Entanglement properties of composite quantum systems

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We present here an overview of our work concerning entanglement properties of composite quantum systems. The characterization of entanglement, i.e. the possibility to assert if a given quantum state is entangled with others and how much entangled it is, remains one of the most fundamental open questions in quantum information theory. We discuss our recent results related to the problem of separability and distillability for distinguishable particles, employing the tool of witness operators. Finally, we also state our results concerning quantum correlations for indistinguishable particles.

I. INTRODUCTION

The processing of quantum information differs in a fundamental way from the processing of classical information: rather than allowing only boolean values “0” and “1” for a bit, a quantum bit or qubit is implemented by the quantum state of a two-level system, which can be in any superposition of “|0⟩” and “|1⟩”, namely |ψ⟩ = α|0⟩ + β|1⟩. If several quantum states are involved, rather than dealing only with one string of bit values, e.g., “001011”, the state of the composite system of qubits can be in a superposition of such strings, e.g., |Ψ⟩ = a|001011⟩ + b|110100⟩ + c|010010⟩ + .... In general such a state cannot be written as a tensor product of states of its subsystems and, therefore, it is called entangled.

Entanglement is a key feature for most of the protocols used in quantum information such as, e.g., quantum teleportation, quantum cryptography, superdense coding, quantum algorithms and quantum error correction. Indeed the resources needed to implement a particular protocol of quantum information are closely linked to the entanglement properties of the states used in the protocol. Therefore, it is highly desirable to characterize the entanglement properties of quantum systems bearing in mind that this is a fundamental open problem of quantum theory but also that it is essential for the implementation of any possible task that relies on quantum bits.

In this manuscript we summarize our efforts in striving at some understanding of the properties of entanglement for composite quantum systems of distinguishable and indistinguishable particles. In the former case, one assumes that the involved quantum systems can be addressed separately. This happens either because the subsystems are located at different places so that their wavefunctions do not spatially overlap, or because they differ in some degrees of freedom permitting thus to distinguish them. Until quite recently, this has been the most common approach considered in the framework of quantum information. However, the experimental progress in achieving quantum bits and quantum gates by means of solid state physics (quantum dots) and optical microtraps with neutral atoms, demands a new formalism which includes the statistical nature of the particles involved. In the last part of this manuscript we address this question.

In the frame of the DFG-Schwerpunkt on “Quanteninformationsverarbeitung” (quantum information processing) we have addressed these subjects in two different projects. The manuscript aims to give a comprehensive summary of our results for a reader familiar with the subject of separability and distillability. This summary, however, is by no means exhaustive. Important contributions to the above projects concerning entanglement measures, catalysis of entanglement and quantum game theory are presented elsewhere [1].

The manuscript is organized as follows: Sections II-IV deal with the characterization of entanglement of composite quantum systems of distinguishable particles. In section II we first briefly state the problem of separability, i.e., the question when the state of a composite quantum system does not contain any quantum correlations or entanglement, and then report our results concerning this question. In section III we address the problem of distillability, i.e., the question when the state of a mixed composite quantum system can be transformed to a maximally entangled pure state by using local operations and classical communication. We report thereafter our progress concerning this subject. Section IV deals with witness operators. We state our achievements in constructing, optimizing and implementing witness operators to detect entanglement. Also, a connection between a witness detecting a given state and the distillability and activability properties of the state is presented there. Finally, in section V we address the study of quantum correlations in composite systems of identical particles and apply some of the formalisms previously developed for distinguishable particles to indistinguishable ones.
II. SEPARABILITY OF COMPOSITE QUANTUM SYSTEMS

In this section, before presenting our results, we define the problem of separability versus entanglement for a given quantum system. The reader interested in a tutorial description of the subject is addressed to references [2] and [3].

For simplicity, let us restrict ourselves here to the simplest case of composite systems: bipartite systems (traditionally denoted as Alice and Bob) of finite, but otherwise arbitrary dimensions. Physical states of such systems are, in general, mixed and are described by density matrices, i.e. hermitian, positive semi-definite linear operators of trace one (i.e. $\rho = \rho^\dagger$, $\rho \geq 0$, $\text{Tr}\rho = 1$), acting in the Hilbert space of the composite system $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$. Without losing generality we will assume that $\text{dim}\mathcal{H}_A = M \geq 2$ and $\text{dim}\mathcal{H}_B = N \geq M$.

Before proceeding further we introduce here some definitions that we will use throughout the paper. Given a density matrix $\rho$, we denote its kernel by $K(\rho) = \{ |\phi\rangle : \rho |\phi\rangle = 0 \}$, its range by $R(\rho) = \{ |\phi\rangle : \exists |\psi\rangle \}$, and its rank by $r(\rho) = \text{dim} R(\rho) = NM - \text{dim} K(\rho)$. Also the notion of partial transposition will be used throughout. The operation of partial transposition of a density matrix $\rho$ means the transposition with respect to only one of the subsystems. If we express $\rho$ in Alice’s and Bob’s orthonormal product basis,

$$\rho = \sum_{i,j=1}^{M} \sum_{k,l=1}^{N} \langle i,k | \rho | j,l \rangle | i,k \rangle \langle j,l | = \sum_{i,j=1}^{M} \sum_{k,l=1}^{N} \langle i,k | \rho | j,l \rangle | i \rangle_A \langle j | \otimes | k \rangle_B \langle l |,$$

(1)

then, the partial transposition with respect to Alice’s system is given by:

$$\rho_T^A = \sum_{i,j=1}^{M} \sum_{k,l=1}^{N} \langle i,k | \rho | j,l \rangle | i \rangle_A \langle j \otimes | k \rangle_B \langle l |.$$

(2)

Note that $\rho_T^A$ is basis-dependent, but its spectrum is not. For the partial transpose $\rho_T^A$ it might hold that $\rho_T^A \geq 0$, but this does not have to be true! As $(\rho_T^A)_T^B = \rho_T$, and as $\rho_T \geq 0$ always holds, positivity of $\rho_T^A$ implies positivity of $\rho_T^B$ and vice versa. A density matrix $\rho$ that fulfills $\rho_T^A \geq 0$ is termed PPT state for positive partial transpose, otherwise it is called NPPT state for non-positive partial transpose.

A. The separability problem

An essential step towards the understanding of entanglement is to first identify separable states, i.e., states that contain classical correlations only or no correlations at all. The mathematical definition of such states (separable states) in terms on convex combinations of product states was given by Werner in [4].

Def. 1 A given state $\rho$ is separable iff

$$\rho = \sum_{i=1}^{k} p_i \rho_i^A \otimes \rho_i^B,$$

(3)

where $\sum_i p_i = 1$, and $p_i \geq 0$.

Notice that the above definition states that a separable state can be prepared by Alice and Bob by means of local operations (unitary operations, measurements, etc.) and classical communication (LOCC). However, the question whether a given state can be decomposed as a convex sum of product states like in eq. (3) is by no means trivial – in fact there are no algorithms to check if such a decomposition for a given state $\rho$ exist.

An entangled state is defined via the negation of the above definition. A given state $\rho$ is entangled iff it cannot be decomposed as in Equation (3). Thus, the separability versus entanglement problem can be formulated as: Given a composite quantum state described by $\rho$, can it be decomposed as a convex combination of product states or not?

A major step in the answer of this problem and in the characterization of separability was done by Peres [5] and the Horodecki family [6] by providing a necessary condition for separability: the positivity of the partial transposition. Their results can be summarized in the following theorem:

Theorem 1 If a density matrix $\rho$ is separable then $\rho_T^A \geq 0$. If $\rho_T^A \geq 0$ in Hilbert spaces of dimensions $2 \times 2$ or $2 \times 3$ then $\rho$ is separable.

Notice that being PPT does not imply separability, except for low dimensional Hilbert spaces! Let us mention here, that also in [6], the problem of separability was rigorously reformulated in terms of the theory of positive maps. We will discuss about positive and completely positive maps in the forthcoming sections.
B. Results on the separability problem

An important tool for studying the properties of states with respect to their separability is the method of subtracting projectors onto product vectors from the given state. This method was developed in [7] and [8]: if there exists a product vector $|e, f\rangle \in R(\rho)$, the projector onto this vector (multiplied by some coefficient $\lambda > 0$) can be subtracted from $\rho$, such that the remainder is positive definite. A similar technique can be used for PPT states $\rho$: if there exists a product vector $|e, f\rangle \in R(\rho)$, such that $|e^*, f\rangle \in R(\rho^{T_A})$, the projector onto this vector (again multiplied by some $\lambda > 0$) can be subtracted from $\rho$, such that the remainder is positive definite and PPT. This observation allows to construct decompositions of a given $\rho$ of the form

$$\rho = \lambda \sigma + (1 - \lambda) \delta,$$

where $\sigma$ is separable, while $\delta$ is a so-called edge state, i.e. a state from which “nothing else” can be subtracted. In the case of decompositions for general entangled states, $\delta$ has no product vectors in the range. In the case of decompositions for PPT states $\delta$ can be taken as PPT edge state, i.e. a state that does not contain any product vector $|e, f\rangle \in R(\rho)$, such that $|e^*, f\rangle \in R(\rho^{T_A})$. The decompositions (4) can be optimized, by demanding $\lambda$ to be maximal [7]. Such an optimal decomposition is illustrated in Figure 1. For separable states an important question (related to the optimization of the detection of entangled states [9]) concerns minimal decompositions, i.e. those containing minimal number of projectors on product vectors. In particular in Ref. [8] it has been shown that in $2 \times 2$ systems the minimal decomposition of separable states contains a number of projectors which is equal to the rank of the state. Minimal decompositions can also be considered in the form of pseudo-mixtures, where not all coefficients multiplying the projectors entering the decomposition are positive, see section IVB.

![Figure 1](image.png)

**FIG. 1.** Illustration of the decomposition of $\rho$ into a separable state $\sigma$ and an edge state $\delta$: $\rho = \lambda \sigma + (1 - \lambda) \delta$

In the following we list the major results obtained by applying the decompositions (4) and constructing edge states in various systems, which has become a basic tool of the so-called Innsbruck-Hannover programme [10].

General properties of optimal separable approximations (decompositions) have been studied in Ref. [11] for the states $\rho$ of bipartite quantum systems of arbitrary dimensions $M \times N$. For two qubit systems ($M=N=2$) the best separable approximation has a form of a mixture of a separable state and a projector onto a pure entangled state. We have formulated the necessary condition that the pure state in the best separable approximation is not maximally entangled. This result allowed Wellens and Kuś [12] to obtain an analytic form of the optimal decomposition in the $2 \times 2$ case and to relate the value of $\lambda$ to the Wootters’ concurrence [13]. We have demonstrated that the weight of the entangled state in the best separable approximation in arbitrary dimensions provides a good entanglement measure. We have proven that in general, for arbitrary $M$ and $N$, the best separable approximation corresponds to a mixture of a separable and an entangled state which are both unique. We have developed also a theory of optimal separable approximations for states with positive partial transpose, and discussed procedures of constructing such decompositions.

The decomposition techniques and investigations of edge states have then be applied to $2 \times N$ systems in [14] and [15]. We have analyzed the separability properties of PPT density operators supported on $C^2 \otimes C^N$. We have shown that if $r(\rho) = N$, then it is separable, and that bound entangled states have rank larger than $N$. We have also solved the separability problem for low rank states: we have given a separability criterion for a generic density operator such that the sum of its rank and the one of its partial transpose does not exceed $3N$. If it exceeds this number we show that one can subtract projectors onto product vectors until decreasing it to $3N$, while keeping the positivity of $\rho$ and its partial transpose. This automatically gives us a sufficient criterion for separability for general density...
operators. We also prove that all density operators that remain invariant (or, more generally close to being invariant) after partial transposition with respect to the first system are separable. Finally, in Ref. [14] we have also presented a simple elementary proof of the Peres-Horodecki separability criterion in $2 \times 2$-dimensional systems.

The results for $2 \times N$ systems were then generalized to $M \times N$ systems [16], where we have also been able to solve the separability problem for low rank states. We have considered low rank density operators $\varrho$ supported on a $M \times N$ Hilbert space for arbitrary $M \leq N$ and with a positive partial transpose $\varrho^{T_A} \geq 0$. For rank $r(\varrho) \leq N$ we have proven that having a PPT is necessary and sufficient for $\varrho$ to be separable; in this case we have also provided its minimal decomposition in terms of pure product states. It follows from this result that there are no bound entangled states of rank 3 having a PPT. We have also presented a necessary and sufficient condition for the separability of generic density matrices for which the sum of the ranks of $\varrho$ and $\varrho^{T_A}$ satisfies $r(\varrho) + r(\varrho^{T_A}) \leq 2MN - M - N + 2$. This separability condition has the form of a constructive check, providing thus also a pure product state decomposition for separable states, and it works in those cases where a system of coupled polynomial equations has a finite number of solutions, as expected in the generic case.

The same research programme can also be applied to $2 \times 2 \times N$ systems [17]. We have investigated separability and entanglement of mixed states in $C^2 \otimes C^2 \otimes C^N$ three-party quantum systems. We have shown that all states $\varrho$ with positive partial transposes that have rank $r(\varrho) \leq N$ are separable. For the three-qubit case ($N=2$) we have proven that all PPT states $\varrho$ that have positive partial transposes and rank $r(\varrho) = 3$ are separable. We provided also constructive separability checks for the states $\varrho$ that have the sum of the rank of $\varrho$ and the ranks of partial transposes with respect to all subsystems smaller than $15N-1$.

We have studied also the problem of separability and entanglement properties of completely positive maps acting on operators acting in the composite Hilbert space of Alice and Bob [18,19]. We have studied when a physical operation can produce entanglement between two systems that are initially disentangled. The formalism that we have developed allows to show that one can perform certain non-local operations with unit probability by performing local measurements on states that are very weakly entangled. This formalism is a generalization of the Jamiołkowski isomorphism, that connect maps with operators, to the case of maps acting on tensor product spaces. We have associated with every completely positive map (CPM) acting on states of Alice and Bob, an operator acting on two copies of Alice’s and Bob’s space. The isomorphism connects separable CPMs with separable states, PPT CPMs with PPT entangled states, and so on. It provides a powerful tool to classify CP maps, using results known for states.

Last, but not least, we have applied our methods and techniques to study states in infinite-dimensional Hilbert spaces, i.e. continuous variable states. A particularly important class of such states, that is very frequently used in experiments with photons, is formed by the so-called Gaussian states. Gaussian states can be defined by the requirement that their associated Wigner function has a Gaussian form. We have been able to solve the separability problem of Gaussian states for two parties each having an arbitrary number of photon (harmonic oscillator) modes ([20], for a review see [21]), and for three parties each having one harmonic mode [22]. For bipartite systems of arbitrarily many modes the necessary and sufficient condition consists in an iterative transformation of the correlation matrix of a given state and provides an operational criterion, since it can be checked by a simple computation with arbitrary accuracy. Moreover, it allows us to find a pure product-state decomposition of any given separable Gaussian state. Our criterion is independent of the one based on partial transposition, and obviously, since it detects all entangled states, it is strictly stronger than the PPT criterion. We have also derived a necessary and sufficient condition for the separability of tripartite three mode Gaussian states, that is easy to check for any such state. We have given a classification of the separability properties of those systems and have shown how to determine for any state to which class it belongs. We have also shown that there exist genuinely tripartite bound entangled states (see III) and have pointed out how to construct and prepare such states.

III. THE DISTILLABILITY PROBLEM

For many applications in quantum information processing one needs a maximally entangled state of two parties, i.e. a state in $M \times N$ dimensions of the form

$$| \Psi_{\text{max}} \rangle = \frac{1}{\sqrt{M}} \sum_{i=1}^{M} |i, i\rangle .$$

(5)

However, even if an experimental source that creates such a state is available, during storage or transmission along a noisy channel the state will interact with the environment and evolve into a mixed state, thus loosing the property of being maximally entangled.
The idea of distillation and purification, i.e., enhancement of the entanglement of a given mixed state by local operations and classical communication (LOCC) was proposed by Bennett et al. [23], Deutsch et al. [24] and Gisin [25]. Again, for Hilbert spaces of composite systems with dimension lower or equal to 6, any mixed entangled state can always be distilled to a pure maximally entangled state. Since for such systems entanglement is equivalent to non-positivity of the partial transpose, we conclude that for systems in $2 \times 2$ and $2 \times 3$ dimensions all NPPT states are distillable [26]. It was shown by the Horodecki family [27] that the PPT property implies undistillability. Somehow surprisingly, in higher dimensions there exist states that are entangled but cannot be distilled. These states, namely PPT entangled states, are called bound entangled states, contrary to free entangled states which can be distilled. In general, the distillability problem can be formulated as: Given a composite quantum state described by $\rho$, is it distillable or undistillable?

The problem of distillability can be rigorously formulated [27] so that it reduces to the following theorem:

**Theorem 2** $\rho$ is distillable iff there exists a state $|\psi\rangle$ from a $2 \times 2$-dimensional subspace, $|\psi\rangle = a|e_1\rangle|f_1\rangle + b|e_2\rangle|f_2\rangle$, such that

$$\langle \psi | (\rho^T_A) \otimes K | \psi \rangle < 0$$

for some $K$.

### A. Results on the distillability problem

As mentioned above, in finite dimensions there exist so-called *bound entangled* states, which are entangled, but their entanglement cannot be distilled. One possibility of the construction of such states was given in [28]. There we have presented a family of bound entangled states in $3 \times 3$ dimensions. Their density matrix depends on 7 independent parameters and has 4 different non-vanishing eigenvalues. This construction can e.g. be useful when testing whether some new entanglement criterion detects bound entanglement.

Apart from several examples for bound entangled states with positive partial transpose we have some evidence that also bound entanglement, i.e., entanglement that cannot be distilled, of states with non-positive partial transpose exists: in [29] we study the distillability of a certain class of bipartite density operators which can be obtained via depolarization starting from an arbitrary one. This class is a one-parameter family of states that consist of a weighted sum of projectors onto the symmetric and the antisymmetric subspace. Our results suggest that non-positivity of the partial transpose of a density operator is not a sufficient condition for distillability, when the dimension of both subsystems is higher than two. This conjecture has been found independently in [30], and is still an open problem.

The present understanding of the decomposition of mixed states into separable, undistillable entangled and distillable entangled states is shown in figure 2.

![FIG. 2. Schematic representation of the set of all states, decomposed into the various subsets explained in the text](image)

We have also addressed the distillability and bound entanglement question in the contexts of infinite dimensional Hilbert spaces [31]. We have introduced and analyzed the definition of generic bound entanglement for the case of continuous variables. We have provided some examples of bound entangled states for that case, and discussed their physical sense in the context of quantum optics. We have raised the question of whether the entanglement of these states is generic. As a byproduct, we have obtained a new many-parameter family of bound entangled states.
with positive partial transpose in Hilbert spaces of arbitrary finite dimension. We have also pointed out that the “entanglement witnesses” (see section IV) and positive maps revealing the corresponding bound entanglement can be easily constructed.

Furthermore, we have studied how rare separable and non-distillable states of continuous variables [18] are. In finite dimensional Hilbert spaces, we have earlier demonstrated that the volumes of the set of separable states and PPT entangled states are both non-zero, and that there exists a vicinity of the identity operator that contains separable states only [32]. This turned out not to be the case for continuous variable systems. Also we have proven that the set of non–distillable continuous variable states is nowhere dense in the set of all states, i.e., the states of infinite–dimensional bipartite systems are generically distillable. This automatically implies that the sets of separable states, entangled states with positive partial transpose, and bound entangled states are also nowhere dense in the set of all states. All these properties significantly distinguish quantum continuous variable systems from the spin like ones. The aspects of the definition of bound entanglement for continuous variables has also been analyzed in the context of the theory of Schmidt numbers. In particular, the main result was generalized to the set of states of arbitrary Schmidt number and to the single copy regime.

IV. WITNESS OPERATORS FOR THE DETECTION OF ENTANGLEMENT

A. Definition and geometrical interpretation of witness operators

A very useful tool to detect entanglement is the so-called entanglement witness. An entanglement witness is an observable \( W \) which reveals the entanglement (if any) of a given state \( \rho \). This concept, which was introduced and studied in [6,33], reformulates the problem of separability in terms of witness operators:

**Theorem 3** A density matrix \( \rho \) is entangled iff there exists a Hermitian operator \( W \) with \( \text{Tr}(W\rho) < 0 \) and \( \text{Tr}(W\sigma) \geq 0 \) for any separable state \( \sigma \).

We say that the witness \( W \) “detects” the entanglement of \( \rho \). The existence of entanglement witnesses is just a consequence of the Hahn-Banach theorem, that states: *Let \( S \) be a convex, compact set, and let \( \rho \notin S \). Then there exists a hyper-plane that separates \( \rho \) from \( S \).*

Figure 3 illustrates the concept of an entanglement witness \( W \), represented by a hyper–plane (dashed line) that separates the state \( \rho \) from the convex compact set \( S \). We have also depicted in the figure, a optimal entanglement witness \( W_{\text{opt}} \) (represented by straight line) together with other optimal witnesses. Optimal witnesses are tangent to the set of separable states (The concept of optimization will be explained in the next subsection). One can immediately grasp from the figure, that, in order to completely characterize the set of separable states \( S \) one should find all the witnesses tangent to \( S \). Unfortunately, infinitely many witnesses are needed for such a task!

![Figure 3. Geometrical picture of entanglement witnesses and their optimization.](image)

Witness operators are also related to maps. Indeed, there is an isomorphism that connects maps with operators known as Jamiołkowski isomorphism: each entanglement witness \( W \) on an \( M \times N \) space defines a positive map \( \mathcal{E} \)
that transforms positive operators on an $M$ or $N$-dimensional Hilbert space into positive operators on an $M$ or $N$-dimensional space [34]. The maps corresponding to entanglement witnesses are positive, but not completely positive (i.e. there is an extension $1 \otimes E$ which is not positive), and thus allow to “detect” the entanglement of $\rho$. Entanglement witnesses for PPT states and the corresponding maps have the property of being non-decomposable. A witness is called decomposable iff it can be written in the form $W = P + Q^T A$ with both $P$ and $Q$ positive. Otherwise it is non-decomposable. Correspondingly a map is decomposable iff it can be represented as a combination of positive maps and partial transposition and it is non-decomposable otherwise.

### B. Results on witness operators

How does one construct an entanglement witness? In [35] we provide a canonical form of mixed states in bipartite quantum systems in terms of a convex combination of a separable state and an edge state, as defined in section II. We construct entanglement witnesses for all edge states, and present a canonical form of non-decomposable entanglement witnesses and the corresponding positive maps. We present a characterization of separable states using a special class of entanglement witnesses.

An entanglement witness $W$ is called optimal, if there exists no entanglement witness that detects states further to the ones detected by $W$. Geometrically, this corresponds to the hyperplane defined by the witness being tangent to the set of separable states, see figure 3. In [36] we give necessary and sufficient conditions for entanglement witnesses to be optimal. We show how to optimize a general witness, and then we particularize our results to witnesses that can detect PPT entangled states, i.e. non-decomposable witnesses. This method also permits the systematic construction of non-decomposable positive maps.

The tool of witness operators can be applied to give a finer classification of entangled states by detecting their so-called Schmidt number. The Schmidt number of a mixed state was introduced in [37] as a generalization of the Schmidt rank for pure states: it characterizes the maximal Schmidt rank of the pure states in the “most simple” decomposition of $\rho$, i.e. the one that needs the lowest maximal Schmidt rank. The definition of the Schmidt number $k$ is given by

$$\rho = \sum_i p_i |\Psi_i^r\rangle\langle \Psi_i^r| , \quad k = \min_{\{dec\}} (r_{\max}),$$

where $r_i$ denotes the Schmidt rank of the state $|\Psi_i\rangle$, the minimization is done over all possible decompositions of $\rho$, and $r_{\max} = \max_i (r_i)$ is the maximal Schmidt rank of a given decomposition. In [38] we investigate the Schmidt number of an arbitrary mixed state by constructing a Schmidt number witness that detects it. We present a canonical form of such witnesses and provide constructive methods for their optimization. In this context we also find strong evidence that all bound entangled states with positive partial transpose in two qutrit systems have Schmidt number

$$| \sum_i c_i a_i\rangle\langle a_i | \otimes | b_i\rangle\langle b_i |,$$

where the coefficients $c_i$ are real and fulfill $\sum_i c_i = 1$. As local projection measurements can be performed with present day technology, some simple measurements then tell the experimentalist whether his given state is indeed

$$W = \sum_i c_i |a_i\rangle\langle a_i | \otimes | b_i\rangle\langle b_i | ,$$
entangled. The general solution to the optimization problem of finding the minimal number of measurements is yet unknown. We discuss a realistic example for two qubits, and suggest the first method for the detection of bound entanglement with local measurements.

The tool of witness operators is not only useful for addressing the separability problem, but also for studying the distillability problem: In [41] we introduce a formalism that connects entanglement witnesses and the distillation and activation properties of a state. We apply this formalism to two cases: First, we rederive the results presented in [42], namely that one copy of any bipartite state with non-positive partial transpose is either distillable, or activable. Second, we show that there exist three-partite NPPT states, with the property that two copies can neither be distilled, nor activated.

Finally, an overview of our programme that investigates quantum correlations and entanglement in terms of convex sets is given in [10]. There we present a unified description of optimal decompositions of quantum states and the optimization of witness operators that detect whether a given state belongs to a given convex set. We illustrate this abstract formulation with several examples, and discuss relations between optimal entanglement witnesses and n-copy non-distillable states with non-positive partial transpose.

V. QUANTUM CORRELATIONS IN SYSTEMS OF FERMIONIC AND BOSONIC STATES

The notion of entanglement discussed in the previous sections applies to situations where the parties are separated by macroscopic distances. Various mechanisms to create entanglement or to perform quantum gate operations, e.g. in the context of quantum dots [43] or neutral atoms in optical microtraps [44], however require a direct interaction at short distances between indistinguishable particles. We have developed a framework to study quantum correlations in such situations where the bosonic or fermionic character of indistinguishable particles become important. We have furthermore described a possible implementation of a quantum logic gate for neutral atoms in optical microtraps and studied bosonic correlations in this case.

A. What is different with indistinguishable particles?

To illustrate the consequences of indistinguishability consider two fermions located in a double well potential as a schematic model of electrons in quantum dots and assume the qubit to be implemented in the spin degree of freedom. Let the initial situation be such that each well contains one electron. Even if they are prepared completely independently, their pure quantum state has to be written in terms of Slater determinants in order to respect the indistinguishability. Operator matrix elements between such Slater determinants contain terms due to the antisymmetrization, but if the spatial wavefunctions of electrons located in different wells have only vanishingly small overlap, then the matrix elements will tend to zero for any physically meaningful operator. This situation is generically realized if the supports of the single-particle wavefunctions are essentially centered around locations being sufficiently apart from each other, or the particles are separated by a sufficiently large energy barrier. In this case the antisymmetrization has no physical effect and for all practical purposes it can be neglected.

If the two wells are moved closer together, or the energy barrier is lowered, such that the electrons are no longer completely localized in one well, then the fermionic statistics is clearly essential and the two-electron wave-function has to be antisymmetrized. Note that in this situation the space of states written in terms of single-particle states no longer has a tensor product structure because the actual state space is just a subspace of the complete tensor product. As a consequence of this fact any antisymmetrized state formally resembles an entangled state although these correlations are not useful as individual particles cannot be accessed. To emphasize this fundamental difference between distinguishable and indistinguishable particles, we will use the term quantum correlations to characterize useful correlations in systems of indistinguishable particles as opposed to correlations arising purely from their statistics.

We remark that there are different possible ways to quantify quantum correlations. An approach which can be seen as complementary to the one which we will describe here was discussed by Zanardi [45] who ignored the original tensor product structure through partitioning of the physical space into subsystems and introducing a tensor product structure in terms of modes. The entangled entities then are no longer particles but modes.
B. Results on quantum correlations for indistinguishable particles

Let us consider the case of two identical fermions sharing an $N$-dimensional single-particle space $\mathcal{H}_N$. The total Hilbert space is $\mathcal{A}(\mathcal{H}_N \otimes \mathcal{H}_N)$ where $\mathcal{A}$ denotes the antisymmetrization operator. A general state vector can be written as

$$|w\rangle = \sum_{i,j=1}^{N} w_{ij} f_i^\dagger f_j^\dagger |\Omega\rangle$$

(9)

with fermionic creation operators $f_i^\dagger$ acting on the vacuum $|\Omega\rangle$. The antisymmetric coefficient matrix $w_{ij}$ fulfills the normalization condition $\text{tr}(w^\ast w) = -1/2$. Under a unitary transformation of the single-particle space, $f_i^\dagger \mapsto \sum_j U_{ji} f_j^\dagger$, $w$ transforms as $w \mapsto U w U^T$.

**Theorem 4** For every pure two-fermion state $|w\rangle$ there exists a unitary transformation of the single particle space such that in the new basis of creation operators $f_i^\dagger$ the state is of the form

$$|w\rangle = 2 \sum_{k=1}^{m} z_k f_{2k}^\dagger f_{2k-1}^\dagger |\Omega\rangle$$

(10)

with $2 \cdot m \leq N$ and $z_k$ real and positive.

Each term in this decomposition corresponds to an elementary Slater determinant which is an analogue of a product state in systems consisting of distinguishable parties. Thus, when expressed in such a basis, $|w\rangle$ is a sum of elementary Slater determinants where each single-particle basis state enters at most one term. In this basis the number $m$ of Slater determinants is furthermore minimal and these Slater determinants are thus the analogues of the products states occurring in the Schmidt decomposition of a bi-partite state of distinguishable particles. Therefore we call $C$ the fermionic Slater rank of $|w\rangle$ [46], and an expansion of the form (10) a Slater decomposition of $|w\rangle$. For bosons there exists a similar expansion in terms of elementary two-boson Slater permanents representing doubly occupied states [47].

For two fermions the smallest single-particle space allowing for non-trivial correlations is four-dimensional. In this case a quantity analogous to the concurrence introduced by Wootters as an entanglement measure for two distinguishable qubits [13] can be constructed in the following way:

**Theorem 5** Let $|w\rangle$ be a two-fermion state in a four-dimensional single-particle space. Then the concurrence $C(|w\rangle)$, defined as

$$C(|w\rangle) = \frac{1}{2} \sum_{i,j,k,l=1}^{4} \epsilon^{ijkl} w_{ij} w_{kl},$$

(11)

($\epsilon$ is the fully antisymmetric unit tensor) has the following properties: (i) $C(|w\rangle)$ is invariant under unitary transformations of the single-particle space, (ii) $0 \leq C(|w\rangle) \leq 1$ and (iii) $C(|w\rangle) = 0$ iff $|w\rangle$ has Slater rank one and $C(|w\rangle) = 1$ iff $|w\rangle$ has maximal Slater rank, i.e. Slater rank two.

The concurrence $C(|w\rangle)$ thus fully characterizes quantum correlations in the case of pure states and for $N = 4$. For mixed two-fermion states in a four-dimensional single-particle space characterized by a density matrix $\rho$ a Slater number can be defined similar to the Schmidt number for mixed states of two qubits as the maximal Slater rank of a decomposition of $\rho$ into pure states minimized over all decompositions. Also we can define the mixed state concurrence as

$$C(\rho) = \inf_{\{\rho_i, |w_i\rangle\}} \left\{ \sum_i p_i C(|w_i\rangle) \right\}$$

(12)

where the infimum is taken over all decompositions of $\rho$. With this definition we find:

**Theorem 6** Let $\rho = \sum_i p_i |w_i\rangle \langle w_i|$ be a mixed two-fermion state. Define $|\tilde{w}_i\rangle = \sum_{i,j,k,l=1}^{4} \epsilon^{ijkl} w_{ij} f_{2k}^\dagger f_{2k-1}^\dagger |\Omega\rangle$ and $\tilde{\rho} = \sum_i p_i |\tilde{w}_i\rangle \langle \tilde{w}_i|$ and let $\lambda_i$ be the real and non-negative eigenvalues of $\rho \tilde{\rho}$ in descending order of magnitude. Then

$$C(\rho) = \max(0, \lambda_1 - \sum_{i=2}^{6} \lambda_i)$$

(13)
and $\rho$ has Slater number one iff $C(\rho) = 0$, i.e. iff $\lambda_1 \leq \sum_{i=2}^{6} \lambda_i$.

Notice that in a similar way the concurrence can be defined and calculated for pure and mixed states of two bosons in a two-dimensional single-particle space.

For higher-dimensional single-particle spaces there exist necessary and sufficient criteria to determine the Slater rank of pure fermionic and bosonic states by contracting their coefficient matrix $w$ with the $\epsilon$-tensor [47]. These become only necessary criteria when applied to mixed states and apparently a full and explicit characterization of higher-dimensional two-boson and two-fermion mixed states is not possible. Furthermore for the case of more than two particles a straight-forward generalization of the Slater decomposition cannot be given. This is again similar to the case of more than two qubits where a Schmidt decomposition of a general pure state does not exist [48]. Consider for example states of three fermions in a six-dimensional Hilbert space. It is in general not possible to find a unitary transformation of the single-particle space that brings a given state to a form $|\psi\rangle \propto z_1 f^1_1 f^1_2 f^1_3 |\Omega\rangle + z_2 f^2_4 f^2_5 f^2_6 |\Omega\rangle$, which would be the analogue of the two-fermion Slater decomposition. There however exist criteria to identify pure uncorrelated states, i.e. states that can be written as a single Slater determinant [47].

Finally we notice that for the case of two fermions or bosons in higher-dimensional single particle spaces ($N > 4$ for fermions, $N > 2$ for bosons) the concepts of witnesses can be applied [46,47]. As explained in section IV for the case of distinguishable particles, $k$-edge states can be introduced as states that become non-positive when $\epsilon \langle w^{<k} | w^{<k} \rangle$ is subtracted for some state $| w^{<k} \rangle$ of Slater rank $< k$. Then fermionic and bosonic $k$-Slater witnesses can be defined that detect states of Slater number $k$. These witnesses can furthermore be optimized as demonstrated in section IV.

C. Implementation of an entangling gate with bosons

In [44] we investigate quantum computation with bosonic neutral atoms in optical microtraps [49]. In contrast to other methods with the qubit being implemented in an internal degree of freedom, we study the case where the qubit is implemented in the motional state of the atoms, i.e., in the two lowest vibrational states of each trap. The quantum gate operation is performed by adiabatically approaching two traps each containing one particle such that tunneling and cold collisions occur and thus the bosonic character of the atoms is important. We especially address the implementation of a $\sqrt{SWAP}$-gate, i.e., a two-qubit gate that transforms states $|0\rangle_A |1\rangle_B$ and $|1\rangle_A |0\rangle_B$ to maximally entangled states while leaving $|0\rangle_A |0\rangle_B$ and $|1\rangle_A |1\rangle_B$ unchanged. The fidelity of the gate operation is evaluated as a function of the degree of adiabaticity in moving the traps and for rubidium atoms in state-of-the-art optical microtraps we obtain gate durations in the range of a few tens of milliseconds. Taking into account error mechanisms like spontaneous scattering of photons we calculate error rates of the gate operation and show that proof-of-principle experiments should be possible.

VI. SUMMARY

The characterization and classification of entangled states is a very challenging open problem of modern quantum theory. We have presented some approaches and partial solutions to this problem. The methods we used are the optimal decomposition of a given state into a separable and an entangled state, and the tool of witness operators. We have summarized various advances in the separability and distillability problem, and addressed the question of experimental implementation of witness operators. However, many open questions still remain to be solved.

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