d$, where d is the dimension of a subsystem.

Proposition 2. The algorithm computes a generalized Schmidt decomposition of an arbitrary multipartite pure state with an arbitrary given precision.

Proof. For simplicity we give the proof for a pure state of three qubits. Generalization to an arbitrary system is given below. In order to find a generalized Schmidt decomposition with a given precision ε we need to find five parameters μ_i with $\sum_{i=1}^5 |\mu_i|^2 = 1$ and a product basis $\{|ijk\rangle\}$ such that the state

$$|\psi_{\mathrm{approx}}\rangle = \mu_1|000\rangle + \mu_2|110\rangle + \mu_3|101\rangle + \mu_4|011\rangle + \mu_5|111\rangle \tag{15}$$

is closer to $|\psi\rangle$ than ε; that is, $D(|\psi\rangle,|\psi_{\mathrm{approx}}\rangle) \leqslant \varepsilon$ with the trace distance $D(|\psi\rangle,|\phi\rangle) = \sqrt{1 - |\langle\psi|\phi\rangle|^2}$. This is accomplished by the state

$$|\psi_n\rangle = \frac{1}{N}\sum_{i,j,k} b_{ijk}|ijk\rangle_n, \tag{16}$$

where $|ijk\rangle_n = |i_n^{(1)}\rangle|j_n^{(2)}\rangle|k_n^{(3)}\rangle$ are the basis states after n iterations of the algorithm. The coefficients b_{ijk} are defined as follows: $b_{100} = b_{010} = b_{001} = 0$, and $b_{ijk} = (\langle\psi|ijk\rangle_n)^\star$ otherwise. N assures normalization of $|\psi_n\rangle$. The trace distance between $|\psi\rangle$ and $|\psi_n\rangle$ becomes $D(|\psi\rangle,|\psi_n\rangle) = \sqrt{|\langle\psi|100\rangle_n|^2 + |\langle\psi|010\rangle_n|^2 + |\langle\psi|001\rangle_n|^2}$. Using Proposition 1 we see that $\lim_{n\to\infty} D(|\psi\rangle,|\psi_n\rangle) = 0$. The wanted approximation $|\psi_{\text{approx}}\rangle$ is obtained by a state $|\psi_n\rangle$ such that $D(|\psi\rangle,|\psi_n\rangle) \leqslant \varepsilon$. ■

Thus, we showed that the algorithm presented in the beginning of this section computes a generalized Schmidt decomposition of the given pure state. As the generalized Schmidt decomposition is, in general, not unique [22,23], the result of the computation may depend on the choice of the initial product state $|\phi_0\rangle$. In particular, the final overlap $1 - |\langle 000|\psi\rangle|^2$ does not have to be the geometric measure of entanglement, even for an infinite number of iterations.

Finally, we note that all results presented in this section can be extended to an arbitrary number of qubits. Then the equations have to be changed accordingly. For four qubits, Eq. (12) becomes $\langle 1000|\psi\rangle = \langle 0100|\psi\rangle = \langle 0010|\psi\rangle = \langle 0001|\psi\rangle = 0$. Moreover, the results even hold if the subsystems are not qubits, but have arbitrary dimensions. For simplicity, we consider a pure state of three qutrits in the following. Again, $|000\rangle = \lim_{n\to\infty} |\phi_n\rangle$ denotes the product state which is achieved after infinite number of iterations. Using the same arguments as in the proof of Proposition 1 we see

$$\langle 100|\psi\rangle = \langle 010|\psi\rangle = \langle 001|\psi\rangle = 0, \tag{17}$$

$$\langle 200|\psi\rangle = \langle 020|\psi\rangle = \langle 002|\psi\rangle = 0, \tag{18}$$

where $|1\rangle$ and $|2\rangle$ are arbitrary states orthogonal to $|0\rangle$ on the corresponding subspace. In order to find a generalized Schmidt decomposition we also have to find specific states $|1\rangle$ and $|2\rangle$ for each subspace. Let $|\psi\rangle = \sum_{i=0}^{2}\sum_{j=0}^{2}\sum_{k=0}^{2} a_{ijk}|ijk\rangle$ be the expansion of the state in a product basis containing $|000\rangle$. Then consider the un-normalized state $|\tilde{\psi}\rangle = \sum_{i=1}^{2}\sum_{j=1}^{2}\sum_{k=1}^{2} a_{ijk}|ijk\rangle$. Since in the present stage of the algorithm we only have the knowledge about the state $|000\rangle = |0^{(1)}\rangle|0^{(2)}\rangle|0^{(3)}\rangle$, the state $|\tilde{\psi}\rangle$ can be computed as follows. Starting from the state $|\psi\rangle$ we compute the un-normalized state $|\alpha\rangle = |\psi\rangle - |000\rangle\langle 000|\psi\rangle$. In the second step we compute $|\beta\rangle = |\alpha\rangle - \sum_{i<j} |0^{(i)}0^{(j)}\rangle\langle 0^{(i)}0^{(j)}|\alpha\rangle$. In the final step we get $|\tilde{\psi}\rangle = |\beta\rangle - \sum_i |0^{(i)}\rangle\langle 0^{(i)}|\beta\rangle$. The state $|\tilde{\psi}\rangle$ is an un-normalized pure state of three qubits, and according to Proposition 1 applying the algorithm to it will give us the desired product basis $\{|ijk\rangle\}$ with the property $\langle 211|\psi\rangle = \langle 121|\psi\rangle = \langle 112|\psi\rangle = 0$. The expansion of the state $|\psi\rangle$ in the final product basis $\{|ijk\rangle\}$ is a generalized Schmidt decomposition of $|\psi\rangle$ [23]. Let $\{|ijk\rangle_n\}$ be the computed product basis after n iterations of the algorithm. The approximated generalized Schmidt decomposition of $|\psi\rangle$ becomes

$$|\psi_n\rangle = \frac{1}{N}\sum_{i,j,k} b_{ijk}|ijk\rangle_n, \tag{19}$$

with $b_{iij} = b_{iji} = b_{jii} = 0$ for $i < j$ and $b_{ijk} = a_{ijk}$ otherwise. N assures normalization of $|\psi_n\rangle$. The precision of the approximation is then given by $D(|\psi\rangle,|\psi_n\rangle) = \sqrt{\sum_{i<j}(|\langle iij|\psi\rangle|^2 + |\langle iji|\psi\rangle|^2 + |\langle jii|\psi\rangle|^2)}$. In the same way we can find a generalized Schmidt decomposition for any multipartite pure state with an arbitrary precision.

B. Mixed states

The main idea of the algorithm for mixed states is a consequence of the fact, that the geometric measure of entanglement may also be written as [24]

$$E_G(\rho) = 1 - \max_{\sigma\in S} F(\rho,\sigma), \tag{20}$$

where S denotes the set of separable states and $F(\rho,\sigma) = (\mathrm{Tr}[\sqrt{\sqrt{\rho}\sigma\sqrt{\rho}}])^2$ is the fidelity. Let $|\psi\rangle \in \mathcal{H}\otimes\mathcal{H}_a$ be a purification of ρ. It can be written as

$$|\psi\rangle = \sum_i \sqrt{p_i}|\psi_i\rangle \otimes |i\rangle, \tag{21}$$

with probabilities p_i and $\rho = \sum_i p_i|\psi_i\rangle\langle\psi_i|$. According to Uhlmann's theorem [3, p. 410] and using (20) we can also write

$$E_G(\rho) = 1 - \max_{\mathrm{Tr}_a[|\phi\rangle\langle\phi|]\in S} |\langle\psi|\phi\rangle|^2, \tag{22}$$

where the maximization is done over all states $|\phi\rangle \in \mathcal{H}\otimes\mathcal{H}_a$ which are purifications of a separable state. Note that any $|\phi\rangle$ can be written in the form

$$|\phi\rangle = \sum_j \sqrt{q_j}|\phi_j\rangle \otimes U^\dagger|j\rangle, \tag{23}$$

with pure separable states $|\phi_j\rangle \in S$, probabilities q_j, a unitary U acting on the Hilbert space $\mathcal{H}_a$, and $\langle i|j\rangle = \delta_{ij}$.

From (22) we see, that we can get an approximation of E_G by maximizing the overlap $|\langle\psi|\phi\rangle|$ over all states $|\phi\rangle$ of the form (23). Our approach for this maximization is the following.

(1) For fixed q_i and $|\phi_i\rangle$ we find a unitary U in (23) such that the overlap $|\langle\psi|\phi\rangle|$ is maximal.

(2) For fixed U and q_i we find states $|\phi_i\rangle$ in (23) such that the overlap $|\langle\psi|\phi\rangle|$ is maximal. Note that this is, in general, only possible for bipartite states. For multipartite states we compute $|\phi_i\rangle$ such that the overlap $|\langle\psi|\phi\rangle|$ does not decrease.

(3) For fixed U and $|\phi_i\rangle$ we find probabilities q_i in (23) such that the overlap $|\langle\psi|\phi\rangle|$ is maximal.

Steps (1)–(3) are iterated until the increase of the overlap $|\langle\psi|\phi\rangle|$ is smaller than a small parameter $\varepsilon > 0$. When the algorithm stops, the approximation of the geometric measure of entanglement is given by $\tilde{E}_G(\rho) = 1 - |\langle\psi|\tilde{\phi}\rangle|^2$, where $|\tilde{\phi}\rangle$ is the final state of the form (23).

In the following section we discuss the properties of the algorithm. Note that the order of the steps presented above can also be changed without changing these properties.

C. Properties

In the following we discuss some properties of the algorithm presented above. In the first step the probabilities q_i and the separable pure states $|\phi_i\rangle$ are fixed. The product $|\langle\psi|\phi\rangle|$ can be maximized using Uhlmann's theorem [3, p. 410]; it is maximal if U is chosen such that the following holds:

$$A = \sqrt{AA^\dagger}U^\dagger, \tag{24}$$

where A is a matrix defined as $A = \sum_{i,j}\sqrt{p_i q_j}\langle\phi_j|\psi_i\rangle|i\rangle\langle j|$. Note that Eq. (24) is the polar decomposition of A, which can be computed efficiently for any matrix A [25].

In the second step of the algorithm we fix U, which was found in the step before. The probabilities q_i are also unchanged. In order to maximize the overlap $|\langle\psi|\phi\rangle|$ the separable states $|\phi_i\rangle$ have to be changed to the states $|\phi_i'\rangle$ for which holds

$$\langle\psi_i'|\phi_i'\rangle = \sqrt{F_s(|\psi_i'\rangle)}, \tag{25}$$

with the states $|\psi_i'\rangle = \frac{1}{\sqrt{p_i'}}\sum_j u_{ij}\sqrt{p_j}|\psi_j\rangle$, where $u_{ij} = \langle i|U|j\rangle$ are elements of U in the computational basis, and $p_i' > 0$ is chosen such that $|\psi_i'\rangle$ is normalized. For bipartite states $|\psi_i'\rangle$ this step is evaluated according to the discussion in Sec. II A 1. If $|\psi_i'\rangle$ is multipartite, the closest separable state $|\phi_i'\rangle$ cannot be found in general. However, there is a way to circumvent this problem as follows. We apply the algorithm described in Sec. II A 2 to the state $|\psi_i'\rangle$ with the initial product state $|\phi_i\rangle$, thus getting a final product state $|\phi_i'\rangle$. The state $|\phi_i'\rangle$ is not necessarily the closest separable state to $|\psi_i'\rangle$; however, it will be closer to $|\psi_i'\rangle$ than the initial product state $|\phi_i\rangle$. However, if we replace $|\phi_i\rangle$ by $|\phi_i'\rangle$, we get a better approximation of the geometric measure of entanglement. This can be seen by noting that for the overlaps of the purifications holds: $|\langle\psi|\phi'\rangle| \geqslant |\langle\psi|\phi\rangle|$, where in $|\phi'\rangle$ all product states $|\phi_i\rangle$ were replaced with $|\phi_i'\rangle$.

In the last step of the iteration we fix U which was found in the first step, and the separable states $|\phi_i'\rangle$ which were found in the second step. Using the method of Lagrange multipliers we find the optimal probabilities:

$$q_i' = \frac{p_i'|\langle\psi_i'|\phi_i'\rangle|^2}{\sum_k p_k'|\langle\psi_k'|\phi_k'\rangle|^2}. \tag{26}$$

Let $\tilde{E}_n(\rho)$ be the approximation of the geometric measure of entanglement after n iterations of the algorithm. We now prove the main property of the algorithm.

Proposition 3. The approximated value of the geometric measure of entanglement never increases in a step of the iteration:

$$\tilde{E}_{n+1}(\rho) \leqslant \tilde{E}_n(\rho). \tag{27}$$

Proof. It is sufficient to show that the overlap of the purifications $|\langle\psi|\phi\rangle|$ does not decrease in any step of the algorithm. This is seen directly from the definition of the algorithm in Sec. II B. ∎

D. Implementation

First we set a small parameter $\varepsilon > 0$. The algorithm starts with a random decomposition $\{p_i,|\psi_i\rangle\}_{i=1}^{d^2}$ into d^2 elements of the state $\rho = \sum_{i=1}^{d^2} p_i|\psi_i\rangle\langle\psi_i|$ and a separable decomposition $\{q_i,|\phi_i\rangle\}_{i=1}^{d^2}$ of a random separable state $\sigma = \sum_{i=1}^{d^2} q_i|\phi_i\rangle\langle\phi_i|$, where we demand that $p_i > 0$ and $q_i > 0$ for all $1 \leqslant i \leqslant d^2$. The steps (1)–(3) from the Sec. II B can be implemented as follows,

(1) Find the singular value decomposition of the matrix $A = \sum_{i,j}\sqrt{p_i q_j}\langle\phi_j|\psi_i\rangle|i\rangle\langle j|$, that is, $A = VDW$ with unitary matrices V, W and diagonal non-negative matrix D. Define $U = W^\dagger V^\dagger$, noting that (24) is fulfilled.

(2) Define un-normalized states

$$|\alpha_i\rangle = \sum_{j=1}^{d^2} u_{ij}\sqrt{p_j}|\psi_j\rangle, \tag{28}$$

with $u_{ij} = \langle i|U|j\rangle$. Compute $p_i' = \langle\alpha_i|\alpha_i\rangle$ and $|\psi_i'\rangle = \frac{1}{\sqrt{p_i'}}|\alpha_i\rangle$ for all i. For bipartite states compute separable pure states $|\phi_i'\rangle \in S$ such that $\langle\psi_i'|\phi_i'\rangle = \sqrt{F_s(|\psi_i'\rangle)}$. For multipartite states find product states $|\phi_i'\rangle$ which are closer to $|\psi_i'\rangle$ than the states $|\phi_i\rangle$ computed in the step before. This can be done applying the algorithm presented in Sec. II A 2 to the state $|\psi_i'\rangle$ with the initial product state $|\phi_i\rangle$.

(3) Compute $q_i' = \frac{p_i'|\langle\psi_i'|\phi_i'\rangle|^2}{\sum_k p_k'|\langle\psi_k'|\phi_k'\rangle|^2}$.

After performing steps (1)–(3) define a new separable state $\sigma' = \sum_i q_i'|\phi_i'\rangle\langle\phi_i'|$, which is an approximation of the closest separable state to ρ. If $F(\rho,\sigma') - F(\rho,\sigma) > \varepsilon$, set $|\psi_i\rangle = |\psi_i'\rangle$, $|\phi_i\rangle = |\phi_i'\rangle$, $p_i = p_i'$ and $q_i = q_i'$ for all i and go back to step (1); otherwise stop. The computed approximation is $\tilde{E}_G(\rho) = 1 - F(\rho,\sigma')$.

E. Convergence

One of the most important questions regarding algorithms computing entanglement is whether the algorithm converges to the exact value of the entanglement measure, at least for infinite number of steps. For a general multipartite state with more than two parties the algorithm will converge to the wrong value with some nonzero probability, depending on the initial separable state. This is due to the fact that the algorithm for pure multipartite states presented in Sec. II A 2 does not necessarily compute the correct value, since it can converge to a local minimum [21,26].

For bipartite mixed states there is no full answer to this question, and testing the algorithm on bipartite states with known geometric measure of entanglement we did not observe convergence to a wrong value. However, it can be shown that for some states and some special choice of the purifications $|\psi\rangle$ and $|\phi\rangle$ the algorithm does not compute the correct value even after an infinite number of iterations. To see this we consider a separable state $\rho \in S$ with rank r such that any separable decomposition of ρ has more elements than r. The existence of such states is assured [5]. Let now $\{p_i,|\psi_i\rangle\}_{i=1}^r$ be a decomposition of ρ which is optimal among all decompositions with r elements; that is, the average entanglement $\sum_{i=1}^r p_i E_G(|\psi_i\rangle)$ is minimal among all decompositions into r elements. Further, let $|\phi_i\rangle$ be the closest separable state to $|\psi_i\rangle$ and we also choose $q_i = \frac{p_i|\langle\psi_i|\phi_i\rangle|^2}{\sum_k p_k|\langle\psi_k|\phi_k\rangle|^2}$. Now we start the algorithm with the decompositions $\{p_i,|\psi_i\rangle\}_{i=1}^r$ and $\{q_i,|\phi_i\rangle\}_{i=1}^r$, as described in the previous section. Then the unitary U which maximizes the overlap of the purifications $|\psi\rangle = \sum_i\sqrt{p_i}|\psi_i\rangle\otimes|i\rangle$ and $|\phi\rangle = \sum_j\sqrt{q_j}|\phi_j\rangle\otimes U^\dagger|j\rangle$ is given by $U = \mathbb{1}$. In the second step the algorithm will maximize the overlaps $\langle\phi_i|\psi_i\rangle$, which are already optimal. The same is true for the last step of the algorithm, where the probabilities q_j are optimized. Thus, the algorithm preserves the initial separable state and does not compute the correct value even for infinite number of steps.

To avoid the problem mentioned above the algorithm should always start with a separable state chosen at random, that is, with random initial probabilities q_i and random separable pure states $|\phi_i\rangle$. Moreover, the number of initial nonzero probabilities q_i should be at least $(\dim \mathcal{H})^2$.

In the following section we test the algorithm and present some applications for states with unknown geometric measure of entanglement.

III. APPLICATIONS

A. Testing the algorithm

1. Two qubits

If ρ is a two-qubit state, the geometric measure of entanglement is given by (9). We applied our algorithm with $\varepsilon = 10^{-15}$ to 10^3 random states of two qubits and tested the computed value $\tilde{E}_G$ against the exact value given in (9). The maximal deviation $\tilde{E}_G - E_G$ from the exact value was 6×10^{-11}. The average number of steps made by the algorithm was 291.

2. Isotropic states

We also tested our algorithm on the isotropic states in dimension $d \times d$; these are states of the form

$$\rho = p|\Phi^+\rangle\langle\Phi^+| + \frac{1-p}{d^2}\mathbb{1}, \qquad (29)$$

with the maximally entangled state $|\Phi^+\rangle = \frac{1}{\sqrt{d}}\sum_{i=1}^{d}|ii\rangle$. For these states an exact expression for the geometric measure of entanglement was given in [9]; the states are entangled if and only if $p > \frac{1}{1+d}$. We applied our algorithm to the state (29) for $2 \leqslant d \leqslant 3$ with the parameter $\varepsilon = 10^{-15}$ for $p = 0.01n$ and $0 \leqslant n \leqslant 99$. The difference between the approximated value $\tilde{E}_G$ and the exact value E_G was always less than 10^{-10}.

In order to do the test for $d = 4$ within a reasonable time some modifications had to be applied. First, we minimized only over decompositions into $d^2 = 16$ instead of $d^4 = 256$ pure states. Further, for $d = 4$ the test was done on entangled states only, that is, for $p = 0.01n$ with $20 < n \leqslant 99$. The difference between the approximation $\tilde{E}_G$ and the exact value E_G never exceeded 10^{-13}. The results are summarized in Table I. There $\bar{N}$ denotes the average number of steps made by the algorithm.

For the cases tested above the algorithm always converged into the correct value of E_G within the precision given in Table I with a single run of the algorithm. Note that in general more than one run with different initial parameters should be done to avoid convergence into a wrong value. Further, we see from Table I that the parameter ε should not be used directly to quantify the precision of the approximation, although the deviation from the exact value is very small.

TABLE I. Precision of the approximation $\tilde{E}_G - E_G$ and the average number of steps $\bar{N}$ for the isotropic states (29) with parameter $\varepsilon = 10^{-15}$.

d	2	3	4
$\tilde{E}_G - E_G$	$<10^{-13}$	$<10^{-10}$	$<10^{-13}$
$\bar{N}$	80	516	2259

3. Four qubits

In Ref. [27] the authors computed the geometric measure of entanglement for a class of mixed states of four qubits. We tested our algorithm on the state $\rho(t)$, which for $t = 0$ is defined as the four-qubit cluster state

$$|\mathrm{CL}_4\rangle = \tfrac{1}{2}(|0000\rangle + |0011\rangle + |1100\rangle - |1111\rangle). \qquad (30)$$

For $t > 0$ the diagonal terms of ρ are left invariant, and the off-diagonal components decay exponentially with t; that is,

$$\rho_{kl}(t) = \begin{cases} \rho_{kl}(0) & \text{for} \quad k = l, \\ e^{-t}\rho_{kl}(0) & \text{for} \quad k \neq l \end{cases}. \qquad (31)$$

We applied our algorithm with parameter $\varepsilon = 10^{-15}$ on the states $\rho(t)$ with $t = 0.01n$ for all $1 \leqslant n \leqslant 100$. The discrepancy between the approximated value and the exact value given in [27] was always smaller than 10^{-14}.

The same test was done for the state $\tilde{\rho}(t)$, which for $t = 0$ is defined as the four-qubit W state

$$|W_4\rangle = \tfrac{1}{2}(|0001\rangle + |0010\rangle + |0100\rangle + |1000\rangle), \qquad (32)$$

and for $t > 0$ the off-diagonal components decay exponentially as given in (31). There the discrepancy between the approximation and the exact value was always smaller than 10^{-11}.

Finally, we tested our algorithm on the four-qubit state $\bar{\rho}(t)$, which for $t = 0$ is defined as the symmetrized Dicke state,

$$|D_4\rangle = \frac{1}{\sqrt{6}}(|0011\rangle + |0101\rangle + |1001\rangle + |1100\rangle + |0110\rangle + |1010\rangle). \qquad (33)$$

Again, for $t > 0$ the off-diagonal components decay as in (31). The test was done with $t = 0.01n$ for all $1 \leqslant n \leqslant 100$, the difference $\tilde{E}_G - E_G$ was always smaller than 10^{-12}. The results are summarized in Table II. There $\bar{N}$ denotes the average number of iterations made by the algorithm.

Note that the optimizations above were done over pure state decompositions into 2^4 elements instead of 2^8. This reduction was needed in order to do the computation within a reasonable time. Moreover, we note that for very small parameter $t = 0.01$ we sometimes observed convergence into a wrong value. This is due to the fact that for small t the state $\rho(t)$ is almost pure. As was mentioned in Sec. II E the algorithm can converge to wrong values for pure multipartite states. In these cases the algorithm was started again with random initial parameters. To get an impression we mention that for the last example $\bar{\rho}(0.01)$ the algorithm sometimes converged to $\tilde{E}_G - E_G \approx 8 \times 10^{-4}$.

We also mention that the examples given here were computed on a standard computer. The computation time

TABLE II. Precision of the approximation $\tilde{E}_G - E_G$ and the average number of steps $\bar{N}$ for the four-qubit states presented in the text with parameter $\varepsilon = 10^{-15}$.

$\rho(0)$	$\lvert\mathrm{CL}_4\rangle$	$\lvert W_4\rangle$	$\lvert D_4\rangle$
$\tilde{E}_G - E_G$	$<10^{-14}$	$<10^{-11}$	$<10^{-12}$
$\bar{N}$	12	173	126

for a single state of three and four qubits was on the order of 1 min. If in the four-qubit case the optimization is done over decompositions into 2^8 instead of 2^4 pure states, the computation time increases at least by the factor 2^4. In general, for an n-partite system of qudits with dimensions d, the computation time scales at least with the number of pure states in the decomposition, given by d^{2n}.

4. Comparison with other algorithms

A significant difference between our algorithm and the algorithms presented in [15,16] is the fact that our algorithm implies only the solution of the eigenproblem and finding a singular value decomposition. For both problems efficient numerical algorithms exist [25], implying that each step of our algorithm can be done efficiently. The algorithms based on conjugate gradients usually imply a line search [15]. It is not known to us whether a line search can in general be done efficiently for the problem considered here.

As noted in Sec. III A 1, the average number of iterations made by our algorithm for random two-qubit states with parameter $\varepsilon = 10^{-15}$ was 291. This is comparable to the performance of the conjugate gradient algorithm; for comparison, see Fig. 1 in [16].

B. On additivity of entanglement

A measure of entanglement E is called additive, if for any two states ρ^{AB} and σ^{AB} holds [6]:

$$E(\rho^{AB} \otimes \sigma^{AB}) = E(\rho^{AB}) + E(\sigma^{AB}), \tag{34}$$

where the entanglement between the parties A and B is considered.

For pure states $|\psi^{AB}\rangle$ and $|\phi^{AB}\rangle$ we see that

$$F_s(|\psi^{AB}\rangle \otimes |\phi^{AB}\rangle) = F_s(|\psi^{AB}\rangle)F_s(|\phi^{AB}\rangle), \tag{35}$$

with $F_s(\rho) = \max_{\sigma\in s} F(\rho,\sigma)$ and the fidelity $F(\rho,\sigma) = (\mathrm{Tr}[\sqrt{\sqrt{\rho}\sigma\sqrt{\rho}}])^2$. From (35) we see that the geometric measure of entanglement is not additive. Note that for the entanglement of formation nonadditivity has also been proved [28].

We consider the *logarithmic entanglement*

$$E_{\log}(\rho) = -\log_2 F_s(\rho), \tag{36}$$

which is additive for pure bipartite states, as is seen from (35). In general, $F_s(\rho^{AB} \otimes \sigma^{AB}) \geqslant F_s(\rho^{AB})F_s(\sigma^{AB})$ holds, and thus the logarithmic entanglement is subadditive:

$$E_{\log}(\rho^{AB} \otimes \sigma^{AB}) \leqslant E_{\log}(\rho^{AB}) + E_{\log}(\sigma^{AB}). \tag{37}$$

We use our algorithm to test the inequality (37). Note that for two-qubit states ρ we get $F_s(\rho) = \frac{1}{2}(1 + \sqrt{1 - C(\rho)^2})$. We take ρ^{AB} and σ^{AB} to be random states of two qubits and apply the algorithm to $\rho^{AB} \otimes \sigma^{AB}$ with parameter $\varepsilon = 10^{-7}$. This procedure is repeated 100 times; each time the computed approximation $\tilde{F}_s(\rho^{AB} \otimes \sigma^{AB})$ was slightly below $F_s(\rho^{AB})F_s(\sigma^{AB})$, which means that we could not disprove additivity of logarithmic entanglement in this way. The difference $F_s(\rho^{AB})F_s(\sigma^{AB}) - \tilde{F}_s(\rho^{AB} \otimes \sigma^{AB})$ was always smaller than 10^{-5}.

C. Applications to three qubits

In this section we apply our algorithm to three-qubit states with unknown value of E_G. If d is the dimension of the total Hilbert space, then for any ρ there always exists an optimal decomposition with at most d^2 elements [24]. A decomposition $\{p_i,|\psi_i\rangle\}$ of a state $\rho = \sum_i p_i|\psi_i\rangle\langle\psi_i|$ is called optimal if its average entanglement is equal to the geometric measure of entanglement: $\sum_i p_i E_G(|\psi_i\rangle) = E_G(\rho)$. In order to make sure that the algorithm always has the chance to find the optimal decomposition, all minimizations in this section were done over decompositions into $d^2 = 2^6 = 64$ pure states. In order to do the computation within a reasonable time we used the parameter $\varepsilon = 10^{-7}$.

1. Isotropic states

Isotropic states of three qubits have the form

$$\rho = p|\mathrm{GHZ}\rangle\langle\mathrm{GHZ}| + \frac{1-p}{8}\mathbb{1}, \tag{38}$$

with $|\mathrm{GHZ}\rangle = \frac{1}{\sqrt{2}}(|000\rangle + |111\rangle)$. They are known to be fully separable if and only if $p \leqslant \frac{1}{5}$ [29]. We apply our algorithm to these states with parameter $\varepsilon = 10^{-7}$ for $p > \frac{1}{5}$. The result is shown in Fig. 1 (solid line). The plot can be compared to the geometric measure of entanglement of the isotropic states of two qubits; see the dashed line in Fig. 1. In the limit $p \to 1$ the state becomes the pure GHZ state with $E_G(|\mathrm{GHZ}\rangle) = \frac{1}{2}$ [9].

2. XX model

As a final example we apply our algorithm to the isotropic XX model of three qubits in a constant magnetic field. The corresponding Hamiltonian is given by [30,31]

$$H = \frac{B}{2}\sum_{i=1}^{3}\sigma_i^z + J\sum_{i=1}^{3}(\sigma_i^x\sigma_{i+1}^x + \sigma_i^y\sigma_{i+1}^y), \tag{39}$$

with periodic boundary conditions $\sigma_4^x = \sigma_1^x$ and $\sigma_4^y = \sigma_1^y$. In thermal equilibrium the system is found in the mixed state $\rho = \frac{e^{-\frac{H}{kT}}}{Z}$ with $Z = \mathrm{Tr}[e^{-\frac{H}{kT}}]$. In the following we set $k = 1$.

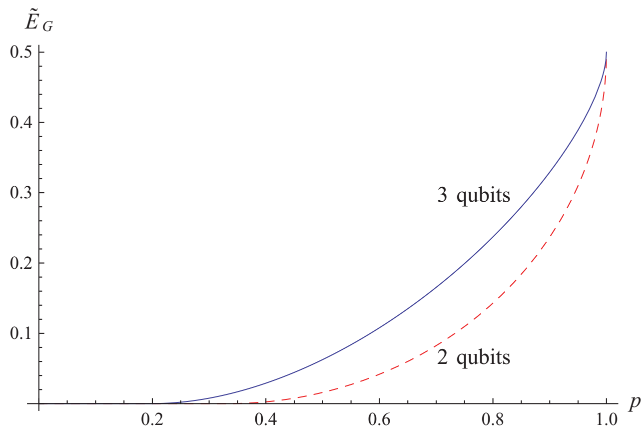

FIG. 1. (Color online) Approximation of the geometric measure of entanglement $\tilde{E}_G$ for isotropic states of three qubits given in (38) as a function of p (solid line) compared to the two-qubit case (dashed line).

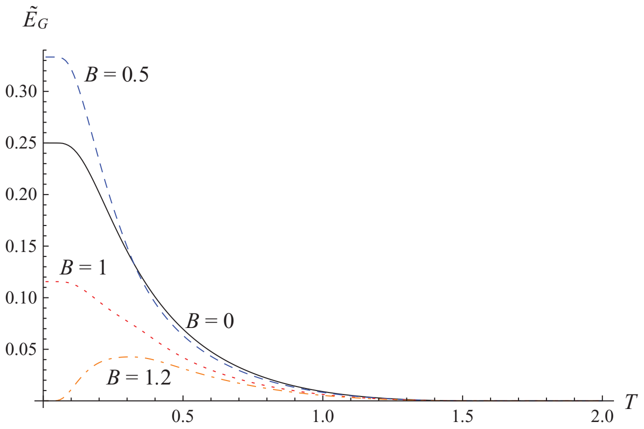

FIG. 2. (Color online) Approximation of the geometric measure of entanglement $\tilde{E}_G$ plotted as function of the temperature T for $\rho = \frac{e^{-\frac{H}{kT}}}{Z}$ with H given in (39). The parameter J is set to $\frac{1}{2}$ and $k = 1$.

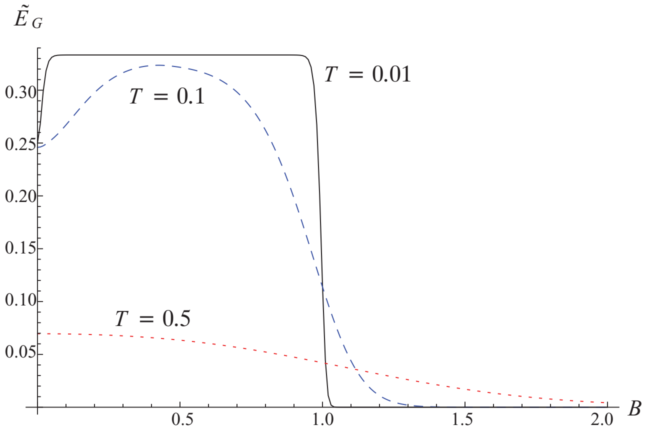

FIG. 3. (Color online) Approximation of the geometric measure of entanglement $\tilde{E}_G$ for fixed values of T plotted as a function of the magnetic field B. The parameter J is set to $\frac{1}{2}$ and $k = 1$.

The results of the approximation with parameter $\varepsilon = 10^{-7}$ are shown in Fig. 2. They can be compared to the results for two qubits in ([32], Fig. 4). For different values of the magnetic field B we observe a different behavior of the system in the low temperature limit. This behavior is explained in the following.

Note that the Hamiltonian (39) has four nondegenerate eigenvalues $\pm\frac{3}{2}B$, and $4J \pm \frac{1}{2}B$. Further, the following two eigenvalues are degenerated twice: $-2J \pm \frac{1}{2}B$. For vanishing magnetic field the ground state of the system is a mixture of the four eigenstates corresponding to the eigenvalue $-2J$ with equal probabilities. In this case we get $\tilde{E}_G \approx \frac{1}{4}$ for $T \to 0$;see the solid curve in Fig. 2. For small nonzero magnetic field $0 < B < 2J$ the ground state of the system is the mixture of the eigenstates corresponding to the eigenvalue $-2J - \frac{1}{2}B$. As can be seen from the dashed curve in Fig. 2, for $T \to 0$ the approximation becomes $\tilde{E}_G \approx \frac{1}{3}$ in this case. In the case $B = 2J$, there are three eigenstates corresponding to the smallest eigenvalue $-3J$. The approximated value for $T \to 0$ in this case becomes $\tilde{E}_G \approx 0.116$; see the dotted curve in Fig. 2. Finally, for $B > 2J$ the ground state is the product state $|111\rangle$, and the entanglement vanishes for $T \to 0$, as is seen from the dot-dashed curve in Fig. 2.

In Fig. 3 we show the plot of $\tilde{E}_G$ as a function of the magnetic field B for three different temperatures T. For $T \to 0$ we observe that $\tilde{E}_G$ becomes a nonanalytic function of B for two different values of the magnetic field, namely for $B = 0$ and $B = 2J$. This is a significant difference to the two-qubit case, where such behavior occurred only for a single value of B ([32], Fig. 5).

IV. CONCLUDING REMARKS

In this paper we presented an algorithm for approximating the geometric measure of entanglement for arbitrary multipartite mixed states. The algorithm is based on a connection between the geometric measure of entanglement and the fidelity [24]. It is easily implementable, since it implies only the solution of an eigenproblem and finding a singular value decomposition. We tested our algorithm on bipartite and multipartite mixed states, where an exact formula for the geometric measure of entanglement is known. In all cases we found convergence to the exact value. For two qubits, the performance of our algorithm is comparable to the performance of the algorithms based on conjugate gradients. We also applied our algorithm to the isotropic state of three qubits, and the three-qubit XX model with external magnetic field.

In our tests on bipartite mixed states with known value of the geometric measure of entanglement our algorithm always converged to the correct value within a given precision. It remains an open question whether this is always the case. For quantum states with more than two parties the algorithm can converge to wrong values with nonzero probability. In general, more than one run of the algorithm with different initial parameters should be performed.

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(Streltsov *et al.*, 2011c) Phys. Rev. A **84**, 022323.

Journal: Physical Review A
Impact Factor 2011: 2,878
Contribution: first author, scientific work and preparation of the manuscript, 90%

Are General Quantum Correlations Monogamous?

Alexander Streltsov,[1] Gerardo Adesso,[2] Marco Piani,[3] and Dagmar Bruß[1]
[1]*Heinrich-Heine-Universität Düsseldorf, Institut für Theoretische Physik III, D-40225 Düsseldorf, Germany*
[2]*School of Mathematical Sciences, University of Nottingham, University Park, Nottingham NG7 2RD, United Kingdom*
[3]*Institute for Quantum Computing and Department of Physics and Astronomy, University of Waterloo, Waterloo, Ontario N2L 3G1, Canada*
(Received 16 December 2011; published 1 August 2012)

Quantum entanglement and quantum nonlocality are known to exhibit monogamy; that is, they obey strong constraints on how they can be distributed among multipartite systems. Quantum correlations that comprise and go beyond entanglement are quantified by, e.g., quantum discord. It was observed recently that for some states quantum discord is not monogamous. We prove, in general, that any measure of correlations that is monogamous for all states and satisfies reasonable basic properties must vanish for all separable states: only entanglement measures can be strictly monogamous. Monogamy of other than entanglement measures can still be satisfied for special, restricted cases: we prove that the geometric measure of discord satisfies the monogamy inequality on all pure states of three qubits.

DOI: 10.1103/PhysRevLett.109.050503 PACS numbers: 03.67.−a

Entanglement, nonclassical correlations, and nonlocal correlations are all forms of correlations between two or more subsystems of a composite quantum system that are different from strictly classical correlations and, in general, different from each other. One of the characteristic traits of classical correlations is that they can be freely shared. A party A can have maximal classical correlations with two parties B and C simultaneously. This is no longer the case if quantum entanglement or nonlocal correlations are concerned [1]. The limits on the shareability of those types of nonclassical correlations are known as monogamy constraints, see Fig. 1 for illustration. Strict monogamy inequalities have been proven that constrain the distribution of particular measures of entanglement and nonlocal correlations (the latter expressed in terms of violation of some Bell-type inequality [2]) among the subsystems of a multipartite system [3–11]. These relations can be seen as a particular case of trade-off relations that, in general, may relate and constrain different quantifiers of correlations [10,12]. Monogamy is the crucial property of correlations that makes quantum key distribution secure [1,13], even in no-signalling theories more general than quantum mechanics.

Nonclassical correlations that go beyond entanglement, often quantified, e.g., via the quantum discord [14,15], have recently attracted considerable attention [16,17]. While entanglement captures the nonseparability of two subsystems [18,19], quantum discord detects nonclassical properties even in separable states. Different attempts were presented to connect the new concept of quantum discord to quantum entanglement [20–26] and to broadcasting [27–29]. Several experimental results have been reported in [30–33]. Quantum discord, as well as related quantifiers of quantum correlations [17,22,23,34–44], have also been linked to better-than-classical performance in quantum computation and communication tasks, even in the presence of limited or strictly vanishing entanglement [30,45–53]. An important question to understand the role of quantum correlations as signatures of genuine nonclassical behavior is whether they distribute in a monogamous way among multipartite systems.

A bipartite measure of correlations $\mathcal{Q}$ satisfies monogamy if [3,19]

$$\mathcal{Q}^{A|BC}(\rho_{ABC}) \geq \mathcal{Q}^{A|B}(\rho_{AB}) + \mathcal{Q}^{A|C}(\rho_{AC}) \qquad (1)$$

holds for all states ρ_{ABC}. Here, $\rho_{AB} = \mathrm{Tr}_C(\rho_{ABC})$ denotes the reduced state of parties A and B, and analogously for ρ_{AC}. The vertical bar is the familiar notation for the bipartite split. The concept of monogamy is visualized in Fig. 1.

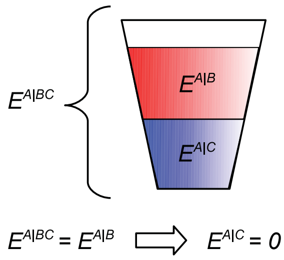

FIG. 1 (color online). Entanglement is monogamous: for a fixed amount of entanglement between A and BC, the more entanglement exists between A and B, the less can exist between A and C. Quantitatively, this is expressed using the monogamy relation, see Eq. (1) in the main text. In particular, the latter implies—for a monogamous measure of entanglement E—that $E^{A|C} = 0$ if $E^{A|BC} = E^{A|B}$. In this Letter we show that the monogamy relation does not hold, in general, for any quantum correlation measure beyond entanglement, i.e., for any measure that does not vanish on separable states.

If $\mathcal{Q}$ denotes, in particular, an entanglement measure [18,19], then there are a number of choices that satisfy monogamy for pure states of qubits, including the squared concurrence [3] and the squared negativity [54], as well as their continuous variable counterparts for multimode Gaussian states [5,6]. The only known measure that is monogamous in all dimensions is the squashed entanglement [10,55]. Other entanglement measures, such as the entanglement of formation, do not satisfy the monogamy relation [3]. There is no known *a priori* rule about whether a given entanglement measure is monogamous or not. It is natural to ask whether a given measure for general quantum correlations is monogamous. Certain measures of general quantum correlations, such as quantum discord, were shown to violate monogamy by finding explicit examples of states for which the inequality (1) does not hold [56–61]. Those examples, however, do not exclude the possibility that other measures of quantum correlations, akin to the quantum discord, could exist that do satisfy a monogamy inequality.

In this Letter we address the issue of whether monogamy, in general, can extend to general quantum correlations beyond entanglement. Quantitatively, this question can be formulated as follows: Does there exist a measure of correlations $\mathcal{Q}$ that obeys the monogamy relation (1) and is nonzero on a separable state? We will put this question to rest by proving that all measures for quantum correlations beyond entanglement (i.e., that are nonvanishing on at least some separable state) and that respect some basic properties are not monogamous in general. These basic properties of the correlation measure $\mathcal{Q}$ are the following:

(1) positivity, i.e.,

$$\mathcal{Q}^{A|B}(\rho_{AB}) \geq 0; \tag{2}$$

(2) invariance under local unitaries $U_A \otimes V_B$, i.e.,

$$\mathcal{Q}^{A|B}(\rho_{AB}) = \mathcal{Q}^{A|B}(U_A \otimes V_B \rho_{AB} U_A^\dagger \otimes V_B^\dagger); \tag{3}$$

(3) no increase upon attaching a local pure ancilla, i.e.,

$$\mathcal{Q}^{A|B}(\rho_{AB}) \geq \mathcal{Q}^{A|BC}(\rho_{AB} \otimes |0\rangle\langle 0|_C). \tag{4}$$

These properties are valid for several measures of correlations known in the literature, including all entanglement measures [18,19]. In particular, positivity and invariance under local unitaries are standard requirements [62]. For the quantum discord defined in Refs. [14,15], which is an asymmetric quantity, Eq. (4) can be verified by inspection and is valid independently of whether the ancilla is attached on the side where the measurement entering the definition of discord is to be performed or on the unmeasured side. In a more general scenario, quantum correlations can be defined as the minimal distance to the set of classically correlated states [23,38,39,41]. In this case, Eq. (4) follows from the fact that any "reasonable" distance does not change upon attaching an ancilla: $D(\rho,\sigma) = D(\rho \otimes |0\rangle\langle 0|, \sigma \otimes |0\rangle\langle 0|)$. The same arguments can be applied to measures that are defined via measurements on local subsystems [36]. Alternatively, quantum correlations may be investigated and quantified in terms of the minimal amount of entanglement necessarily created between the system and a measurement apparatus realizing a complete projective measurement [22,23,26,63]. Equation (4) also holds in this case, which can be seen solely using the properties of entanglement measures.

We are now in position to prove the following theorem.

Theorem 1. A measure of correlations $\mathcal{Q}$ that respects Eqs. (2)–(4), and is also monogamous according to (1) must vanish for all separable states.

Proof.— Consider a measure $\mathcal{Q}$ respecting the hypothesis and a generic separable state $\rho_{AC} = \sum_i p_i |\psi_i\rangle\langle\psi_i|_A \otimes |\phi_i\rangle\langle\phi_i|_C$. In the following, we will concentrate on a special extension of ρ_{AC}, defined as

$$\rho_{ABC} = \sum_i p_i |\psi_i\rangle\langle\psi_i|_A \otimes |i\rangle\langle i|_B \otimes |\phi_i\rangle\langle\phi_i|_C, \tag{5}$$

with orthogonal states $\{|i\rangle_B\}$. Observe that ρ_{ABC} has the same amount of correlations $\mathcal{Q}^{A|BC}$ as the state

$$\sigma_{ABC} = \sum_i p_i |\psi_i\rangle\langle\psi_i|_A \otimes |i\rangle\langle i|_B \otimes |0\rangle\langle 0|_C, \tag{6}$$

since both states are related by a local unitary on BC. On the other hand, Eq. (4) implies that σ_{ABC} does not have more correlations than the reduced state σ_{AB}. Taking these two observations together, we obtain $\mathcal{Q}^{A|B}(\sigma_{AB}) \geq \mathcal{Q}^{A|BC}(\rho_{ABC})$. Now, we invoke the monogamy relation for the state ρ_{ABC}, which leads us to the inequality

$$\mathcal{Q}^{A|B}(\sigma_{AB}) \geq \mathcal{Q}^{A|B}(\rho_{AB}) + \mathcal{Q}^{A|C}(\rho_{AC}). \tag{7}$$

The final ingredient in the proof is the fact that the two states ρ_{AB} and σ_{AB} are equal. From the positivity of the measure, it follows immediately that $\mathcal{Q}^{A|C}$ must vanish on the state ρ_{AC}. Since the latter is a generic separable state, $\mathcal{Q}$ must vanish on all separable states. ■

The power of Theorem 1 lies in its generality. Under very weak assumptions, it rules out the existence of monogamous correlations beyond entanglement. Note that the arguments used in the proof of Theorem 1 are strong enough to show that the violation of monogamy appears even in three-qubit systems. This can be seen starting from Eq. (5), with each subsystem being a qubit. The measure $\mathcal{Q}$ violates monogamy if it is nonzero on some separable two-qubit state of rank two. This is the case for quantum discord and any related measures of quantum correlations.

As we have argued below Eq. (4), the properties (2)–(4) are satisfied by all reasonable measures of quantum correlations known to the authors. However, in general, it cannot be excluded that the measure under study violates one of the properties given in Eqs. (2) and (3), or (4). Alternatively, we assume that some of these properties cannot be proven. In this situation, Theorem 1 does not tell us whether $\mathcal{Q}$ is monogamous or not. Then, it is still possible to show that a monogamous measure $\mathcal{Q}$ must be zero on all separable states if it remains finite for a fixed dimension of one subsystem, i.e., if

$$\mathcal{Q}^{A|B} \leq f(d_A) < \infty \tag{8}$$

for fixed d_A, and some function f. To see this, we use the fact that any separable state ρ_{AB} has a symmetric extension $\rho_{AB_1\cdots B_n}$ such that $\rho_{AB} = \rho_{AB_i}$ holds for all $1 \leq i \leq n$, where n is an arbitrary positive integer [64–67]. Equation (8) implies that the measure $\mathcal{Q}^{A|B_1\cdots B_n}(\rho_{AB_1\cdots B_n})$ is finite for all n, including the limit $n \to \infty$. On the other hand, if $\mathcal{Q}$ is monogamous, it has to fulfill the following inequality:

$$\mathcal{Q}^{A|B_1\cdots B_n}(\rho_{AB_1\cdots B_n}) \geq n\mathcal{Q}^{A|B}(\rho_{AB}). \tag{9}$$

However, if the measure $\mathcal{Q}$ is nonzero on the separable state ρ_{AB}, one can always choose some n which is large enough such that Eq. (9) is violated, and thus $\mathcal{Q}$ cannot be monogamous.

So far we have presented two different ways to show that a given measure of quantum correlations $\mathcal{Q}$ violates monogamy, namely, Theorem 1 and Eq. (8). At this stage, it is natural to ask whether these two results have the same power, i.e., whether they allow us to draw the same conclusions about the structure of a given measure $\mathcal{Q}$. As already noted above, the proof of Theorem 1 allows us to rule out monogamy even for the simplest case of three qubits, as long as the measure $\mathcal{Q}$ does not vanish on some separable state of two qubits having rank not larger than two. On the other hand, this argument does not apply to Eqs. (8) and (9). Indeed, if $\mathcal{Q}$ is nonzero on some separable two-qubit state ρ_{AB}, Eqs. (8) and (9) only allow the statement that the measure $\mathcal{Q}$ violates monogamy for some extension $\rho_{AB_1\ldots B_n}$. In particular, if $n > 2$, this result does not provide any insight about the monogamy of the measure for three-qubit states.

We move on to observe that monogamy [Eq. (1)], together with positivity [Eq. (2)], invariance under local unitary [Eq. (3)], and no increase under attaching a local ancilla [Eq. (4)] imply no increase under local operations. This is due to the fact that any quantum operation Λ admits a Stinespring dilation: $\Lambda[\rho_B] = \mathrm{Tr}_C(U_{BC}\rho_B \otimes |0\rangle\langle 0|_C U_{BC}^\dagger)$; i.e., any quantum operation can be seen as resulting from a unitary operation on a larger-dimensional Hilbert space. Thus, for $\mathcal{Q}$ respecting Eqs. (1)–(4), one finds

$$\begin{aligned}\mathcal{Q}^{A|B}(\rho_{AB}) &\geq \mathcal{Q}^{A|BC}(\rho_{AB} \otimes |0\rangle\langle 0|_C)\\ &= \mathcal{Q}^{A|BC}(U_{BC}\rho_{AB} \otimes |0\rangle\langle 0|_C U_{BC}^\dagger)\\ &\geq \mathcal{Q}^{A|B}(\mathrm{Tr}_C(U_{BC}\rho_{AB} \otimes |0\rangle\langle 0|_C U_{BC}^\dagger))\\ &\quad + \mathcal{Q}^{A|C}(\mathrm{Tr}_B(U_{BC}\rho_{AB} \otimes |0\rangle\langle 0|_C U_{BC}^\dagger))\\ &\geq \mathcal{Q}^{A|B}(\Lambda_B[\rho_{AB}]).\end{aligned} \tag{10}$$

No-increase under local operations [68], and thus, *a fortiori*, monogamy [the latter together with the almost trivial properties (2)–(4)] imply the following.

Theorem 2. A measure of correlations $\mathcal{Q}$ that is nonincreasing under operations on at least one side must be maximal on pure states; that is, for any ρ_{AB} on $\mathbb{C}^d \otimes \mathbb{C}^d$ there exists a pure state $|\psi\rangle\langle\psi|_{AB} \in \mathbb{C}^d \otimes \mathbb{C}^d$ such that $\mathcal{Q}^{A|B}(|\psi\rangle\langle\psi|_{AB}) \geq \mathcal{Q}^{A|B}(\rho_{AB})$.

Proof.—Immediate when one uses the fact that any state ρ_{AB} can be seen as the result of the application of a channel Λ_B (Λ_A) on any purification $|\psi\rangle_{AB}$ of ρ_A (ρ_B) (see, for example, [55]). Suppose that the measure $\mathcal{Q}$ is nonincreasing under quantum operations on A. Then:

$$\mathcal{Q}^{A|B}(|\psi\rangle\langle\psi|_{AB}) \geq \mathcal{Q}^{A|B}(\Lambda_A[|\psi\rangle\langle\psi|_{AB}]) = \mathcal{Q}^{A|B}(\rho_{AB}). \tag{11}$$

■

This simple theorem is relevant, in particular, for the case of symmetric measures of quantum correlations. Several such measures were proposed in Refs. [23,38,41]. Some of these measures have counterintuitive properties. In particular, in [23] it was shown that for the relative entropy of quantumness, there exist mixed states ρ_{AB} that have more quantum correlations than any pure state $|\psi\rangle_{AB}$. The theorem just proven can be interpreted as a signature of the fact that general quantum correlations can increase under local operations (and *a fortiori* as a signature of the lack of monogamy) [41].

Theorem 1 and the reasoning in its proof amount essentially to the following insight about the violation of monogamy: if there is a separable state ρ_{AB} with nonzero correlations $\mathcal{Q}$, then there exists a mixed state ρ_{ABC} which proves that the measure under scrutiny is not monogamous: $\mathcal{Q}^{A|BC}(\rho_{ABC}) < \mathcal{Q}^{A|B}(\rho_{AB}) + \mathcal{Q}^{A|C}(\rho_{AC})$. On the other hand, crucially, a measure of correlations can still respect monogamy when evaluated on pure states $\rho_{ABC} = |\psi\rangle\langle\psi|_{ABC}$. As will be demonstrated in the following, the geometric measure of discord has exactly this property for three qubits. Before we present this result, we recall the definition of this measure.

The geometric measure of discord D_G was defined in Ref. [39] as the minimal square Hilbert-Schmidt distance to the set of classical-quantum states (CQ):

$$D_G^{A|B}(\rho_{AB}) = \min_{\sigma_{AB}\in CQ} \|\rho_{AB} - \sigma_{AB}\|_2^2. \tag{12}$$

Here, we used the 2-norm, also known as Hilbert-Schmidt norm, $\|\rho - \sigma\|_2 = \sqrt{\mathrm{Tr}(\rho - \sigma)^2}$, and the minimum is taken over all classical-quantum states σ_{AB}. These are states which can be written as $\sigma_{AB} = \sum_i p_i |i\rangle\langle i|_A \otimes \sigma_B^i$ with some local orthogonal basis $\{|i\rangle_A\}$. The geometric discord has an operational interpretation in terms of the average fidelity of the remote state preparation protocol for two-qubit systems [69]. As noted above, the geometric measure of discord cannot be monogamous in general, since it is nonzero on some separable states. However, the following holds.

Theorem 3. The geometric measure of discord is monogamous for all pure states $|\psi\rangle_{ABC}$ of three qubits:

$$D_G^{A|BC}(|\psi\rangle\langle\psi|_{ABC}) \geq D_G^{A|B}(\rho_{AB}) + D_G^{A|C}(\rho_{AC}), \quad (13)$$

where $\rho_{AB} = \mathrm{Tr}_C(|\psi\rangle\langle\psi|_{ABC})$ and analogously for ρ_{AC}.

Proof.—We notice that for proving the inequality in Eq. (13), it is enough to show that for any pure state $|\psi\rangle_{ABC}$ there exists a classical-quantum state σ_{ABC} such that

$$D_G^{A|BC}(|\psi\rangle\langle\psi|_{ABC}) \geq \|\rho_{AB} - \sigma_{AB}\|_2^2 + \|\rho_{AC} - \sigma_{AC}\|_2^2. \quad (14)$$

This inequality then automatically implies inequality (13), as, due to the minimization in the geometric measure of discord, the right-hand side of (13) can only be smaller than or equal to the right-hand side of (14). In order to show the existence of the mentioned classical-quantum state σ_{ABC} we choose a specific parametrization for a pure state of three qubits [70]:

$$|\psi_{ABC}\rangle = \sqrt{p}|0\rangle_A(a|00\rangle_{BC} + \sqrt{1-a^2}|11\rangle_{BC}) + \sqrt{1-p}|1\rangle_A[\gamma(\sqrt{1-a^2}|00\rangle_{BC} - a|11\rangle_{BC}) + f|01\rangle_{BC} + g|10\rangle_{BC}]. \quad (15)$$

The real numbers p, a, and f range between 0 and 1, g is complex with $0 \leq f^2 + |g|^2 \leq 1$, and $\gamma = \sqrt{1 - f^2 - |g|^2}$ is also real.

We proceed by evaluating the left-hand side of Eq. (14), using the explicit formula for pure states [71,72]:

$$D_G^{A|BC}(|\psi\rangle\langle\psi|_{ABC}) = 2(1-p)p. \quad (16)$$

In the next step, we define the classical-quantum state $\sigma_{ABC} = \sum_{i=0}^{1} \Pi_A^i \rho_{ABC} \Pi_A^i$ with local projectors in the computational basis: $\Pi_A^i = |i\rangle\langle i|_A$. The evaluation of the right-hand side of Eq. (14) is straightforward:

$$\|\rho_{AB} - \sigma_{AB}\|_2^2 + \|\rho_{AC} - \sigma_{AC}\|_2^2 = 2c(1-p)p \quad (17)$$

with $c = 1 + [4a^2(1-a^2) - 1]\gamma^2$. The proof is complete, if we can show that c cannot be larger than 1. This can be seen by noting that the term $4a^2(1-a^2)$ is maximal for $a^2 = \frac{1}{2}$, which leads to the maximal possible value $c = 1$. ■

Even though quantum correlations beyond entanglement cannot be monogamous in general, Theorem 3 demonstrates that for pure states of three qubits, monogamy of the geometric measure of discord is still preserved. To the best of our knowledge, this is the first instance of a measure of quantum correlations beyond entanglement that satisfies a restricted monogamy inequality. Certainly, this is not a property that all measures of quantum correlations have in common: As shown, e.g., in Ref. [56], the original quantum discord violates monogamy even on some pure states of three qubits.

In conclusion, we have addressed the question of monogamy for quantum correlations beyond entanglement. Using very general arguments, we have proven that any measure of correlations which is nonzero on some separable state unavoidably violates monogamy. Furthermore, we have shown that any monogamous measure of quantum correlations must be maximal on pure states. These results imply severe constraints on any monogamous measure of quantum correlations, and can also be used to witness the violation of monogamy. Finally, we have shown that even though all measures of nonclassical correlations akin to quantum discord cannot be monogamous for all states, they still may obey monogamy in certain restricted situations. In particular, we proved that the geometric measure of discord is monogamous for all pure states of three qubits. It is an open question whether there exists a measure of general quantum correlations which is monogamous for tripartite pure states of arbitrary dimensions. Another open question, which points to a possible future research direction, arises from the generalization of quantum discord to theories which are more general than quantum [73]. We hope that the results presented in this Letter are also useful for this more general scenario. Thus, the answer to the question posed in the title is: General quantum correlations are, in general, not monogamous.

We thank Davide Girolami and Hermann Kampermann for discussions. M. P. acknowledges support by NSERC, CIFAR, Ontario Centres of Excellence. G. A. is supported by a Nottingham Early Career Research and Knowledge Transfer Award. M. P. and G. A. acknowledge joint support by the EPSRC Research Development Fund (Pump Priming Grant No. 0312/09). G. A. acknowledges ESF for sponsoring the workshop during which this work was started. D. B. and A. S. acknowledge financial support by DFG; A. S. was supported by ELES.

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(Streltsov *et al.*, 2012a) Phys. Rev. Lett. **109**, 050503.

Journal: Physical Review Letters
Impact Factor 2011: 7,37
Contribution: first author, scientific work and preparation of the manuscript, 60%

Quantum Cost for Sending Entanglement

Alexander Streltsov,* Hermann Kampermann, and Dagmar Bruß
Institut für Theoretische Physik III, Heinrich-Heine-Universität Düsseldorf, D-40225 Düsseldorf, Germany
(Received 20 March 2012; published 18 June 2012)

Establishing quantum entanglement between two distant parties is an essential step of many protocols in quantum information processing. One possibility for providing long-distance entanglement is to create an entangled composite state within a lab and then physically send one subsystem to a distant lab. However, is this the "cheapest" way? Here, we investigate the minimal "cost" that is necessary for establishing a certain amount of entanglement between two distant parties. We prove that this cost is intrinsically quantum, and is specified by quantum correlations. Our results provide an optimal protocol for entanglement distribution and show that quantum correlations are the essential resource for this task.

DOI: 10.1103/PhysRevLett.108.250501 PACS numbers: 03.67.Hk

Imagine that one wants to send a letter in the old-fashioned way. The postage cost that the sender has to invest depends on the amount of the transmitted substance, quantified by the weight of the letter. If the receiver had already provided some prepaid envelope, the sender may have to add an appropriate stamp if he or she wants to send a heavier letter. Naturally, the allowed weight of the letter is smaller or equal to a limit which is linked to the total postage.

Now, imagine that a sender wants to send quantum entanglement to a receiver. How does the cost that the sender has to invest depend on the amount of entanglement sent, quantified by some entanglement measure? Is this cost reduced when sender and receiver already shared some preestablished entanglement? And what is the nature of this cost—can one pay in classical quantities, or does one have to invest a quantum cost?

One might be tempted to consider these questions and their answers as obvious matters. However, quantum mechanics has often surprised us with puzzling features: counterintuitively, as shown in [1], separable states (i.e., states without entanglement) can be used to distribute entanglement. What is then the resource that makes this process possible and enables entanglement distribution without actually sending an entangled state?

In order to address this question in a well defined and quantitative way we will consider the following setting, see Fig. 1: the sender is called Alice (A), and the distant receiver Bob (B). Each of them has a quantum particle in his or her possession. In addition, they have a third quantum particle or ancilla (C) available, which is at the beginning located in Alice's lab, and then sent (via a noiseless quantum channel) to Bob's lab. This is a general model for any interaction: one can consider the particle C as the intermediate particle that realises the global interaction between A and B. A similar scenario was also considered in a different context in [2,3].

Initially, the total joint quantum state may or may not carry entanglement. In the following, we will be only interested in bipartite entanglement; i.e., two out of the three particles A, B, and C are grouped together. We quantify the initial entanglement between AC and B as $E^{AC|B}$, and the final entanglement, after sending C to Bob, as $E^{A|BC}$. As a quantifier of entanglement we will first use the relative entropy of entanglement, which is a well established and widely studied measure of entanglement for mixed states [4,5]. It is defined as the minimal relative entropy $S(\rho \parallel \sigma) = \mathrm{Tr}[\rho \log\rho] - \mathrm{Tr}[\rho \log\sigma]$ between the given state ρ^{XY} for two parties X and Y and the set of separable states $\mathcal{S}$:

$$E^{X|Y}(\rho^{XY}) = \min_{\sigma^{XY}\in\mathcal{S}} S(\rho^{XY} \parallel \sigma^{XY}). \quad (1)$$

Besides the fact that the relative entropy plays a crucial role in quantum information theory [6], the significance of

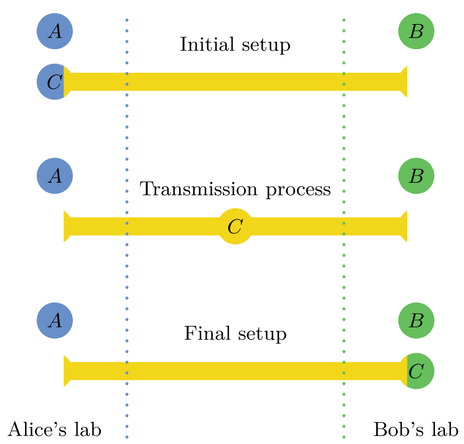

FIG. 1 (color online). Entanglement distribution between Alice and Bob. The upper figure shows the initial setup before the transmission: Alice holds the particles A and C, while Bob is in possession of the particle B. The middle figure shows the transmission process: Alice uses a quantum channel to send C to Bob. The final situation is shown in the lower figure. See also main text.

the relative entropy of entanglement is also provided by its close relation to the distillable entanglement [7].

In a naive approach to our original question, namely determining in a quantitative way the cost for sending a certain amount of entanglement, a natural conjecture would be the inequality $Q^{C|AB} \geq E^{A|BC} - E^{AC|B}$, where Q denotes a yet undefined kind of correlations. This inequality can be interpreted as follows: if initially Alice and Bob share some preestablished entanglement, quantified by $E^{AC|B}$, and wish to achieve final entanglement of $E^{A|BC}$ between them, the ancilla C, sent from Alice to Bob, needs to carry at least an amount of correlations given by the difference of final and initial entanglement. This inequality quantifies the intuition, that entanglement distribution does not come for free, but always requires to invest some correlations. In other words, $Q^{C|AB}$ could be interpreted as the "cost" for sending the entanglement $E^{A|BC} - E^{AC|B}$. Quite surprisingly, it is not the entanglement between C and AB, which plays a crucial role here: as was demonstrated in [1], all steps of the protocol can be successfully implemented without any entanglement between C and the rest of the system. In other words, if some inequality of the conjectured form exists, the quantity Q cannot be a measure of entanglement. However, does the fact that entanglement distribution is possible via separable states mean that the "cost" for this protocol is of classical nature? As we will show in the following, this is not the case: the cost for sending entanglement is of quantum nature.

Even separable states, which by definition can be prepared locally with the help of classical communication, can carry quantum properties; i.e., they can be quantum correlated. A composite quantum state is called strictly classically correlated if its correlations can be described by a joint probability distribution for classical variables of the subsystems [8]. If this is not the case, quantum correlations are manifest in the state. Recently, there has been much interest in characterising quantum correlations [9–15], in interpreting their occurrence in quantum information protocols [16–20], and in particular in determining their role in quantum algorithms [21–25], see also the feature article [26] and the comprehensive review [27]. In the following we will quantify the amount of quantum correlations according to the thermodynamical approach presented in [12,28]. There the authors provided the notion of the information deficit: it quantifies the amount of information which cannot be localised by classical communication between two parties. If only one-way classical communication from party X to party Y is allowed, this leads to the one-way information deficit:

$$\Delta^{X|Y}(\rho^{XY}) = \min_{\{\Pi_i^X\}} S\left(\rho^{XY} \,\|\, \sum_i \Pi_i^X \rho^{XY} \Pi_i^X\right), \qquad (2)$$

where the minimization is done over all local von Neumann measurements $\{\Pi_i^X\}$ on subsystem X.

We will show in the following that the measure defined in Eq. (2) quantifies the cost discussed above, thus revealing the fundamental role of quantum correlations as a resource for the distribution of entanglement:

$$\Delta^{C|AB} \geq E^{A|BC} - E^{AC|B}, \qquad (3)$$

where the entanglement measure $E^{X|Y}$ was defined in Eq. (1). This inequality is our central result; we will discuss its meaning and implications below. We point out that this inequality holds for any dimension of the three subsystems, see Fig. 2 for illustration. The main idea of the proof of Eq. (3) is sketched in Fig. 3. We name the state σ to be the closest separable state to ρ, i.e., $E^{AC|B}(\rho) = S(\rho \,\|\, \sigma)$. We then consider the local measurement $\{\Pi_i^C\}$ on particle C that minimizes the relative entropy of the resulting state ρ' with respect to the original ρ, i.e., $\rho' = \sum_i \Pi_i^C \rho \Pi_i^C$ such that $\Delta^{C|AB}(\rho) = S(\rho \,\|\, \rho')$. In Fig. 3 we also show the state $\sigma' = \sum_i \Pi_i^C \sigma \Pi_i^C$, which results from the application of the same measurement on the state σ. It is crucial to note that the three states ρ, ρ' and σ' lie on a straight line, as shown in Fig. 3:

$$S(\rho||\sigma') = S(\rho||\rho') + S(\rho'||\sigma'). \qquad (4)$$

For proving this equality it is enough to show the relations $\mathrm{Tr}[\rho \log \rho'] = \mathrm{Tr}[\rho' \log \rho']$ and $\mathrm{Tr}[\rho \log \sigma'] = \mathrm{Tr}[\rho' \log \sigma']$, then Eq. (4) immediately follows. These two equalities can be shown in a straight-forward way, by using the idempotent property of the projectors, the cyclic invariance of the trace, and the fact that the projectors Π_i^C sum up to the identity.

The final ingredient in the proof of Eq. (3) is the fact that the relative entropy does not increase under quantum operations [4,29,30]: $S(\Lambda(\rho) \,\|\, \Lambda(\sigma)) \leq S(\rho \,\|\, \sigma)$, and thus $S(\rho' \,\|\, \sigma') \leq S(\rho \,\|\, \sigma)$. Inserting this into Eq. (4) implies the inequality $S(\rho \,\|\, \sigma') \leq \Delta^{C|AB}(\rho) + E^{AC|B}(\rho)$. To complete the proof of Eq. (3), we notice that the state σ' is a tripartite fully separable state, and thus gives an upper bound on the entanglement $E^{A|BC}(\rho) \leq S(\rho \,\|\, \sigma')$.

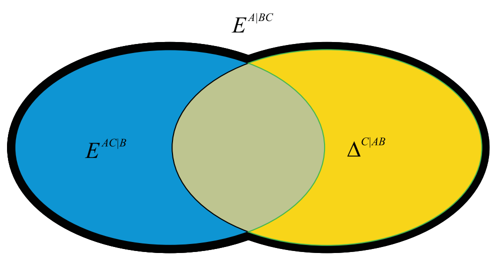

FIG. 2 (color online). Illustration of the main result: The size of the left area represents the entanglement between AC and B, while the size of the right area represents the quantum correlations between C and AB. The total area, enclosed by the black curve, represents the entanglement between A and BC. One can read off the main result: $E^{A|BC} \leq E^{AC|B} + \Delta^{C|AB}$.

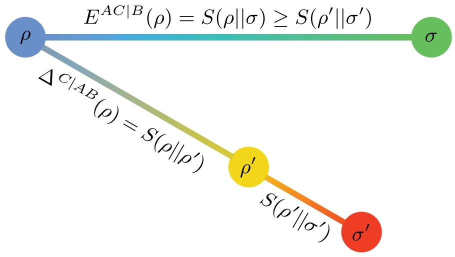

FIG. 3 (color online). Proof of the main result in Eq. (3): The separable state σ is the closest separable state to the given state ρ. The measured state $\rho' = \sum_i \Pi_i^C \rho \Pi_i^C$ is defined such that $\Delta^{C|AB}(\rho) = S(\rho||\rho')$. Application of the same measurement on σ gives the state $\sigma' = \sum_i \Pi_i^C \sigma \Pi_i^C$. The states ρ, ρ', and σ' lie on a straight line; for details see main text.

The techniques presented above can also be applied to a more general measure of entanglement, where the relative entropy $S(\rho_1 \parallel \rho_2)$ is replaced—both for the entanglement measure and the quantum correlation measure—by a general distance $D(\rho_1, \rho_2)$. We only demand that D has the following two properties: (1) D does not increase under any quantum operation, (2) D satisfies the triangle inequality. Then Eq. (4) becomes an inequality: $D(\rho, \sigma') \leq D(\rho, \rho') + D(\rho', \sigma')$, and the proof of Eq. (3) follows from the same arguments as above. Well-known and frequently used examples for distances that fulfil these two properties [31] are, e.g., the trace distance, defined as $D_t(\rho_1, \rho_2) = \frac{1}{2}\,\mathrm{tr}|\rho_1 - \rho_2|$ and the Bures distance [32], defined as $D_B(\rho_1, \rho_2) = 2(1 - \sqrt{F(\rho_1, \rho_2)})$, with $F(\rho_1, \rho_2) = (\mathrm{tr}\sqrt{\sqrt{\rho_1}\rho_2\sqrt{\rho_1}})^2$.

Let us point out that our main result in inequality (3) can be alternatively seen as a restricting link between the correlation properties of the three possible bipartite splits of a tripartite quantum state in any dimension: the entanglement across one of the bipartite splits cannot be larger than the sum of the entanglement across one of the other splits plus the quantum correlations across the remaining split. Thus, the inequality (3) may be interpreted as a type of "monogamy" relation between three entangled parties. This inequality also holds for all permutations of the parties. By permuting the systems A and B in Eq. (3), we obtain the generally valid inequality

$$E^{AC|B} - \Delta^{C|AB} \leq E^{A|BC} \leq E^{AC|B} + \Delta^{C|AB}. \quad (5)$$

This inequality tells us, that the entanglement between A and BC is not independent from the entanglement between AC and B. In particular, in the case of vanishing quantum correlations, i.e. $\Delta^{C|AB} = 0$, we immediately see that these two quantities are equal: $E^{A|BC} = E^{AC|B}$. We also note that for those situations, where $\Delta^{C|AB} = E^{C|AB}$, this happens, e.g., for the relative entropy when the state under consideration is pure, one arrives, using all permutations of inequality (3), at the triangle inequality $|E^{B|AC} - E^{C|AB}| \leq E^{A|BC} \leq E^{B|AC} + E^{C|AB}$. However, we stress again that this symmetric inequality is a special case of the general inequality (5), and is valid only for certain classes of states.

We are now in position to answer the question posed in the first paragraph of this paper: what is the cheapest way for distributing entanglement? In order to answer this question in full generality, we consider the most general distribution protocol, which may contain n uses of the quantum channel together with local operations and classical communication between Alice and Bob. The amount of entanglement sent in this process of entanglement growing cannot be larger than the total cost in the protocol:

$$E_{\mathrm{final}} - E_{\mathrm{initial}} \leq \sum_{i=1}^{n} \Delta_i, \quad (6)$$

where E_{initial} and E_{final} is the amount of entanglement between Alice and Bob before and after the protocol, and Δ_i is the amount of quantum correlations between the sent particle and the remaining system in the ith application of the quantum channel.

In order to prove Eq. (6), we first consider a protocol where the quantum channel is used once from Alice to Bob and once in the other direction, i.e., $n = 2$. Suppose that Alice and Bob start with a state ρ_1, the initial entanglement is $E_{\mathrm{initial}} = E^{AC|B}(\rho_1)$. After sending the particle C to Bob the entanglement between the two parties is given by $E^{A|BC}(\rho_1)$, and the cost for this process is given by $\Delta^{C|AB}(\rho_1)$. Now Alice and Bob locally act on their subsystems, and may additionally communicate classically with each other, thus arriving at the final state ρ_2 with the entanglement $E^{A|BC}(\rho_2)$. In the final step of this single-round protocol Bob sends the particle C back to Alice, and the final entanglement is $E_{\mathrm{final}} = E^{AC|B}(\rho_2)$. The corresponding cost for this final step is given by $\Delta^{C|AB}(\rho_2)$. We will now show that the amount of entanglement sent in the total process cannot be larger than the total cost:

$$E_{\mathrm{final}} - E_{\mathrm{initial}} \leq \Delta^{C|AB}(\rho_1) + \Delta^{C|AB}(\rho_2). \quad (7)$$

This inequality can be seen by applying inequality (3) to the two states ρ_1 and ρ_2 independently, and considering the sum of the both inequalities: $E^{AC|B}(\rho_2) - E^{A|BC}(\rho_2) + E^{A|BC}(\rho_1) - E^{AC|B}(\rho_1) \leq \Delta^{C|AB}(\rho_2) + \Delta^{C|AB}(\rho_1)$. Note that the entanglement $E^{A|BC}(\rho_2)$ is not larger than $E^{A|BC}(\rho_1)$, since the state ρ_2 results from the state ρ_1 after application of local operations and classical communication. This proves the desired inequality (7). To prove the general expression in Eq. (6), we now suppose that the quantum channel is used n times, where n can be even or odd. We can define the states $\rho_1, \ldots, \rho_n$ in an analogous way as above. Using the same argumentation we arrive at Eq. (6).

The result in Eq. (6) can now be used to find the most "economic" way to distribute entanglement. If Alice and

Bob are told to send a fixed amount of entanglement $E = E_{\text{final}} - E_{\text{initial}}$, they can achieve this in the most economic way by choosing a protocol such that the inequality (6) becomes an equality. One possibility to achieve this is the well-known "trivial" one: Alice locally prepares a pure state $|\psi\rangle^{AC}$ with entanglement $E = E^{A|C}$, and sends the particle C to Bob. However, this is not the only possibility: the inequality (6) can also be satisfied without sending entanglement, see the example below. If one considers entanglement to be an expensive resource, one may thus be able to distribute entanglement in a "cheaper" way by sending quantum correlations without entanglement.

The results presented in this Letter provide new powerful tools to understand and quantify entanglement as well as quantum correlations. In this paragraph we 1will demonstrate how Eq. (3) can be used to evaluate the entanglement and the one-way information deficit in the specific state η, which was used in [1] to show that entanglement distribution with separable states is possible:

$$\eta = \frac{1}{3}|\Psi_{\text{GHZ}}\rangle\langle\Psi_{\text{GHZ}}| + \sum_{i,j,k=0}^{1} \beta_{ijk}\Pi_{ijk} \tag{8}$$

with $|\Psi_{\text{GHZ}}\rangle = \frac{1}{\sqrt{2}}(|000\rangle + |111\rangle)$, $\Pi_{ijk} = |ijk\rangle\langle ijk|$, and all β's are zero apart from $\beta_{001} = \beta_{010} = \beta_{101} = \beta_{110} = \frac{1}{6}$. It was shown in [1] that the entanglement is zero between two different cuts: $E^{AC|B} = E^{AB|C} = 0$. As an application of Eq. (3) we will now prove that the remaining two quantities are equal: $E^{A|BC}(\eta) = \Delta^{C|AB}(\eta) = \frac{1}{3}$. This can be seen by considering the relative entropy between η and the state $\eta' = \sum_i \Pi_i^C \eta \Pi_i^C$ with orthogonal projectors $\Pi_i^C = |i\rangle\langle i|^C$ in the computational basis. It can be verified by inspection that $S(\eta \| \eta') = \frac{1}{3}$, and thus $\Delta^{C|AB}(\eta)$ is not larger than $\frac{1}{3}$. On the other hand, the entanglement $E^{A|BC}(\eta)$ is bounded from below by $\frac{1}{3}$. This follows from the two facts that the state η can be used to distil Bell states with probability $\frac{1}{3}$ [1], and that the relative entropy of entanglement is not smaller than the distillable entanglement [7]. In this example, quantum correlations provide the most economic and cheapest resource for entanglement distribution.

In conclusion, we have identified quantum correlations as the key resource for entanglement distribution. They quantify the quantum cost that one has to invest for increasing the entanglement between two distant parties. Explicitly, we proved that the entanglement between two parties cannot grow more than the amount of quantum correlations which the particle carries that mediates the interaction between the two parties. Our result is completely general and is valid regardless of the particular realization of the protocol. Thus it provides a fundamental connection between quantum entanglement on one side and quantum correlations on the other side. Since the study of quantum correlations is believed to be important for understanding the power of quantum computers, our results may find applications far beyond the scope of this work.

We thank Otfried Gühne for helpful discussions. A. S. thanks Kavan Modi, Hugo Cable and Vlatko Vedral for organizing the Quantum Discord Workshop in Singapore, where he had enlightening discussions with Gerardo Adesso, Wojciech H. Zurek, and Animesh Datta. We acknowledge financial support from Deutsche Forschungsgemeinschaft (DFG) and ELES.

Note added.— During the completion of this work we became aware of independent related work by T. K. Chuan *et al.* in [33]. There, the authors derive similar results, and also provide alternative examples for entanglement distribution with separable states.

*streltsov@thphy.uni-duesseldorf.de

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(Streltsov *et al.*, 2012b) Phys. Rev. Lett. **108**, 250501.

Journal: Physical Review Letters
Impact Factor 2011: 7,37
Contribution: first author, scientific work and preparation of the manuscript, 90%

Ich versichere an Eides statt, dass die Dissertation von mir selbständig und ohne unzulässige fremde Hilfe unter Beachtung der “Grundsätze zur Sicherung guter wissenschaftlicher Praxis an der Heinrich-Heine-Universität Düsseldorf” erstellt worden ist.

Düsseldorf, den 31. Januar 2013

(Alexander Streltsov)

Hiermit erkläre ich, dass ich die Dissertation keiner anderen Fakultät bereits vorgelegt habe und keinerlei vorherige erfolglose Promotionsversuche vorliegen.

Düsseldorf, den 31. Januar 2013

(Alexander Streltsov)