# Quantum Correlations in Systems of Indistinguishable Particles

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We discuss quantum correlations in systems of indistinguishable particles in relation to entanglement in composite quantum systems consisting of well separated subsystems. Our studies are motivated by recent experiments and theoretical investigations on quantum dots and neutral atoms in microtraps as tools for quantum information processing. We present analogies between distinguishable particles, bosons, and fermions in low-dimensional Hilbert spaces. We introduce the notion of Slater rank for pure states of pairs of fermions and bosons in analogy to the Schmidt rank for pairs of distinguishable particles. This concept is generalized to mixed states and provides a correlation measure for indistinguishable particles. Then we generalize these notions to pure fermionic and bosonic states in higher-dimensional Hilbert spaces and also to the multi-particle case. We review the results on quantum correlations in mixed fermionic states and discuss the concept of fermionic Slater witnesses. Then the theory of quantum correlations in mixed bosonic states and of bosonic Slater witnesses is formulated. In both cases we provide methods of constructing optimal Slater witnesses that detect the degree of quantum correlations in mixed fermionic and bosonic states.     © 2002 Elsevier Science (USA)

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## 1. INTRODUCTION

The understanding and characterization of quantum entanglement is one of the most fundamental issues of modern quantum theory [1, 2], and a lot of work has been devoted to this topic in recent years [3–6].

In the beginning of modern quantum theory, the notion of entanglement was first noted by Einstein *et al.* [7] and by Schrödinger [8]. While in those days quantum entanglement and its predicted physical consequences were (at least partially) considered as an unphysical property of the formalism (a "paradox"), the modern perspective on this issue is very different. Now quantum entanglement is seen as an experimentally verified property of nature, that provides a resource for a vast variety of novel phenomena and concepts such as quantum computation, quantum cryptography, or quantum teleportation. Accordingly there are several motivations to study the entanglement of quantum states:

I. Interpretational and philosophical motivation. Entanglement plays an essential role in apparent "paradoxes" and counterintuitive consequences of quantum mechanics [7–10].

II. Fundamental physical motivation. The characterization of entanglement is one of the most fundamental open problems of quantum mechanics. It should answer the question: What is the nature of quantum correlations in composite systems [1]?

III. Applied physical motivation. Entanglement plays an essential role in applications of quantum mechanics to quantum information processing, and in particular to quantum computing [11], quantum cryptography [12, 13], and quantum communication [14] (i.e., teleportation [15, 16] and super dense coding [17]). The resources needed to implement a particular protocol of quantum information processing are closely linked to the entanglement properties of the states used in the protocol. In particular, entanglement lies at the heart of quantum computing [2].

IV. Fundamental mathematical motivation. The entanglement problem is directly related to one of the most challenging open problems of linear algebra and functional analysis: characterization and classification of positive maps on $\mathcal{C}^*$ algebras [3–5, 18–20] (for mathematical literature see [21–24]).

While entanglement plays an essential role in quantum communication between parties separated by macroscopic distances, the characterization of quantum correlations at short distances is also an open problem, which has received much less attention so far. In this case the indistinguishable character of the particles involved (electrons, photons, . . .) has to be taken into account. In his classic book, Peres [1] discussed the entanglement in elementary states of indistinguishable particles. These are symmetrizations and antisymmetrizations of product states for bosons and fermions, respectively. It is easy to see that all such states of two-fermion systems, and as well all such states formed by two non-collinear single-particle states in two-boson systems, are necessarily entangled in the usual sense. However, in the case of particles far apart from each other, this type of entanglement is not of physical relevance: "No quantum prediction, referring to an atom located in our laboratory, is affected by the mere presence of similar atoms in remote parts of the universe" [1]. This kind of entanglement between indistinguishable particles being far apart from each other is not the subject of this paper. Our aim here is rather to classify and characterize the quantum correlations between indistinguishable particles at short distances. We discuss below why this problem is relevant for quantum information processing in various physical systems. Perhaps the first attempt to study such quantum correlations in macroscopic

systems was done by Legett [25]. More recently he has formulated the concept of *disconnectivity* [26] of quantum states which is somewhat related to the concepts developed in this review.

This paper is organized as follows: In Section 2 we illustrate the consequences of indistinguishability. In Section 3 we describe analogies between quantum correlations in systems of two indistinguishable fermions, bosons, and two distinguishable parties where we concentrate on the lowest-dimensional Hilbert spaces that allow for non-trivial correlation effects. We derive the fermion and bosons analogues of recent results by Wootters [27], Kraus and Cirac [29], and Khaneja and Glaser [30]. Our results shed new light on a question posed recently by Vollbrecht and Werner: *Why two qubits are special* [31] (see also [32]). In Section 4 we report further results on quantum correlations in pure states of indistinguishable fermions in higher-dimensional cases. Results on mixed fermionic states are summarized in Section 5, and in Section 6 we report further results on identical bosons. We conclude in Section 7.

## 2. QUANTUM CORRELATIONS AND ENTANGLEMENT

### 2.1. Physical Systems: Quantum Dots and Neutral Atoms in Microtraps

Semiconductor quantum dots [33] are a promising approach to the physical realization of quantum computers. In these devices charge carriers (e.g., electrons) are confined in all three spatial dimensions. Their electronic spectrum consists of discrete energy levels since the confinement is of the order of the Fermi wavelength. It is experimentally possible to control the number of electrons in such a dot starting from zero (e.g., in a GaAs heterostructure [34]).

When one wants to use quantum dots for quantum computation it is necessary to define how the qubit (i.e., the basic unit of information) should be physically realized; e.g., the orbital electronic degrees of freedom or the electron spin $\vec{S}$ can be chosen to form the qubit. An advantage of the latter approach is that the decoherence time is much longer for the spin than for the orbital degree of freedom (usually three orders of magnitude [33, 35]).

The implementation of quantum algorithms needs single qubit and two qubit quantum gates [36]. For the spin degree of freedom the former can be achieved by the application of a magnetic field exclusively to a single spin [37]. It is well known [38] that arbitrary computations can be done if, apart from single qubit rotations, a mechanism by which two qubits can be entangled is available (the entangling gate $\sqrt{\text{SWAP}}$, together with single qubit rotations, can be used to produce the fundamental controlled-NOT gate). It was proposed in [37] to realize this mechanism by temporarily coupling two spins in two dots. The coupling, described by a Heisenberg Hamiltonian $H(t) = J(t)\vec{S}_1\vec{S}_2$, can be turned on and off by lowering and raising the tunnel barrier between neighboring quantum dots.

Another interesting type of physical implementation possibilities is neutral atoms in magnetic [39] or optical [40] microtraps. Here each single neutral atom is trapped in a harmonic potential and their collisional interaction can be controlled by temporarily decreasing the distance of the traps or by state-selective switching of the trapping potential.

### 2.2. Consequences of Indistinguishability

We will use a schematic view of two electrons located in a double-well potential to illustrate the consequences of indistinguishability for entanglement. This description applies to the discussed examples of quantum information processing in quantum dots and in optical or magnetical microtraps (replacing electrons by atoms). For this illustration we will assume that the qubit is modeled by the spin degree of freedom, which we will denote by $|\uparrow\rangle$ and $|\downarrow\rangle$. Furthermore we have two spatial wavefunctions labeled $|\phi\rangle$ and $|\chi\rangle$, initially localized in the left and in the right potential well, respectively. Then the complete state-space is four dimensional: $\{|\phi\rangle|\uparrow\rangle, |\chi\rangle|\uparrow\rangle, |\phi\rangle|\downarrow\rangle, |\chi\rangle|\downarrow\rangle\}$.
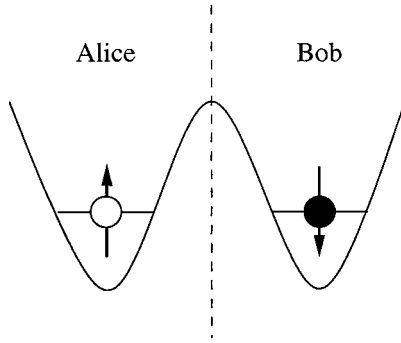
**FIG. 1.** The initial state $|\psi_{\text{init}}\rangle_{AB} = |\phi\rangle|\uparrow\rangle_A \otimes |\chi\rangle|\downarrow\rangle_B$, i.e., the case of separated wells. $|\phi\rangle$ and $|\chi\rangle$ denote the spatial part of the wavefunction localized in the left and in the right well, respectively.

We start with a situation where we have one electron in each well. 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 single Slater determinants contain terms due to the antisymmetrization of coordinates ("exchange contributions" in the language of Hartree–Fock theory). However, if the moduli of $\langle \vec{r}|\phi\rangle$, $\langle \vec{r}|\chi\rangle$ have only vanishingly small overlap, these exchange correlations will also 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.

Such observations clearly justify the treatment of indistinguishable particles separated by macroscopic distances as effectively distinguishable objects. So far, research in quantum information theory has concentrated on this case, where the exchange statistics of particles forming quantum registers could be neglected, or was not specified at all.

Under these conditions we write an initial state $|\psi_{\text{init}}\rangle_{AB} = |\phi\rangle|\uparrow\rangle_A \otimes |\chi\rangle|\downarrow\rangle_B$ where $A$ (Alice) and $B$ (Bob) are (physically meaningful) labels for the particle in the left and the right dot, respectively. The situation is shown in Fig. 1.

Now we want to analyze the situation when the two wells have been moved closer together or the energy barrier has been lowered. In such a situation the probability of finding, e.g., Alice's electron in the right well is non-vanishing. Then the fermionic statistics is clearly essential and the two-electron wavefunction has to be antisymmetrized and reads $|\psi(t_1)\rangle = (1/\sqrt{2})[|\phi\rangle|\uparrow\rangle_1 \otimes |\chi\rangle|\downarrow\rangle_2 - |\chi\rangle|\downarrow\rangle_1 \otimes |\phi\rangle|\uparrow\rangle_2]$. The indices $A$ and $B$ are changed to 1 and 2 here to stress that the enumeration of the particles is completely arbitrary since these labels are not physical: because of the spatial overlap of the wavefunctions the individual particles labeled 1 or 2 are not accessible independently. The situation is shown in Fig. 2.
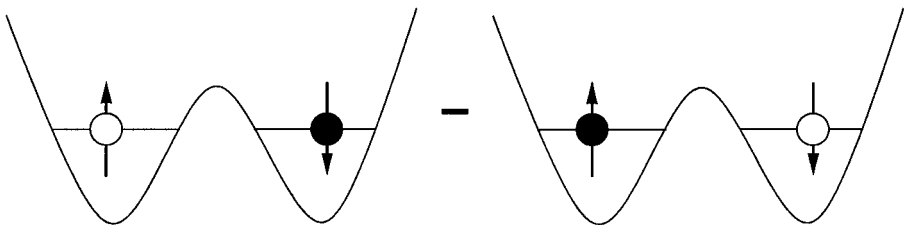


**FIG. 2.** Illustration of $|\psi(t_1)\rangle$, i.e., after lowering the tunnel barrier. The electronic wavefunctions are no longer completely localized in one of the wells.

Note that not only the labeling of the particles but also the notation suggesting a tensor product structure of the space of states is misleading because the actual state space is just a subspace of the complete tensor product [41]. As a consequence of this fact the antisymmetrized state $|\psi(t_1)\rangle$ formally resembles an entangled state although it is clear that this entanglement is not accessible, and therefore cannot be used as a resource in the sense discussed above for distinguishable particles. 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 (thereby following [33]).

Quantum correlations in systems of indistinguishable fermions arise if more than one Slater determinant is involved, i.e., if there is no single-particle basis such that a given state of $N$ indistinguishable fermions can be represented as an elementary Slater determinant (i.e., a fully antisymmetric combination of $N$ orthogonal single-particle states). These correlations are the analogue of quantum entanglement in separated systems and are essential for quantum information processing in non-separated systems.

As an example suppose it is possible to control the coupling $J(t)$ of the electrons such that at time $t_2$

$$|\psi(t_2)\rangle = \frac{1}{2}[|\phi\rangle|\uparrow\rangle_1 \otimes |\chi\rangle|\downarrow\rangle_2 - |\chi\rangle|\downarrow\rangle_1 \otimes |\phi\rangle|\uparrow\rangle_2 + |\phi\rangle|\downarrow\rangle_1 \otimes |\chi\rangle|\uparrow\rangle_2 - |\chi\rangle|\uparrow\rangle_1 \otimes |\phi\rangle|\downarrow\rangle_2]$$

which is illustrated in Fig. 3.

In the given single-particle basis, $|\psi(t_2)\rangle$ is written in terms of two elementary Slater determinants (and evidently there is no basis in which it can be written as a single one). This state contains some useful correlations beyond the required permutation symmetry as can be seen through localizing the particles again by switching off the interaction, i.e., raising the tunneling barrier or moving the wells apart (here we neglect the effects of non-adiabaticity, see [33] for a more detailed study of these effects). This corresponds to a partition of the basis between Alice and Bob, such that Alice's Hilbert space is formed by $\{|\phi\rangle|\uparrow\rangle, |\phi\rangle|\downarrow\rangle\}$ and Bob's by $\{|\chi\rangle|\uparrow\rangle, |\chi\rangle|\downarrow\rangle\}$. Then again the electrons can be viewed as effectively distinguishable, provided that none of the dots
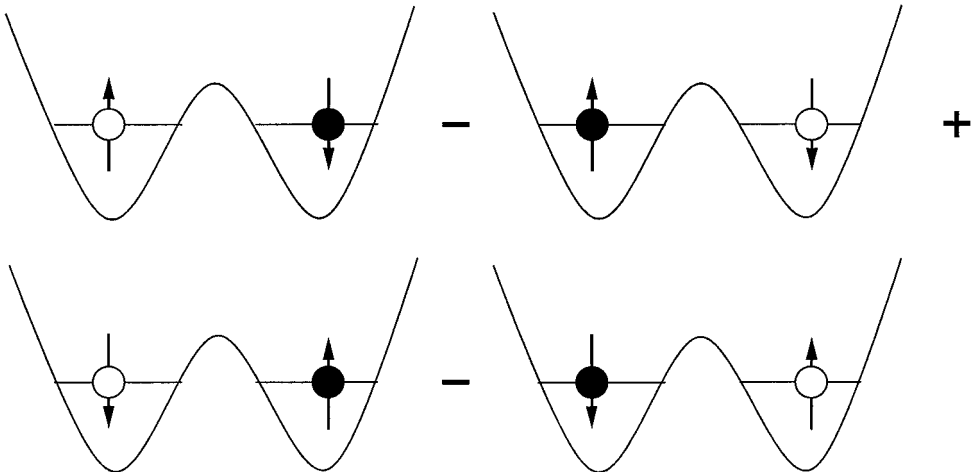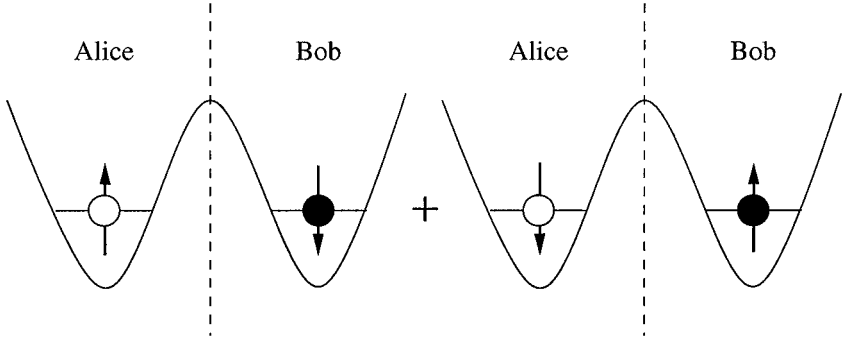


**FIG. 3.** Illustration of $|\psi(t_2)\rangle$.

**FIG. 4.** The final state $|\psi_{\text{final}}\rangle_{AB}$. Raising the tunneling barrier localizes the wavefunctions again.

is occupied by two electrons. This does not happen here because the final state is $|\psi_{\text{final}}\rangle_{AB} = (1/\sqrt{2})[|\phi\rangle|\uparrow\rangle_A \otimes |\chi\rangle|\downarrow\rangle_B + |\phi\rangle|\downarrow\rangle_A \otimes |\chi\rangle|\uparrow\rangle_B]$, where *new* labels $A$ and $B$ are attributed to the particles, corresponding to the dot in which they are found after separation; i.e., the electron found in the left (right) dot is named $A(B)$. $|\psi_{\text{final}}\rangle_{AB}$ is shown in Fig. 4.

The final state $|\psi_{\text{final}}\rangle_{AB}$, shown in Fig. 4, is the Bell state $|\Psi^+\rangle$, i.e., a *maximally entangled* two qubit state (thus the operation performed in this example is the entangling gate $\sqrt{\text{SWAP}}$). In this sense it is reasonable to call $|\psi(t_2)\rangle$ a *maximally correlated* state of two indistinguishable fermions in a four-dimensional single-particle space and to view it as a resource for the production of entangled states of distinguishable particles.

Motivated by these considerations in [43] we have developed a classification of states of two fermions with $2M$ accessible single-particle states. This question was also addressed very recently by Li *et al.* [44] and by Paskauskas and You [45]. In these papers two-boson systems are examined and analogues to earlier results about two-fermion systems [33, 43] are derived. However, Refs. [44, 45] differ in detail about which two-boson states should be considered as analogues of entangled states (in a bipartite system) in a certain limiting case.

Zanardi [41, 42] discusses another approach, ignoring the original tensor product structure through a partition of the physical space into subsystems. The entangled entities then are no longer particles but modes. This approach may be seen as complementary to the one followed here. For completeness we present the corresponding formalism in Appendix A. It is reasonable to consider both kinds of quantum correlations—which one is more useful depends on the particular situation, for instance on their usefulness for concrete applications, e.g., cryptography or teleportation.

## 3. ANALOGIES BETWEEN BOSONS, FERMIONS, AND DISTINGUISHABLE PARTICLES IN LOW-DIMENSIONAL HILBERT SPACES

### 3.1. Pure States: Schmidt Rank and Slater Rank

#### 3.1.1. *Schmidt Rank of Distinguishable Particles*

The "classic" examples for quantum entanglement were studied in systems composed of separated (and therefore distinguishable) subsystems. The most investigated case involves two parties, say $A$(lice) and $B$(ob), having a finite-dimensional Hilbert space $\mathcal{H}_A$ and $\mathcal{H}_B$, respectively. This results in a total space $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$. An important tool for the investigation of such bipartite systems is the bi-orthogonal Schmidt decomposition [1]. It states that for any state vector $|\psi\rangle \in \mathcal{H}$ there exist

bases of $\mathcal{H}_A$ and $\mathcal{H}_B$ such that

$$|\psi\rangle = \sum_{i=1}^{r} z_i(|a_i\rangle \otimes |b_i\rangle), \qquad z_i > 0 \quad \text{and} \quad \sum_{i=1}^{r} z_i^2 = 1, \tag{1}$$

where the basis states fulfill that $\langle a_i|a_j\rangle = \langle b_i|b_j\rangle = \delta_{ij}$. Thus, each vector in both bases for $\mathcal{H}_A$ and $\mathcal{H}_B$ occurs at most in only one product vector in the above expansion. The expression (1) is an expansion of the state $|\psi\rangle$ into a basis of orthogonal product vectors with a minimum number $r$ of nonzero terms. This number can take values between one and $\min\{\dim\mathcal{H}_A, \dim\mathcal{H}_B\}$ and is called the *Schmidt rank* of $|\psi\rangle$. $|\psi\rangle$ is entangled if and only if $r > 1$.

### 3.1.2. *Slater Rank of Fermionic States*

Let us now turn to 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

$$|w\rangle = \sum_{i,j=1}^{n} w_{ij} f_i^\dagger f_j^\dagger |0\rangle \tag{2}$$

with fermionic creation operators $f_i^\dagger$ acting on the vacuum $|0\rangle$. The antisymmetric coefficient matrix $w_{ij}$ fulfills the normalization condition

$$\text{tr}(w^*w) = -\frac{1}{2}. \tag{3}$$

Under a unitary transformation of the single-particle space,

$$f_i^\dagger \mapsto \mathcal{U} f_i^\dagger \mathcal{U}^\dagger = U_{ji} f_j^\dagger, \tag{4}$$

$w$ transforms as

$$w \mapsto UwU^T, \tag{5}$$

where $U^T$ is the transpose of $U$. For any complex *antisymmetric* $n \times n$ matrix $w$ there is a unitary transformation $U$ such that $w' = UwU^T$ has nonzero entries only in $2 \times 2$ blocks along the diagonal [43, 46]. That is,

$$w' = \text{diag}[Z_1, \ldots, Z_r, Z_0] \qquad \text{with } Z_i = \begin{bmatrix} 0 & z_i \\ -z_i & 0 \end{bmatrix}, \tag{6}$$

where $z_i > 0$ for $i \in \{1, \ldots, r\}$, and $Z_0$ is the $(n - 2r) \times (n - 2r)$ null matrix. Each $2 \times 2$ block $Z_i$ corresponds to an elementary Slater determinant. Such elementary Slater determinants are the analogues of product states in systems consisting of distinguishable parties. Thus, when expressed in such a basis, the state $|w\rangle$ is a sum of elementary Slater determinants where each single-particle basis state occurs at most in one term. This property is analogous to the bi-orthogonality of the Schmidt decomposition discussed above. The matrix (6) represents an expansion of $|w\rangle$ into a basis of elementary Slater determinants with a minimum number $r$ of non-vanishing terms. This number is analogous to the Schmidt rank for the distinguishable case. Therefore we shall call it the *fermionic Slater rank* of $|w\rangle$ [43], and an expansion of the above form a *Slater decomposition* of $|w\rangle$.

### 3.1.3. *Slater Rank of Bosonic States*

Similarly, a general state of a system of two indistinguishable bosons in an $n$-dimensional single-particle space reads

$$|v\rangle = \sum_{i,j=1}^{n} v_{ij} b_i^\dagger b_j^\dagger |0\rangle \tag{7}$$

with bosonic creation operators $b_i^\dagger$ acting on the vacuum state. The symmetric coefficient matrix $v_{ij}$ transforms under single-particle transformations just the same as in the fermionic case,

$$v \mapsto U v U^T. \tag{8}$$

For any complex *symmetric* matrix $v$ there exists a unitary transformation $U$ such that the resulting matrix $v' = U v U^T$ is diagonal [44–46], i.e.,

$$v' = \mathrm{diag}(z_1, \ldots, z_r, 0, \ldots, 0) \tag{9}$$

with $z_i \neq 0$ for $i \in \{1, \ldots, r\}$. In such a single particle basis the state $|v\rangle$ is a linear combination of elementary two-boson Slater permanents representing doubly occupied states. Moreover Eq. (9) defines an expansion of the given state $|v\rangle$ into Slater permanents representing doubly occupied states with the smallest possible number $r$ of nonzero terms. We shall call this number the *bosonic Slater rank* of $|v\rangle$.

An expansion of the form (9) for a two-boson system was also obtained very recently in Refs. [44, 45]. Moreover the fermionic analogue (6) of the bi-orthogonal Schmidt decomposition of bipartite systems was also used earlier in studies of electron correlations in Rydberg atoms [47].

Regarding Slater determinant states in fermionic Hilbert spaces we also mention interesting earlier work by Rombouts and Heyde [48] who investigated the question of under what circumstances a given many-fermion wavefunction can be cast as a Slater determinant built up from in general *non-orthogonal* single-particle states. Since a wavefunction of this kind can in general not be written as a single Slater determinant constructed from *orthogonal* single-particle states, i.e., has non-trivial quantum correlations beyond simple antisymmetrization effects, the criteria obtained in [48] do not address the issues here.

As we saw, elementary Slater determinants in two-fermion systems, i.e., states with Slater rank one, are the natural analogues of product states in systems of distinguishable parties. One needs at least a fermionic state of slater rank two to form a quantum correlated state corresponding to a Schmidt rank two state of separated particles. In contrast, in the bosonic case one needs at least a state of Slater rank four to perform the same task. This can already be seen from the fact that for distinguishable particles entangled states need at least a $2 \times 2$ dimensional Hilbert space.

In the following we shall refer to the Schmidt rank or Slater rank of a given pure state also as its *quantum correlation rank*.

## 3.2. Magic Bases, Concurrence, and Dualisation

One of the most important issues in quantum information theory is the qualification and quantification of entanglement between several subsystems in a given state $\rho$. For the case of two *distinguishable* parties, a useful measure of entanglement of pure states is the von Neumann-entropy of reduced density matrices constructed from the density matrix $\rho = |\psi\rangle\langle\psi|$ [49],

$$E(|\psi\rangle) = -\mathrm{tr}_A(\rho_A \log_2 \rho_A) = -\mathrm{tr}_B(\rho_B \log_2 \rho_B), \tag{10}$$

where the reduced density matrices are obtained by tracing out one of the subsystems, $\rho_A = \text{tr}_B \rho$ and vice versa. With the help of the bi-orthogonal Schmidt decomposition of $|\psi\rangle$ one shows that both reduced density matrices have the same spectrum and therefore the same entropy, as stated in Eq. (10). In particular, the Schmidt rank of $|\psi\rangle$ equals the algebraic rank of the reduced density matrices. A pure state is non-entangled if and only if its reduced density matrices are again pure states, and it is maximally entangled if its reduced density matrices are "maximally mixed," i.e., if they have only one nonzero eigenvalue with a multiplicity of $\min\{\dim \mathcal{H}_A, \dim \mathcal{H}_B\}$.

### 3.2.1. *Two Distinguishable Particles*

The lowest-dimensional system of two distinguishable particles having non-trivial entanglement properties consists of just two qubits, i.e., $\dim \mathcal{H}_A = \dim \mathcal{H}_B = 2$. For this system, the entanglement measure (10) takes a particularly simple form if the state $|\psi\rangle$ is expressed in the so-called *magic basis*,

$$|\chi_1\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$$

$$|\chi_2\rangle = \frac{1}{\sqrt{2}}(|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle)$$

$$|\chi_3\rangle = \frac{i}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) \tag{11}$$

$$|\chi_4\rangle = \frac{i}{\sqrt{2}}(|\uparrow\uparrow\rangle - |\downarrow\downarrow\rangle),$$

i.e., $|\psi\rangle = \sum_{i=1}^{4} \alpha_i |\chi_i\rangle$, where an obvious notation has been used. With respect to this basis it holds [27, 50]

$$E(|\psi\rangle) = h\left(\frac{1 + \sqrt{1 - \mathcal{C}(|\psi\rangle)^2}}{2}\right), \tag{12}$$

where $h(x) = -x \log_2(x) - (1 - x) \log_2(1 - x)$ is the binary entropy function and the "concurrence" $\mathcal{C}(|\psi\rangle)$ is defined by $\mathcal{C}(|\psi\rangle) = |\sum_{i=1}^{4} \alpha_i^2|$. Thus, a state is fully entangled if and only if all its coefficients with respect to the magic basis have the same phase. What is furthermore "magic" about this basis is the fact that its elements are (pseudo-)eigenstates of the time reversal operator $\mathcal{D}$ [27],

$$\mathcal{D}|\chi_i\rangle = |\chi_i\rangle \tag{13}$$

with

$$\mathcal{D} = \left((i\sigma_A^y) \otimes (i\sigma_B^y)\right)\mathcal{K}. \tag{14}$$

Here $\sigma_{A,B}^y$ are Pauli matrices in the basis used in the construction of the magic basis (11), and $\mathcal{K}$ is the operator of complex conjugation which acts on a product state of basis vectors as $\mathcal{K}|\mu\nu\rangle = |\mu\nu\rangle$, where $\mu, \nu \in \{\uparrow, \downarrow\}$, and on a general vector as $K \sum_{\mu,\nu} \psi_{\mu\nu}|\mu\nu\rangle = \sum_{\mu,\nu} \psi_{\mu\nu}^*|\mu\nu\rangle$. These relations are part of the definition of $\mathcal{K}$. $\mathcal{D}$ is invariant under arbitrary SU(2) transformations performed independently on the two subsystems, due to the relation $U\sigma^y U^T = \sigma^y$ for any $U \in$ SU(2). It was pointed out in Ref. [31] that this property is particular to the $2 \times 2$ matrix $\sigma^y$ and does not have a true analogue in higher dimensions. However, in the following we will encounter similar invariance relations

in higher-dimensional spaces where the manifold of transformations is restricted to a physically motivated subgroup of the unitary group.

Using the time reversal operator $\mathcal{D}$, the concurrence can be written as $\mathcal{C}(|\psi\rangle) = |\langle\tilde{\psi}|\psi\rangle|$ with $|\tilde{\psi}\rangle = \mathcal{D}|\psi\rangle$. Moreover, since the entanglement measure $E(|\psi\rangle)$ is a monotonous function of $\mathcal{C}(|\psi\rangle)$ with both functions ranging from zero to one, one can equally well use $\mathcal{C}(|\psi\rangle)$ as a measure of entanglement [27, 51], as we shall do in the following.

The definition of the magic basis (and as well of the complex conjugation operator $\mathcal{K}$) refers explicitly to certain bases in the two subsystems. However, using the above invariance property, it is straightforward to show that switching to different local bases has only trivial effects without any physical significance. In particular, the concurrence is invariant under such operations. This can be seen from writing $|\psi\rangle$ in the computational basis as $|\psi\rangle = \sum_{\mu,\nu=\uparrow,\downarrow} \psi_{\mu,\nu}|\mu\nu\rangle$. Then $\mathcal{C}(|\psi\rangle)^2 = 4|\det(\psi)|^2$ and in this context it has been named "tangle" by Wootters [28].

### 3.2.2. Two Fermions

Let us now turn to the case of two fermions. The lowest-dimensional system allowing a Slater rank larger than one has a four-dimensional single-particle space resulting in a six-dimensional two-particle Hilbert space. This case was analyzed first in Ref. [33] where a fermionic analogue of the two-qubit concurrence was found. It can be constructed in the following way: For a given state $|w\rangle = \sum_{i,j=1}^{4} w_{ij} f_i^\dagger f_j^\dagger |0\rangle$ defined by its coefficient matrix $w_{ij}$, define the dual matrix $\tilde{w}_{ij}$ by

$$\tilde{w}_{ij} = \frac{1}{2} \sum_{k,l=1}^{4} \varepsilon^{ijkl} w_{kl}^*, \tag{15}$$

with $\varepsilon^{ijkl}$ being the usual totally antisymmetric unit tensor. Then the concurrence $\mathcal{C}(|w\rangle)$ can be defined as [52]

$$\mathcal{C}(|w\rangle) = |\langle\tilde{w}|w\rangle| = \left| \sum_{i,j,k,l=1}^{4} \varepsilon^{ijkl} w_{ij} w_{kl} \right| = 8|(w_{12}w_{34} + w_{13}w_{42} + w_{14}w_{23})|. \tag{16}$$

Obviously, $\mathcal{C}(|w\rangle)$ ranges from zero to one. Importantly it vanishes if and only if the state $|w\rangle$ has the fermionic Slater rank one, i.e., is an elementary Slater determinant. This statement was proved first in Ref. [33]; an alternative proof can be given using the Slater decomposition of $|w\rangle$ and observing that

$$\det w = \left( \frac{1}{8} \langle\tilde{w}|w\rangle \right)^2. \tag{17}$$

This relation is just a special case of a general expression for the determinant of an antisymmetric $(2K) \times (2K)$ matrix $w$,

$$\det w = \left( \frac{1}{2^K K!} \sum_{i_1,\dots,i_{2K}=1}^{2K} \varepsilon^{i_1\dots i_{2K}} w_{i_1 i_2} \dots w_{i_{2K-1} i_{2K}} \right)^2, \tag{18}$$

which is known as the Pfaffian representation and can be proved readily by the same means. Note the formal analogy to the definition of the tangle of two qubits [28].

Moreover, it is straightforward to show that the concurrence is invariant under arbitrary SU(4) transformations in the single-particle space. More generally, for any two states $|w_1\rangle$, $|w_2\rangle$ being

subjected to a single-particle transformation $\mathcal{U}$, $|w_i\rangle \mapsto |u_i\rangle = \mathcal{U}|w_i\rangle$, $i \in \{1, 2\}$, it holds

$$\langle \tilde{u}_2 | u_1 \rangle = \det \mathcal{U} \langle \tilde{w}_2 | w_1 \rangle. \tag{19}$$

In summary, the concurrence $\mathcal{C}(|w\rangle)$ constitutes, in analogy to the case of two qubits, a measure of "entanglement" for any two-fermion state $|w\rangle$. It ranges from zero for "non-entangled" states (having Slater rank one) to one for "fully entangled" states which are collinear with their duals. In this case the Slater decomposition of $|w\rangle$ consists of two elementary Slater determinants having the same weight.

From the occurrence of the complex conjugation in the definition of the dual state (15) it is obvious that the dualisation of a two-fermion state is an anti-linear operation. In fact, as we will illustrate below, the dualisation of a state $|w\rangle$ again corresponds to time reversal. As another physical interpretation, it can be identified with a particle-hole transformation,

$$\mathcal{U}_{ph} f_i^\dagger \mathcal{U}_{ph}^\dagger = f_i, \qquad \mathcal{U}_{ph}|0\rangle = f_1^\dagger f_2^\dagger f_3^\dagger f_4^\dagger |0\rangle, \tag{20}$$

along with a complex conjugation. The operator of dualisation $\mathcal{D}$, $|\tilde{w}\rangle = \mathcal{D}|w\rangle$, can be written as

$$\mathcal{D} = -\mathcal{U}_{ph}\mathcal{K}, \tag{21}$$

where $\mathcal{K}$ is the anti-linear operator of complex conjugation acting on the single-particle states and the fermionic vacuum as

$$\mathcal{K} f_i^\dagger \mathcal{K} = f_i^\dagger, \qquad \mathcal{K} f_i \mathcal{K} = f_i, \qquad \mathcal{K}|0\rangle = |0\rangle. \tag{22}$$

As a further analogy to the two-qubit case one also has a magic basis, i.e., a basis of (pseudo-) eigenstates of the dualisation operator (21):

$$
\begin{aligned}
|\chi_1\rangle &= \frac{1}{\sqrt{2}}(f_1^\dagger f_2^\dagger + f_3^\dagger f_4^\dagger)|0\rangle \\[4pt]
|\chi_2\rangle &= \frac{1}{\sqrt{2}}(f_1^\dagger f_3^\dagger + f_4^\dagger f_2^\dagger)|0\rangle \\[4pt]
|\chi_3\rangle &= \frac{1}{\sqrt{2}}(f_1^\dagger f_4^\dagger + f_2^\dagger f_3^\dagger)|0\rangle \\[4pt]
|\chi_4\rangle &= \frac{i}{\sqrt{2}}(f_1^\dagger f_2^\dagger - f_3^\dagger f_4^\dagger)|0\rangle \\[4pt]
|\chi_5\rangle &= \frac{i}{\sqrt{2}}(f_1^\dagger f_3^\dagger - f_4^\dagger f_2^\dagger)|0\rangle \\[4pt]
|\chi_6\rangle &= \frac{i}{\sqrt{2}}(f_1^\dagger f_4^\dagger - f_2^\dagger f_3^\dagger)|0\rangle.
\end{aligned}
\tag{23}
$$

Expressed in this basis, the concurrence of a state $|w\rangle = \sum_{i=1}^{6} \alpha_i |\chi_i\rangle$ just reads $\mathcal{C}(|w\rangle) = |\sum_{i=1}^{6} \alpha_i^2|$. Therefore, $|w\rangle$ has a concurrence of modulus one if and only if all its coefficients with respect to the magic basis have the same phase.

Like in the two-qubit case, the definition of the complex conjugation operator $\mathcal{K}$ and the magic basis refers to a certain choice of basis in the single-particle space. However, due to the invariance properties described above, this does not have physically significant consequences.

A four-dimensional single-particle space can formally be viewed as the Hilbert space of a spin-$\frac{3}{2}$-object. Having two indistinguishable fermions in this system means coupling two spin-$\frac{3}{2}$ states to total spin states that are antisymmetric under particle exchange. This leads to the two multiplets with even total spin, i.e., $S = 2$ and $S = 0$. When the single-particle states labeled so far by $i \in \{1, 2, 3, 4\}$ are interpreted as states of a spin-$\frac{3}{2}$ particle with $S^z = \frac{3}{2} - (i - 1)$ ($\hbar = 1$) these multiplet states read explicitly

$$
\begin{aligned}
|2, 2\rangle &= f_1^\dagger f_2^\dagger |0\rangle \\
|2, 1\rangle &= f_1^\dagger f_3^\dagger |0\rangle \\
|2, 0\rangle &= \frac{1}{\sqrt{2}} (f_1^\dagger f_4^\dagger + f_2^\dagger f_3^\dagger) |0\rangle \\
|2, -1\rangle &= f_2^\dagger f_4^\dagger |0\rangle \\
|2, -2\rangle &= f_3^\dagger f_4^\dagger |0\rangle \\
|0, 0\rangle &= \frac{i}{\sqrt{2}} (f_1^\dagger f_4^\dagger - f_2^\dagger f_3^\dagger) |0\rangle.
\end{aligned}
\tag{24}
$$

The phase of the last singlet state has been adjusted such that the dualisation operator reads in this ordered basis

$$
\mathcal{D} =
\begin{pmatrix}
0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & -1 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 \\
0 & -1 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1
\end{pmatrix}
\mathcal{K}
\tag{25}
$$

which is nothing but the time reversal operator acting on the two multiplets $S = 2$ and $S = 0$. Thus, the operation of dualisation can also be interpreted as a time reversal operation performed on appropriate spin objects. However, this interpretation is not necessarily the physically most natural one: the notion of dualisation and entanglement-like quantum correlations between indistinguishable fermions was first investigated for the case of two electrons (carrying a spin of $\frac{1}{2}$) in a system of two quantum dots [33]. There the interpretation of $\mathcal{D}$ as the anti-linear implementation of a particle-hole transformation, rather than time reversal of formal spin objects, seems clearly more appropriate. Therefore we shall retain the general term dualisation for such an operation in the two kinds of systems investigated so far, and also in the case of a bosonic system to be explored below.

### 3.2.3. *Two Bosons*

Having established all these analogies between two qubits and a system of two fermions sharing a four-dimensional single particle space, it is natural to ask whether similar observations can be made for a system of two bosons. The bosonic system showing properties analogous to those discussed before consists of two indistinguishable bosons in a two-dimensional single-particle space. This is the smallest-dimensional system admitting states with a bosonic Slater rank greater than one. It can be viewed as the symmetrized version of the two-qubit system, and its two-boson space represents therefore the Hilbert space of a spin-1-object.

A general state vector of this system reads $|v\rangle = \sum_{i,j=1}^{4} v_{ij} b_i^\dagger b_j^\dagger |0\rangle$ with a coefficient matrix

$$v = \begin{pmatrix} A & B \\ B & C \end{pmatrix} \tag{26}$$

being subject to the normalization condition $2|A|^2 + 4|B|^2 + 2|C|^2 = 1$. The appropriate dualisation operator is

$$\mathcal{D} = \mathcal{R}\mathcal{K}, \tag{27}$$

where $\mathcal{K}$ is the complex conjugation operator with analogous properties as above, and the operator $\mathcal{R}$ acts in the single-particle space as

$$b_a^\dagger \mapsto \mathcal{R} b_a^\dagger \mathcal{R}^\dagger = \sum_{b=1}^{2} -i\sigma_{ba}^y b_b^\dagger; \tag{28}$$

i.e., $\mathcal{R}$ exchanges the state labels inferring a sign. When expressed in the ordered basis $((1/\sqrt{2})b_1^\dagger b_1^\dagger |0\rangle$, $b_1^\dagger b_2^\dagger |0\rangle$, $(1\sqrt{2})b_2^\dagger b_2^\dagger |0\rangle)$ the dualisation operator reads

$$\mathcal{D} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & -1 & 0 \\ 1 & 0 & 0 \end{pmatrix} \mathcal{K} \tag{29}$$

which is, as natural, just the time reversal operator for a spin-1-object. Now the concurrence $\mathcal{C}(|v\rangle)$ can be defined as the modulus of the scalar product of $|v\rangle$ with its dual $|\tilde{v}\rangle = \mathcal{D}|v\rangle$ and expressed as

$$\mathcal{C}(|v\rangle) = |\langle \tilde{v}|v\rangle| = |4(AC - B^2)| = |4 \det v|. \tag{30}$$

The last equation makes it immediately obvious that $\mathcal{C}(|v\rangle)$ is invariant under SU(2) transformations in the single-particle space and is zero if and only if $|v\rangle$ has bosonic Slater rank one. Therefore this quantity has properties that are completely analogous to the two other cases before. A magic basis of the two-boson space is given by

$$|\chi_1\rangle = \frac{1}{2}(b_1^\dagger b_1^\dagger + b_2^\dagger b_2^\dagger)|0\rangle$$

$$|\chi_2\rangle = \frac{i}{2}(b_1^\dagger b_1^\dagger - b_2^\dagger b_2^\dagger)|0\rangle \tag{31}$$

$$|\chi_3\rangle = i(b_1^\dagger b_2^\dagger)|0\rangle.$$

Again, the concurrence is maximal, i.e., $\mathcal{C}(|v\rangle) = 1$, if and only if the coefficients of $|v\rangle$ in the magic basis have all the same phase.

### 3.3. Mixed States and Unified Correlation Measure: Wootters' Formula and Its Analogues

We now turn to the case of mixed states characterized by a density matrix $\rho$. For a general bipartite system (not necessarily consisting of just two qubits) the *entanglement of formation* of a state $\rho$ is

defined by the expression [53, 54]

$$\mathcal{E}_F(\rho) = \inf_{\{p_i, |\psi_i\rangle\}} \left\{ \sum_i p_i E(|\psi_i\rangle) \right\}, \tag{32}$$

where $E$ is the entanglement measure (10) for pure states, and the infimum is taken over all decompositions $\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$ of the density matrix $\rho$ in terms of normalized but in general not orthogonal states $|\psi_i\rangle$ and positive coefficients $p_i$ with $\sum_i p_i = 1$.

In the case of two qubits an equivalent entanglement measure is, following Wootters [27], given by

$$\mathcal{C}(\rho) = \inf_{\{p_i, |\phi_i\rangle\}} \left\{ \sum_i p_i \mathcal{C}(|\phi_i\rangle) \right\}, \tag{33}$$

where the concurrence $\mathcal{C}$ enters directly instead of via the entropy expression (12). This possibility relies on the fact that $E(|\psi\rangle)$ for a pure state $|\psi\rangle$ is a monotonous function of the modulus of its concurrence, and the infimum in (32) is actually realized by a decomposition of $\rho$ where each state $|\psi\rangle$ has the same concurrence, such that the summation becomes trivial [27].

Furthermore $\mathcal{C}$ can be given by a closed expression avoiding the minimization entering (33), namely

$$\mathcal{C}(\rho) = \max\{0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4\}, \tag{34}$$

where $\lambda_1, \lambda_2, \lambda_3, \lambda_4$ are, in descending order of magnitude, the square roots of the singular values of the matrix $\rho\tilde{\rho}$ with $\tilde{\rho} = \mathcal{D}\rho\mathcal{D}^{-1}$. The singular values of the (in general non-hermitian) matrix $\rho\tilde{\rho}$ can readily be shown to be always real and non-negative.

The formula (34) was first conjectured and proved for a subclass of density matrices by Hill and Wootters [50], and it was proved for the general case shortly afterwards by Wootters [27].

The expression (33) can obviously be read as a unified correlation measure for all of the three cases discussed above, namely two qubits, two indistinguishable fermions in a four-dimensional single-particle space, and finally two indistinguishable bosons in a two-dimensional single-particle space. This unified measure ranges from zero to one and vanishes for pure states with correlation rank one. Moreover this quantity is invariant under "local unitary transformations," i.e., independent SU(2) transformation in the two qubit spaces, or, for indistinguishable particles, unitary transformations of the single-particle Hilbert space. Moreover, in all three systems, the dualisation operation has the property that for any two pure states $|\psi\rangle$, $|\chi\rangle$ and their duals $|\tilde{\psi}\rangle$, $|\tilde{\chi}\rangle$, the identity $\langle\tilde{\psi}|\chi\rangle = \langle\tilde{\chi}|\psi\rangle$ holds.

These three properties are sufficient to take Wootters' proof [27] over to the other two cases. Therefore, the correlation measure $\mathcal{C}(\rho)$ of a general mixed state of two fermions sharing a four-dimensional single-particle space can be expressed as

$$\mathcal{C}_{\mathcal{F}}(\rho) = \max\{0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4 - \lambda_5 - \lambda_6\}, \tag{35}$$

and the analogous expression for the two-boson system reads

$$\mathcal{C}_{\mathcal{B}}(\rho) = \max\{0, \lambda_1 - \lambda_2 - \lambda_3\}. \tag{36}$$

Again, in full analogy to the two-qubit case, the $\lambda_i$ are, in descending oder of magnitude, the square roots of the singular values of $\rho\tilde{\rho}$ with $\tilde{\rho} = \mathcal{D}\rho\mathcal{D}^{-1}$ being the appropriately dualised density matrix. As in Ref. [27] one can show that the singular values of $\rho\tilde{\rho}$ are always real and non-negative.

In Ref. [43] we have given a somewhat alternative proof of Eqs. (34), (35), (36) by discussing the matrix

$$C_{ij} = \langle \tilde{\psi}_i | \psi_j \rangle \tag{37}$$

which arises from the decompositions $\rho = \sum_i |\psi_i\rangle\langle\psi_i|$ of a given density matrix in terms of (in general non-normalized) states $|\psi_i\rangle$.

### 3.4. Invariance Group of the Dualisation and General Unitary Transformations

To simplify the notation we shall in the following denote analogous quantities referring to the three systems above, namely two qubits, two fermions, and two bosons, in the form $[\cdot, \cdot, \cdot]$. As an example, the unified correlation measure reads

$$\mathcal{C}(\rho) = \max\left\{ 0, \lambda_1 - \sum_{i=2}^{d} \lambda_i \right\}, \tag{38}$$

where $d = [4, 6, 3]$ is the dimension of the full Hilbert space of each system.

Let us denote the group of (special) unitary transformations of the appropriate total Hilbert space by $G = [\mathrm{SU}(4), \mathrm{SU}(6), \mathrm{SU}(3)]$, and the group of "local transformations" (acting on the qubit spaces, or on the appropriate single-particle space) by $H = [\mathrm{SU}(2) \otimes \mathrm{SU}(2), \mathrm{SU}(4), \mathrm{SU}(2)]$. In the following we do not distinguish between $H$ and its [4, 6, 3]-dimensional representation in the full Hilbert space.

For a given state $|\Psi\rangle$ expressed in the magic basis, $|\Psi\rangle = \sum_{i=1}^{d} \alpha_i |\chi_i\rangle$, the action of the dualisation operator is

$$\mathcal{D}|\Psi\rangle = \sum_{i=1}^{d} \alpha_i^* |\chi_i\rangle. \tag{39}$$

Therefore, within the magic basis, the dualisation operator $\mathcal{D}$ acting on the coordinate vector with components $\alpha_i$ is just $\mathcal{D} = \mathbf{1}_{d \times d} \mathcal{K}$. We now investigate the subgroup $M$ of $G$ consisting of all unitary transformations $\mathcal{U}$ that leave scalar products of the form $\langle \tilde{\Psi}_1 | \Psi_2 \rangle$ invariant, i.e., $\langle \tilde{\Phi}_1 | \Phi_2 \rangle = \langle \tilde{\Psi}_1 | \Psi_2 \rangle$ for $|\Psi_i\rangle \mapsto |\Phi_i\rangle = \mathcal{U}|\Psi_i\rangle$, $i \in \{1, 2\}$ with two arbitrary states $|\Psi_i\rangle$. Such transformations must leave the dualisation operator invariant,

$$\mathcal{U}\mathcal{D}\mathcal{U}^\dagger = \mathcal{D} \tag{40}$$

which means in a magic basis

$$\mathcal{U}\mathcal{U}^T = \mathbf{1}. \tag{41}$$

It follows that $\mathcal{U}$ is, in a magic basis, real and orthogonal, $\mathcal{U} \in \mathrm{O}(d)$, $d = [4, 6, 3]$, and, since $\det \mathcal{U} = 1$, $\mathcal{U} \in \mathrm{SO}(d)$. In a general basis $\mathcal{U}$ is an element of the corresponding equivalent representation of $\mathrm{SO}(d)$. Thus, $M$ is just the special orthogonal group $\mathrm{SO}(d)$. Moreover, since $H$ is certainly contained in $M$, and $\mathrm{SO}(d)$ is in all three cases a representation of $H$, we have $M = H$. This result can of course also be achieved by a straightforward construction of $M$ in terms of its generators.

The fact that the group of "local transformations" is in all three cases identical to the unitary invariance group of the dualisation operator is peculiar to these small systems studied here. As an example, consider a system of $2n$ qubits. The generalization of the operator $\mathcal{D}$ is obvious, and, since the number of qubits is even, one also finds magic bases. Then the argument leading to the condition

(40) can be repeated in a straightforward way, with the conclusion that the invariance group of $\mathcal{D}$ is essentially $SO(2^{2n})$, containing $2^{2n-1}(2^{2n} - 1)$ independent parameters. In contrast, $H$ consists just of copies of $SU(2)$ and has $6n$ parameters. Thus only for $n = 1$ we find $M = H$; for larger $n$, $H$ is a proper subgroup of $M$. Similar arguments can be made for the generalization of the other two-particle systems to larger Hilbert spaces.

As we saw, $H$ contains in all of the three cases above all unitary transformations which turn the states of a given magic basis into another magic basis. This result is the key ingredient to prove a recent result by Kraus and Cirac for the two-qubit case [29] (also derived independently Khaneja and Glaser [30]). Here we shall just state the general result: Any unitary transformation $\mathcal{U} \in G$ of the full Hilbert space can be written in any magic basis as

$$\mathcal{U} = \mathcal{V}_1 \mathcal{U}_d \mathcal{V}_2 \tag{42}$$

with $\mathcal{V}_1, \mathcal{V}_2 \in H$ and $\mathcal{U}_d \in G$ diagonal. Thus, $\mathcal{U}_d$ contains $d - 1 = [3, 5, 2]$ independent parameters in the phase factors on its diagonal. Since the operations $\mathcal{V}_1, \mathcal{V}_2$ do not change the concurrence of any state, Eq. (42) constitutes a decomposition of a unitary transformation into parts which preserve "entanglement" and a part that does not. Therefore this decomposition is very helpful in the study of generation and deletion of entanglement in the course of a unitary transformation [29].

The proof of the statement made in Eq. (42) for all three cases is completely analogous to the one given in the appendix of Ref. [29] for the two-qubit case. For all systems the dimensions of the groups involved on the r.h.s. of Eq. (42) add up to give the dimension of the l.h.s. For analogous systems with larger Hilbert spaces such a decomposition of unitary transformations is in general not possible, as one can see from similar dimensional arguments as given above.

### 3.5. Summary

In this section we have studied three different two-body systems:

- Two distinguishable qubits with a four-dimensional total Hilbert space.
- Two indistinguishable fermions with a four-dimensional single-particle Hilbert space. The total two-particle space is six-dimensional.
- Two indistinguishable bosons in a two-dimensional single-particle space. The total two-particle space is three-dimensional.

These three systems share a series of properties:

- They represent the smallest systems (regarding the dimensions of the Hilbert spaces) which allow for nontrivial correlation effects, i.e., a correlation rank larger than one.
- In all three cases there is a *correlation measure*, the concurrence, related to an appropriately defined time reversal operator (dualisation). In the fermionic case this operator can be also interpreted as the anti-linear implementation of a particle-hole-transformation.
- In all three cases a *magic basis* exists that consists of states being invariant under the dualisation operator. Maximally correlated states (with a concurrence of one) have real coefficients (up to a common phase factor) when expressed in the magic basis.
- In the fermionic and bosonic case there are perfect analogues of Wootters' formula [27] for the correlation measure of mixed two-qubit states.
- In all three systems a general unitary transformation $\mathcal{U}$ of the full Hilbert space can be written (in the magic basis) as

$$\mathcal{U} = \mathcal{V}_1 \mathcal{U}_d \mathcal{V}_2, \tag{43}$$

where $\mathcal{U}_d$ is diagonal and $\mathcal{V}_1$, $\mathcal{V}_2$ are appropriate single-particle transformations. The result for the two-qubit case was derived recently in Refs. [29, 30].

- In all three cases the group of single-particle transformations and the group of unitary invariance transformations of the dualisation operator coincide. In higher-dimensional cases the invariance group of the dualisation operator is larger than the group of single-particle transformations.

Recently Verstraete *et al.* derived an explicit expression for a global unitary transformation which maximizes the entanglement of a given mixed state of two qubits [55]. Given the analogies derived above, we conjecture that the results of Ref. [55] can be applied to the other two systems studied here.

In fact all these analogies can be derived from the following observation: as explained a two-fermion system in a four-dimensional single-particle space can be realized by two electrons on two neighboring quantum dots, taking into account only the lowest orbital states and the spin degree of freedom. After a projection onto the subspace where each dot contains one and only one electron a two-qubit system remains. Finally we arrive at a system of two bosons in a two-dimensional single-particle space by symmetrization. In this sense the system of two fermions is the most general one. Therefore, the question of "why two qubits are special," posed recently by Vollbrecht and Werner [31], can be formulated more generally: *What is special about two fermions in a four-dimensional single-particle space?*

## 4. QUANTUM CORRELATIONS OF PURE FERMIONIC AND BOSONIC STATES IN HIGHER-DIMENSIONAL HILBERT SPACES

### 4.1. Two-Fermion States

As shown above, correlations of pure states of two fermions with a four-dimensional single-particle Hilbert space are characterized by the concurrence $\mathcal{C}(|w\rangle)$. In particular this quantity vanishes if and only if $|w\rangle$ has Slater rank one. As soon as larger Hilbert spaces are considered there is no straightforward extension of the concurrence. However, performing the Slater decomposition is always possible and thus correlations of a two-fermion system can be characterized by the Slater rank. Here we introduce criteria for pure states in a single-particle space of arbitrary (even) dimension $d = 2K$ that allow us to specify the Slater rank without explicitly performing the decomposition.

To begin, notice that in the case of $2K = 4$ the concurrence vanishes if and only if the general expression (18) for the determinant of an antisymmetric $2K \times 2K$-matrix is zero. Using this for general dimension $2K$ together with the block structure of $w$ in the canonical form it is clear that $|w\rangle$ has Slater rank $< K$ if and only if

$$\sum_{i_1,\ldots,i_{2K}=1}^{2K} \varepsilon^{i_1\ldots i_{2K}} w_{i_1 i_2} \ldots w_{i_{2K-1} i_{2K}} = 0. \tag{44}$$

Let us first turn to the case of $2K = 6$. Here it only remains to distinguish Slater rank one from Slater rank two/three. This can be done by

LEMMA 4.1.  *Let $|w\rangle = \sum_{i,j=1}^{6} w_{ij} f_i^\dagger f_j^\dagger |0\rangle$ be a two-fermion state in a six-dimensional single-particle space. Then $|w\rangle$ has Slater rank one if and only if $\forall \alpha, \beta$, with $1 \leq \alpha < \beta \leq 6$,*

$$\sum_{i,j,k,l=1}^{6} w_{ij} w_{kl} \varepsilon^{ijkl\alpha\beta} = 0. \tag{45}$$

The proof is given in Appendix B.1.

For $2K > 6$ this result can be generalized to classify the Slater rank of an arbitrary pure state of two fermions. The quantities to be calculated have an analogous structure: Slater rank two or higher is distinguished from Slater rank one by contraction of two $w$-matrices with the $\varepsilon$-tensor. Slater rank one and two can be distinguished from Slater rank three and above by contracting three $w$-matrices and so on until finally states with maximal Slater rank are identified by the full contraction of $K$ matrices. This is collected in the following lemma (see the Appendix for the proof):

LEMMA 4.2.    *A two-fermion state* $|w\rangle = \sum_{i,j=1}^{2K} w_{ij} f_i^\dagger f_j^\dagger |0\rangle \in \mathcal{A}(\mathcal{H}_{2K} \otimes \mathcal{H}_{2K})$ *has Slater rank* $<N$ *if and only if* $\forall \alpha_1, \ldots, \alpha_{2(K-N)}$, *with* $1 \leq \alpha_1 < \cdots < \alpha_{2(K-N)} \leq 2K$,

$$\sum_{i_1,\ldots,i_{2N}=1}^{2K} w_{i_1 i_2} \ldots w_{i_{2N-1} i_{2N}} \varepsilon^{i_1 \ldots i_{2N} \alpha_1 \ldots \alpha_{2(K-N)}} = 0. \tag{46}$$

### 4.2. Three- and Multi-Fermion States

Three identical fermions in a $2K$-dimensional single particle space $\mathcal{H}_{2K}$ live in a total Hilbert space $\mathcal{A}(\mathcal{H}_{2K} \otimes \mathcal{H}_{2K} \otimes \mathcal{H}_{2K})$. In the usual notation a general pure state is written

$$|w\rangle = \sum_{i,j,k=1}^{2K} w_{ijk} f_i^\dagger f_j^\dagger f_k^\dagger |0\rangle, \tag{47}$$

where $w$ is completely antisymmetric and fulfills the normalization condition

$$\sum_{i,j,k=1}^{2K} w_{ijk}^* w_{ijk} = \frac{1}{6}. \tag{48}$$

Because every single-particle state for fermions can only be occupied once, a particle-hole transformation $\mathcal{U}_{\mathrm{ph}}$ (cf. Eq. (20)) allows us to treat the cases $d = 2K = 4$ and $d = 5$ more easily: three fermions acting in a four-dimensional single-particle space are mapped by $\mathcal{U}_{\mathrm{ph}}$ onto one fermion (and thus such a state is never correlated) while a five-dimensional three-fermion state is mapped onto two fermions in five dimensions. This five-dimensional state can then always be embedded into a four-dimensional single particle space because the rank of the coefficient matrix is always even. Thus for $d = 4$ a state of three fermions is always non-correlated; for $d = 5$ the concurrence from Section 3.2 can be used. The lowest non-trivial systems of three fermions act in a single particle space of dimension $2K = 6$.

In the case of distinguishable particles it is well known that a straightforward generalization of the bi-orthogonal Schmidt decomposition to systems of more than two parties is not possible [56–58]. Not every three-quantum-bit state can be transformed via local unitary transformations into a sum of tri-orthogonal product states; i.e.,

$$|\psi\rangle = d_0 |0\rangle_A \otimes |0\rangle_B \otimes |0\rangle_C + d_1 |1\rangle_A \otimes |1\rangle_B \otimes |1\rangle_C \tag{49}$$

is not always possible.

Counting of dimensions shows that also for three fermions a canonical form consisting of a sum of elementary Slater determinants cannot exist. In the case of $2K = 6$ this would mean finding a unitary transformation $\mathcal{U}$ of the single particle space such that

$$w'_{lmn} = \sum_{i,j,k=1}^{2K} w_{ijk} U_{li} U_{mj} U_{nk} = z_1 \varepsilon^{lmn456} + z_2 \varepsilon^{123lmn}, \tag{50}$$

i.e., $|w'\rangle \propto z_1 f_1^\dagger f_2^\dagger f_3^\dagger |0\rangle + z_2 f_4^\dagger f_5^\dagger f_6^\dagger |0\rangle$, where by adjusting the phases of the basis states the $z_k$ can be chosen real and non-negative. In general such a form depends on $\lfloor 2K/3 \rfloor$ real numbers ($\lfloor x \rfloor$ is the largest integer $\leq x$), while a general three-fermion state has

$$2\left[\binom{2K}{3}\right] = \frac{(2K)^3 - 3(2K)^2 + 4K}{3} \tag{51}$$

parameters (including normalization and an overall phase). A unitary transformation $\mathcal{U}$ of the $2K$-dimensional single particle space has $(2K)^2$ real parameters. For the case of $2K = 6$ this means that a general state is described by 40 parameters while the desired Slater decomposed form only has two parameters. But then the 36 real numbers that can be chosen for the unitary transformation are not enough in general to solve the corresponding set of linear equations.

It is interesting that questions on multi-fermion pure states can be answered by projecting them onto pure states of fewer particles. For this purpose let us define an operator $R_{|a\rangle}$ with $|a\rangle = \sum_i a_i f_i^\dagger |0\rangle$, which projects the three-fermion state $|w\rangle$ on a two-fermion state $|\hat{w}\rangle$ supported at most on the single-particle space orthogonal to $|a\rangle$ and which is defined through the equation

$$|\hat{w}\rangle = R_{|a\rangle}|w\rangle = R_{|a\rangle} \sum_{i,j,k=1}^{2K} w_{ijk} f_i^\dagger f_j^\dagger f_k^\dagger |0\rangle = 3 \sum_{i,j=1}^{2K} \sum_{k=1}^{2K} w_{ijk} a_k f_i^\dagger f_j^\dagger |0\rangle. \tag{52}$$

The first thing to be noticed is that a decomposition of $|w\rangle$ into elementary non-overlapping Slater determinants only exists if there is a set $\{|e^\alpha\rangle\}_{\alpha=1,\ldots,2K}$, $\langle e^{\alpha_1}|e^{\alpha_2}\rangle = \delta^{\alpha_1\alpha_2}$ and $\mathcal{H}_{2K} = \mathrm{span}\{|e^\alpha\rangle\}$ such that $R_{|e^\alpha\rangle}|w\rangle$ has Slater rank one or is zero and $R_{|e^\alpha\rangle}|w\rangle$ is orthogonal to $R_{|e^\beta\rangle}|w\rangle$ if $\alpha \neq \beta$. In the basis where $|w\rangle$ has the desired block form this set is given by the set of basis vectors.

Following the definition of non-correlated states for two-fermion systems a three-fermion state is non-correlated if and only if it can be written as

$$|w\rangle = f_1^\dagger f_2^\dagger f_3^\dagger |0\rangle \tag{53}$$

in some basis. This is simply a Slater decomposable state with Slater rank one. These are also the states called "separable" in Ref. [44]. We first remark that here the particle-hole transformation does not help to identify or even to quantify quantum correlations as it did via the concurrence in the two-fermion case, because for a three-fermion state $|w\rangle$ we have $|\langle \tilde{w}|w\rangle| = |\langle w|(\mathcal{UK})^\dagger|w\rangle| \equiv 0$. This is analogous to three distinguishable qubits where $\langle \psi|(i\sigma_A^y) \otimes (i\sigma_B^y) \otimes (i\sigma_C^y)\mathcal{K}|\psi\rangle \equiv 0$ (cf. Eq. (14)) [31].

Instead of a direct translation of the concurrence there is a necessary and sufficient criterion for three-fermion pure states having Slater rank one, by using the projection defined above (the proof is given in Appendix B.1).

LEMMA 4.3.    *A three-fermion state* $|w\rangle = \sum_{i,j,k=1}^{2K} w_{ijk} f_i^\dagger f_j^\dagger f_k^\dagger |0\rangle \in \mathcal{A}(\mathcal{H}_{2K} \otimes \mathcal{H}_{2K} \otimes \mathcal{H}_{2K})$ *is not correlated* (*has Slater rank one*) *if and only if* $\forall |a\rangle \in \mathcal{H}_{2K}$,

$$R_{|a\rangle}|w\rangle = 3 \sum_{i,j=1}^{2K} \sum_{k=1}^{2K} w_{ijk} a_k f_i^\dagger f_j^\dagger |0\rangle \tag{54}$$

*has Slater rank one or is equal to the* $2K$-*dimensional zero.*

This lemma can be combined together with Lemma 4.2 (which allowed us to calculate the Slater rank of two-fermion states) to give

LEMMA 4.4. *A three-fermion pure state* $|w\rangle = \sum_{i,j,k=1}^{2K} w_{ijk} f_i^\dagger f_j^\dagger f_k^\dagger |0\rangle$ *has Slater rank one if and only if* $\forall \alpha_1, \ldots, \alpha_{2(K-2)}, 1 \le \alpha_1 < \cdots < \alpha_{2(K-2)} \le 2K$, *and* $\forall \vec{a} \in \mathcal{C}^{2K}$,

$$\sum_{i,j,k,l,m,n=1}^{2K} w_{ijk} a_i w_{lmn} a_l \varepsilon^{jkmn\alpha_1 \ldots \alpha_{2(K-2)}} = 0. \tag{55}$$

As an example consider

$$|w\rangle = x f_1^\dagger f_2^\dagger f_3^\dagger |0\rangle + y f_3^\dagger f_5^\dagger f_6^\dagger |0\rangle, \qquad w_{ijk} = \frac{1}{3}(x \varepsilon^{ijk456} + y \varepsilon^{12i4jk})|0\rangle, \qquad |x|^2 + |y|^2 = 1. \tag{56}$$

By Lemma 4.3, $|w\rangle$ does not have Slater rank one because for $\vec{a} = (0, 0, 1, 0, 0, 0)^T$

$$R_{|a\rangle}|w\rangle \propto x f_1^\dagger f_2^\dagger |0\rangle + y f_5^\dagger f_6^\dagger |0\rangle \tag{57}$$

has Slater rank two. Also evaluation of Lemma 4.4 shows that $|w\rangle$ does not have Slater rank one because it gives rise to the five conditions

$$a_3^2 x y = 0, \qquad a_1 a_3 x y = 0, \qquad a_2 a_3 x y = 0, \qquad a_3 a_5 x y = 0, \qquad a_3 a_6 x y = 0 \tag{58}$$

which are obviously violated by some choices of $\vec{a}$ as long as $x$ and $y$ are nonzero. Notice that also $|w\rangle$ cannot be written by a transformation of the single-particle space as a sum of orthogonal Slater determinants as

$$|w'\rangle \propto z_1 (f')_1^\dagger (f')_2^\dagger (f')_3^\dagger |0\rangle + z_2 (f')_4^\dagger (f')_5^\dagger (f')_6^\dagger |0\rangle, \quad \text{i.e., } w' \propto z_1 f_1^\dagger f_2^\dagger f_3^\dagger |0\rangle + z_2 f_4^\dagger f_5^\dagger f_6^\dagger |0\rangle, \tag{59}$$

because $R_{|b\rangle}|w'\rangle \ne 0$ for all $|b\rangle$ but $R_{|b\rangle}|w\rangle = 0$ for $|b\rangle = f_4^\dagger |0\rangle$ (or, equivalently, $\mathrm{rank}(w') > \mathrm{rank}(w)$). All the comments and results for three-fermion states can be carried over to systems consisting of $N$ identical fermions in a Hilbert space $\mathcal{A}(\mathcal{H}_{2K} \otimes \cdots \otimes \mathcal{H}_{2K})$. Here the lowest non-trivial dimension of the single-particle space is $2N$ since otherwise a treatment through a particle-hole transformation is easier. A general pure state reads

$$|w\rangle = \sum_{i_1,\ldots,i_N=1}^{2K} w_{i_1 \ldots i_N} f_{i_1}^\dagger \ldots f_{i_N}^\dagger |0\rangle, \qquad \sum_{i_1,\ldots,i_N=1}^{2K} w_{i_1 \ldots i_N}^* w_{i_1 \ldots i_N} = \frac{1}{N!}, \tag{60}$$

where $w$ is antisymmetric in all indices. Again for $N > 2$ a decomposition into orthogonal elementary Slater determinants is not possible in general, but a state equivalent to a pure separable state of distinguishable particles can be said to have Slater rank one if, by a transformation of the single-particle space, it can be cast into the form

$$|w'\rangle = f_1^\dagger \ldots f_N^\dagger |0\rangle. \tag{61}$$

This is a Slater decomposable state with Slater rank one and the definition again coincides with the definition of "separable" in Ref. [44]. The operator $R_{|a\rangle}$ can be generalized to a projector from a

system of $N$ to $N-1$ fermions as

$$R_{|a\rangle}|w\rangle = |\hat{w}\rangle \qquad \text{with } \hat{w}_{i_1...i_{N-1}} = N \sum_{i_N=1}^{2K} w_{i_1...i_N} a_{i_N} \tag{62}$$

and it is clear that the necessary criterion for the existence of a decomposition into orthogonal Slater determinants given above for three fermions also holds for more particles. Furthermore Lemma 4.3 can be translated as follows:

LEMMA 4.5. *A pure $N$-fermion state has Slater rank one if and only if*

$$\forall |a\rangle \in \mathcal{H}_{2K}, \qquad R_{|a\rangle}|w\rangle = N \sum_{i_1,...,i_N=1}^{2K} w_{i_1...i_N} a_{i_N} f_{i_1}^\dagger \cdots f_{i_{N-1}}^\dagger |0\rangle \tag{63}$$

*has Slater rank one or is zero.*

The proof can be found in Appendix B.1. The lemma is maybe easier to handle if it is given in the following form:

LEMMA 4.6. *A pure $N$-fermion state has Slater rank one if and only if $\forall \alpha_i$, with $1 \leq \alpha_1 < \cdots < \alpha_{2(K-2)} \leq 2K$, and for all $\vec{a}^1, \ldots, \vec{a}^{N-2} \in \mathcal{C}^{2K}$,*

$$\sum_{\substack{i_1,...i_N=1 \\ j_1,...j_N=1}}^{2K} w_{i_1...i_N} \alpha_{i_1}^1 \cdots a_{i_{N-2}}^{N-2} w_{j_1...j_N} a_{j_1}^1 \cdots a_{j_{N-2}}^{N-2} \varepsilon^{i_{N-1} i_N j_{N-1} j_N \alpha_1 ... \alpha_{2(K-2)}} = 0. \tag{64}$$

Here Lemma 4.5 is simply used several times, thereby reducing the number of fermions in the system to $N-1$, $N-2$ and so on until Lemma 4.2 can be applied to the resulting two-fermion state.

As an example illustrating this lemma and showing that the straightforward extension of the two-fermion concurrence using the particle-hole transformation fails, let

$$|w\rangle = \sum_{i,j,k,l=1}^{2K} w_{ijkl} f_i^\dagger f_j^\dagger f_k^\dagger f_l^\dagger |0\rangle, \qquad w_{ijkl} = x\varepsilon^{ijkl5678} + y\varepsilon^{ij34kl78} + z\varepsilon^{12ijkl78}. \tag{65}$$

To see that this is a correlated state take $\vec{a} = (0, 1, 0, 0, 0, 0, 0, 0)^{\mathrm{T}}$ to get $R_{|a\rangle}|w\rangle = x f_1^\dagger f_3^\dagger f_4^\dagger |0\rangle + y f_1^\dagger f_5^\dagger f_6^\dagger |0\rangle$, which after some permutation of the basis is proporational to the three-fermion correlated state from Eq. (56). Thus also $|w\rangle$ does not have Slater rank one. Nevertheless

$$|\tilde{w}\rangle = U_{ph}\mathcal{K}|w\rangle = \sum_{\substack{i,j,k,l=1 \\ m,n,o,p=1}}^{2K} \varepsilon^{ijklmnop} w_{ijkl}^* f_m^\dagger f_n^\dagger f_o^\dagger f_p^\dagger |0\rangle \tag{66}$$

and therefore $\langle \tilde{w} \mid w \rangle = 0$ although $|w\rangle$ contains correlations.

## 4.3. Two-Boson States

Next we will apply the concept of assessing correlations by identifying the Slater number to bosonic pure states. Given a two-boson state $|v\rangle = \sum v_{ij} b_i^\dagger b_j^\dagger$ with $v_{ij} = v_{ji}$, a distinction between maximal and non-maximal Slater rank is provided by the vanishing of $\det v$ in the latter case, i.e., by considering the full contraction of $K$ $v$-matrices with two $K$-dimensional $\varepsilon$-tensors. For a finer distinction in the case of a three-dimensional single-particle space we have.

LEMMA 4.1. *Let* $|v\rangle = \sum_{i,j=1}^{3} v_{ij} b_i^\dagger b_j^\dagger |0\rangle$ *be a two-boson state in a three-dimensional single particle space. Then* $|v\rangle$ *has Slater rank one if and only if* $\forall 1 \leq \alpha \leq 3$,

$$\sum_{i,j,k,l=1}^{3} v_{ij} v_{kl} \varepsilon^{ik\alpha} \varepsilon^{jl\alpha} = 0. \tag{67}$$

This can be extended to higher-dimensional single-particle spaces essentially as for fermions. The result is the following lemma which is the bosonic equivalent to Lemma 4.2 (the proof is sketched in Appendix B.2):

LEMMA 4.2. *Let* $|v\rangle$ *be a two-boson state in* $\mathcal{A}(\mathcal{H}_K \otimes \mathcal{H}_k)$. $|v\rangle$ *has Slater rank* $<N$ *if and only if* $\forall \alpha_1, \ldots, \alpha_{K-N}$, *with* $1 \leq \alpha_1 < \alpha_{K-N} \leq K$,

$$\sum_{i_1,\ldots,i_{2N}=1}^{K} v_{i_1 i_2} v_{i_3 i_4} \ldots v_{i_{2N-1} i_{2N}} \varepsilon^{i_1 i_3 \ldots i_{2N-1} \alpha_1 \alpha_{K-N}} \varepsilon^{i_2 i_4 \ldots i_{2N} \alpha_1 \alpha_{K-N}} = 0. \tag{68}$$

## 4.4. Three- and Multi-Boson States

For three bosons in a two-dimensional single-particle space a general state $|v\rangle$ has 8 real parameters while a unitary transformation of the single-particle space has 4. This shows that, similar to the fermionic case, a straightforward generalization of the two-boson Slater decomposition is not possible, i.e., $|v\rangle$ cannot always be written as $|v\rangle = (z_1 b_1^\dagger b_1^\dagger b_1^\dagger + z_2 b_2^\dagger b_2^\dagger b_2^\dagger)|0\rangle$. The same holds for $N$-boson states with $N \geq 3$.

A special case of $N$-boson states that indeed are Slater decomposable are non-correlated states that we are going to define now by generalizing the definition for two-boson systems:

DEFINITION 4.1. A pure $N$-boson state $|v\rangle$ is non-correlated (is Slater decomposable and has Slater rank one) if in some basis it can be written

$$|v\rangle = \frac{1}{\sqrt{N}} b_1^\dagger \ldots b_1^\dagger |0\rangle, \qquad \text{i.e., } v_{i_1 \ldots i_N} = \frac{1}{\sqrt{N}} \prod_{j=1}^{N} \delta_{i_j 1}. \tag{69}$$

It is worth noticing that this definition differs slightly from the one in Ref. [44] where $|v\rangle$ is also called non-correlated if it can be written $|v\rangle = (1/\sqrt{N}) b_1^\dagger \ldots b_N^\dagger |0\rangle$ in some basis where the $b_i^\dagger$ are orthogonal.

If we define an operator $R_{|a\rangle}$ for $|a\rangle = \sum_i a_i b_i^\dagger |0\rangle$ that projects from a system of $N$ to a system of $N-1$ bosons (cf. Eqs. (52) and (62)),

$$|\hat{v}\rangle = R_{|a\rangle} |v\rangle = \sum_{i_1,\ldots,i_N,j=1}^{K} v_{i_1 \ldots i_N} a_j b_j b_{i_1}^\dagger \ldots b_{i_N}^\dagger |0\rangle = N \sum_{i_1 \ldots i_N=1}^{K} v_{i_1 \ldots i_N} a_{i_N} b_{i_1}^\dagger \ldots b_{i_{N-1}}^\dagger |0\rangle \tag{70}$$

(here the result is not necessarily only supported on the single-particle space orthogonal to $|a\rangle$), then an identification of non-correlated states is possible.

LEMMA 4.3. *A pure N-boson state* $|v\rangle$ *has Slater rank one if and only if the* $N-1$*-boson state*

$$R_{|a\rangle} |v\rangle = N \sum_{i_1,\ldots,i_N=1}^{2K} v_{i_1 \ldots i_N} a_{i_N} b_{i_1}^\dagger \ldots b_{i_{N-1}}^\dagger |0\rangle \tag{71}$$

*has Slater rank one or is zero* $\forall |a\rangle \in \mathcal{H}_{2K}$.

It is worth noticing that this lemma is also valid if, instead of Definition 4.1, the definition from Ref. [44] is used. However, concentrating on Definition 4.1, it is possible to iterate Lemma 4.3 until a two-boson state is left and Lemma 4.2 can be applied. Thus we have

LEMMA 4.4.   *An N-boson pure state has Slater rank one if and only if* $\forall \alpha_i$ *with* $1 \leq \alpha_1 < \cdots < \alpha_{K-2} \leq K$, *and for all* $\vec{a}^1, \ldots, \vec{a}^{N-2} \in \mathcal{C}^{2K}$,

$$\sum_{\substack{i_1,\ldots i_N=1 \\ j_1,\ldots j_N=1}}^{K} v_{i_1 \ldots i_N} a_{i_1}^{(1)} \ldots a_{i_{N-2}}^{(N-2)} v_{j_1 \ldots j_N} a_{j_1}^{(1)} \ldots a_{j_{N-2}}^{(N-2)} \varepsilon^{i_{N-1} j_{N-1} \alpha_1 \ldots \alpha_{K-2}} \varepsilon^{i_N j_N \alpha_1 \ldots \alpha_{K-2}} = 0. \tag{72}$$

## 5. QUANTUM CORRELATIONS IN MIXED FERMIONIC STATES

In this section we repeat for the completeness of the present paper the main results of Ref. [43] concerning mixed states of two identical fermions. Part of these results, concerning the two-fermion system with a four-dimensional single particle space, has been already discussed in Section 2. In this case the question of the Slater rank of a given mixed state can be answered exactly. Here we concentrate thus on the general case, for which no exact answers are known in general.

### 5.1. Slater Number of Mixed Fermionic States

Let us now generalize the concepts introduced in Section 2 to the case of fermionic mixed states with a single-particle space of arbitrary dimension. To this end, we define formally the Slater number of a mixed state, in analogy to the Schmidt number for the case of distinguishable parties [59, 60]:

DEFINITION 5.1.    Consider a density matrix $\rho$ of a two-fermion system, and all its possible convex decompositions in terms of pure states, i.e., $\rho = \sum_i p_i |\psi\rangle_i^{r_i} \langle \psi|_i^{r_i}$, where $r_i$ denotes the Slater rank of $|\psi\rangle_i^{r_i}$; the Slater number of $\rho$, $k$, is defined as $k = \min\{r_{\max}\}$, where $r_{\max}$ is the maximum Slater rank within a decomposition, and the minimum is taken over all decompositions.

In other words, there exists a decomposition of $\rho$ that uses pure states with Slater rank not exceeding $k$, and there is no construction that only uses pure states with Slater rank smaller than $k$.

Many of the results concerning Schmidt numbers can be transferred directly to the Slater number. For instance, let us denote the whole space of density matrices in $\mathcal{A}(\mathcal{C}^{2K} \otimes \mathcal{C}^{2K})$ by $Sl_K$, and the set of density matrices that have Slater number $k$ or less by $Sl_k$. $Sl_k$ is a convex compact subset of $Sl_K$. A state from $Sl_k$ will be called a state of (Slater) class $k$. Sets of increasing Slater number are embedded into each other, i.e., $Sl_1 \subset Sl_2 \subset \ldots Sl_k \ldots \subset Sl_K$. In particular, $Sl_1$ is the set of states that can be written as a convex combination of elementary Slater determinants; $Sl_2$ is the set of states of Slater number 2, i.e., those that require at least one pure state of Slater rank 2 for their formation, etc.

The determination of the Slater number of a given state is in general a very difficult task. Similarly, however, as in the case of separability of mixed states of two qubits (i.e., states in $\mathcal{C}^2 \otimes \mathcal{C}^2$), and one qubit–one qutrit (i.e., states in $\mathcal{C}^2 \otimes \mathcal{C}^3$) [61], the situation is particularly simple in the case of small $K$. For $K = 1$ there exists only one state (a singlet). For $K = 2$ we have presented in Section 2 a necessary and sufficient condition for a given mixed state to have a Slater number of one. We have also defined the Slater correlation measure in analogy to Wootters' result [27], relating separability to a quantity called concurrence, and to eigenvalues of a certain matrix. One should note, however, that in the considered case of fermionic states there exists no simple analogy of the partial transposition, which is essential for the theory of entangled states of distinguishable particles. In fact, the Peres–Horodecki criterion [61, 62] in $2 \times 2$ and $2 \times 3$ spaces says that a state is separable if and only if its partial transpose is positive semidefinite. The results of Section 2 can be formulated as the following theorem:

THEOREM 5.1.   *Let the mixed state acting in $\mathcal{A}(\mathcal{C}^4 \otimes \mathcal{C}^4)$ have a spectral decomposition $\rho = \sum_{i=1}^{r} |\Psi_i\rangle\langle\Psi_1|$, where $r$ is the rank of $\rho$, and the eigenvectors $|\Psi_i\rangle$ belonging to nonzero eigenvalues $\lambda_i$ are normalized as $\langle\Psi_i|\Psi_j\rangle = \lambda_i \delta_{ij}$. Let $|\Psi_i\rangle = \sum_{a,b} w_{ab}^i f_a^\dagger f_b^\dagger |0\rangle$ in some basis, and define the complex symmetric $r \times r$ matrix $C$ by*

$$C_{ij} = \sum_{abcd} \varepsilon^{abcd} w_{ab}^i w_{cd}^j, \tag{73}$$

*which can be represented using a unitary matrix as $C = U C_d U^T$, with $C_d = \mathrm{diag}[c_1, c_2, \ldots, c_r]$ diagonal and $|c_1| \geq |c_2| \geq \cdots \geq |c_r|$. The state $\rho$ has Slater number 1 if and only if*

$$|c_1| \leq \sum_{i=2}^{r} |c_i|. \tag{74}$$

The above theorem is thus an analogue of the Peres–Horodecki–Wootters result for two-fermion systems having a single particle space of dimension $2K \leq 4$. The situation is much more complicated, when we go to $K > 2$; this is similar to the case of the separability problem in $\mathcal{C}^M \otimes \mathcal{C}^N$ with $MN > 6$. These issues are ivestigated in the next subsection.

At this point it is worth stressing that our formalism can also be used for odd dimensions, i.e., formally for half-integer $K$. Here the situation is again particularly simple for $K = 1.5$ ($2K = 3$). All states have obviously the Slater number one and can thus be written as a convex sum of projectors onto states equivalent to the single state $|0\rangle|1\rangle - |1\rangle|0\rangle$, which implies that the entanglement of formation of any antisymmetric mixed state (treated as a state of two distinguishable particles) is 1 ebit.

## 5.2. Fermionic Slater Witnesses

We now investigate fermionic systems with single-particle Hilbert spaces of dimension $2K > 4$. In this case, a full and explicit characterization of pure and mixed state quantum correlations, such as given above for the two-fermion system with $K = 2$, is apparently not possible. Therefore one has to formulate other methods to investigate the Slater number of a given state. We can, however, as in Ref. [43] follow here the lines of the papers that we have written on entanglement witnesses [63, 64], and Schmidt number witnesses [60]. In the following we skip the proofs, which are discussed in detail in Ref. [43].

In order to determine the Slater number of a fermionic density matrix $\rho$ we note that due to the fact that the sets $Sl_k$ are convex and compact, any density matrix of class $k$ can be decomposed into a convex combination of a density matrix of class $k - 1$, and a remainder $\delta$ [65]:

PROPOSITION 5.1.   *Any state of class $k$, $\rho_k$, can be written as a convex combination of a density matrix of class $k - 1$ and a so-called $k$-edge state $\delta$,*

$$\rho_k = (1 - p)\rho_{k-1} + p\delta, \qquad 1 \geq p > 0, \tag{75}$$

*where the edge state $\delta$ has Slater number $\geq k$.*

The decomposition (75) is obtained by subtracting projectors onto pure states of Slater rank smaller than $k$, $P = |\psi^{<k}\rangle\langle\psi^{<k}|$ such that $\rho_k - \lambda P \geq 0$. Here $|\psi^{<k}\rangle$ stands for pure states of Slater rank $r < k$. Denoting by $K(\rho)$, $R(\rho)$, and $r(\rho)$ the kernel, range, and rank of $\rho$, respectively, we observe that $\rho' \propto \rho - \lambda|\psi\rangle\langle\psi|$ is non-negative if and only if $|\psi\rangle \in R(\rho)$ and $\lambda \leq \langle\psi|\rho^{-1}|\psi\rangle^{-1}$ (see [65]). The idea behind this decomposition is that the edge state $\delta$ which has generically lower rank contains all the information concerning the Slater number $k$ of the density matrix $\rho_k$.

As in the case of the Schmidt number, there is an optimal decomposition of the form (75) with $p$ minimal. Alternatively, restricting ourselves to decompositions $\rho_k = \sum_i p_i |\psi\rangle_i^{r_i} \langle\psi|_i^{r_i}$ with all $r_i \leq k$, we can always find a decomposition of the form (75) with $\delta \in Sl_k$. We define below more precisely what an edge state is.

DEFINITION 5.2.    A fermionic $k$-edge state $\delta$ is a state such that $\delta - \varepsilon |\psi^{<k}\rangle\langle\psi^{<k}|$ is not positive, for any $\varepsilon > 0$ and $|\psi^{<k}\rangle$.

The edge states are thus characterized by the following

*Criterion 5.1.*    A mixed state $\delta$ is a $k$-edge state if and only if there exists no $|\psi^{<k}\rangle$ such that $|\psi^{<k}\rangle \in R(\delta)$.

Now we are in the position of defining a fermionic $k$-Slater witness ($k$-SlW, $k \geq 2$):

DEFINITION 5.3.    A hermitian operator $W$ is a fermionic Slater witness (SlW) of class $k$ if and only if $\mathrm{Tr}(W\sigma) \geq 0$ for all $\sigma \in Sl_{k-1}$, and there exists at least one fermionic $\rho \in Sl_k$ such that $\mathrm{Tr}(W\rho) < 0$.

It is straightforward to see that every SlW that detects $\rho$ given by (75) also detects the edge state $\delta$, since if $\mathrm{Tr}(W\rho) < 0$ then necessarily $\mathrm{Tr}(W\delta) < 0$, too. Thus, the knowledge of all SlWs of $k$-edge states fully characterizes all $\rho \in Sl_k$. Below, we show how to construct for any edge state a SlW which detects it. Most of the technical proofs used to construct and optimize fermionic Slater witnesses are practically equivalent to those presented in Ref. [63] for entanglement witnesses.

All the operators we consider in this subsection act in $\mathcal{A}(\mathcal{C}^{2K} \otimes \mathcal{C}^{2K})$. Let $\delta$ be a $k$-edge state, $C$ an arbitrary positive operator such that $\mathrm{Tr}(\delta C) > 0$, and $P$ a positive operator whose range fulfills $R(P) = K(\delta)$. We define $\varepsilon \equiv \inf_{|\psi^{<k}\rangle} \langle\psi^{<k}|P|\psi^{<k}\rangle$ and $c \equiv \sup\langle\psi|C|\psi\rangle$. Note that $c > 0$ by construction and $\varepsilon > 0$, because $R(P) = K(\delta)$ and therefore, since $R(\delta)$ does not contain any $|\psi^{<k}\rangle$ by the definition of edge state, $K(P)$ cannot contain any $|\psi^{<k}\rangle$ either. This implies:

LEMMA 5.1.    *Given a fermionic $k$-edge state $\delta$, then*

$$W = P - \frac{\varepsilon}{c}C \tag{76}$$

*is a fermionic $k$-SlW which detects $\delta$.*

The simplest choice of $P$ and $C$ consists in taking projections onto $K(\delta)$ and the identity operator on the antisymmetric space $\mathbb{I}_a$, respectively. As we will see below, this choice provides us with a canonical form of a fermionic $k$-SlW.

PROPOSITION 5.2.    *Any fermionic Slater witness can be written in the canonical form,*

$$W = \tilde{W} - \varepsilon\mathbb{I}_a, \tag{77}$$

*such that $R(\tilde{W}) = K(\delta)$, where $\delta$ is a $k$-edge state and $0 < \varepsilon \leq \inf_{|\psi^{<k}\rangle} \langle\psi|\tilde{W}|\psi\rangle$.*

It is useful to consider also

DEFINITION. 5.4.    A $k$-Slater witness $W$ is *tangent* to $Sl_{k-1}$ at $\rho$ if $\exists$ a state $\rho \in Sl_{k-1}$ such that $\mathrm{Tr}(W\rho) = 0$.

Similar methods to the ones used in Ref. [43] allow us to prove Proposition 5.2 and to observe that

*Observation 5.1.*    The fermionic state $\rho$ is of Slater class $k - 1$ if and only if for all fermionic $k$-SW's tangent to $Sl_{k-1}$, $\mathrm{Tr}(W\rho) \geq 0$.

### 5.2.1. *Optimal Fermionic Slater Witnesses*

We will now discuss the optimization of a fermionic Slater witness. As proposed in [60, 63] an entanglement witness (Schmidt witness) W is optimal if there exists no other witness that detects more states than it. The same definition can be applied to fermionic Slater witnesses. We say that a fermionic $k$-Slater witness $W_2$ is finer than a fermionic $k$-Slater witness $W_1$, if $W_2$ detects more fermionic states than $W_1$. Analogously, we define a $k$-Slater witness $W$ to be optimal when there exists no finer witness than itself. Let us define the set of $|\psi\rangle$ pure states of Slater rank $k-1$ for which the expectation value of the $k$-Slater witness $W$ vanishes,

$$T_W = \{|\psi\rangle \text{ such that } \langle\psi|W|\psi\rangle = 0\}, \tag{78}$$

i.e., the set of pure tangent states of Slater rank $<k$. $W$ is an optimal $k$-SlW if and only if $W - \varepsilon P$ is not a $k$-SlW, for any positive operator $P$. If the set $T_W$ spans the whole Hilbert space $\mathcal{A}(\mathcal{C}^{2K} \otimes \mathcal{C}^{2K})$, then $W$ is an optimal $k$-SlW. If $T_W$ does not span $\mathcal{A}(\mathcal{C}^{2K} \otimes \mathcal{C}^{2K})$, then we can optimize the witness by subtracting from it a positive operator $P$, such that $PT_W = 0$. For example, for Slater witnesses of class 2 this is possible, provided that $\inf_{|e\rangle \in \mathcal{C}^{2K}} [P_e^{-1/2} W_e P_e^{-1/2}]_{\min} > 0$. Here for any $X$ acting on $\mathcal{A}(\mathcal{C}^{2K} \otimes \mathcal{C}^{2K})$ we define

$$X_e = [\langle e, .|X|e, .\rangle - \langle e, .|X|., e\rangle - \langle ., e|X|e, .\rangle + \langle ., e|X|., e\rangle], \tag{79}$$

as an operator acting in $\mathcal{C}^{2K}$, and $[X]_{\min}$ denotes its minimal eigenvalue (see [63]). An example of an optimal witness of Slater number $k$ in $\mathcal{A}(\mathcal{C}^{2K} \otimes \mathcal{C}^{2K})$ is given by

$$W = \mathbb{1}_a - \frac{K}{k-1}\mathcal{P}, \tag{80}$$

where $\mathcal{P}$ is a projector onto a "maximally correlated state," $|\Psi\rangle = (1/\sqrt{K}) \sum_{i=1}^{K} f_{2i}^\dagger f_{2i+1}^\dagger |0\rangle$. The reader can easily check that the above witness operator has mean value zero in the states $f_{2i}^\dagger f_{2i+1}^\dagger |0\rangle$ for $i = 1, 2$, but also for all states of the form $g_1^\dagger g_2^\dagger |0\rangle$ where

$$g_1^\dagger = f_1^\dagger e^{i\varphi_{11}} + f_2^\dagger e^{i\varphi_{12}} + f_3^\dagger e^{i\varphi_{21}} + f_4^\dagger e^{i\varphi_{22}}, \tag{81}$$

$$g_2^\dagger = -f_1^\dagger e^{-i\varphi_{12}} + f_2^\dagger e^{-i\varphi_{11}} - f_3^\dagger e^{-i\varphi_{22}} + f_4^\dagger e^{-i\varphi_{21}}, \tag{82}$$

for arbitrary $\varphi_{ij}, i, j = 1, 2$. The set $T_W$ spans in this case the whole Hilbert space $\mathcal{A}(\mathcal{C}^{2K} \otimes \mathcal{C}^{2K})$, *ergo* $W$ is optimal.

### 5.2.2. *Fermionic Slater Witnesses and Positive Maps*

It is interesting also to consider positive maps associated with fermionic Slater witnesses via the Jamiołkowski isomorphism [18]. Such maps employ $W$ acting in $\mathcal{H}_A \otimes \mathcal{H}_B = \mathcal{C}^{2K} \otimes \mathcal{C}^{2K}$ and transform a state $\rho$ acting in $\mathcal{H}_A \otimes \mathcal{H}_C = \mathcal{C}^{2K} \otimes \mathcal{C}^{2K}$ into another state acting in $\mathcal{H}_B \otimes \mathcal{H}_C = \mathcal{C}^{2K} \otimes \mathcal{C}^{2K}$, via the relation $M(\rho) = \text{Tr}_A(W\rho^{T_A})$. Obviously, such maps are positive on separable states: When $\rho$ is separable, then for any $|\Psi\rangle \in \mathcal{H}_B \otimes \mathcal{H}_C$, the mean value of $\langle\Psi|M(\rho)|\Psi\rangle$, becomes a convex sum of mean values of $W$ in some product states $|e, f\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$. Since $W$ acts in fact in the antisymmetric space, we can antisymmetrize these states, i.e., $|e, f\rangle \to (|e, f\rangle - |f, e\rangle)$. Such antisymmetric states have, however, Slater rank 1, and all SlW of class $k \geq 2$ have thus positive mean value in those states. This class of positive maps is quite different from the ones considered in Refs. [63, 64]; they provide thus an interesting class of necessary separability conditions. The particular map associated with the witness (80) is, however, decomposable; i.e., it is a sum of a completely positive map and another

completely positive map composed with the transposition. This follows from the fact that $W^{T_A} = Q$ is a positive operator and from $M(\rho) = \text{Tr}_A(W\rho^{T_A}) = \text{Tr}_A(Q\rho) = M_Q(\rho^{T_A}) = (M_Q \circ T_A)(\rho)$ where $M_Q(X) = \text{Tr}_A(QX^{T_A})$ is a completely positive map because $Q$ is a positive operator.

## 6. QUANTUM CORRELATIONS IN MIXED BOSONIC STATES

Here we present new results that generalize the previous section to the case of bosons. The case of a two-boson system with a two-dimensional single-particle space, where the Slater number of a given mixed state can be calculated directly, has already been discussed (cf. Section 3). The concern of this section is thus a single particle Hilbert space $\mathcal{C}^K$ with $K > 2$. We discuss also the relation of the Slater number and positive definiteness of the partial transpose.

### 6.1. Slater Number of Mixed Bosonic States

Following the results from the previous section we may define formally the Slater number $k$ of a bosonic mixed state.

DEFINITION 5.1′.  Consider a density matrix $\rho$ of a two-boson system, and all its possible convex decompositions in terms of pure states, i.e., $\rho = \sum_i p_i |\psi|_i^{r_i} \langle \psi|_i^{r_i}$, where $r_i$ denotes the Slater rank of $|\psi\rangle_i^{r_i}$; the Slater number of $\rho$, $k$, is defined as $k = \min\{r_{max}\}$, where $r_{max}$ is the maximum Slater rank within a decomposition, and the minimum is taken over all decompositions.

Most of the results concerning Slater numbers for fermions can be transferred directly to the Slater number for bosons. If we denote the whole space of density matrices in $\mathcal{S}(\mathcal{C}^{2K} \otimes \mathcal{C}^{2k})$ by $Sl_K$, and the set of density matrices that have Slater number $k$ or less by $Sl_k$, then $Sl_k$ as in the previous section is a convex compact subset of $Sl_K$; a state from $Sl_k$ will be called a state of (Slater) class $k$. Sets of increasing Slater number are embedded into each other, i.e., $Sl_1 \subset Sl_2 \subset \ldots Sl_k \ldots \subset Sl_K$. In particular, $Sl_1$ is the set of states that can be written as a convex combination of elementary Slater permanents. There exists, however, one very basic difference between bosonic and fermionic systems; in the latter case, namely, the concept of partial transposition seems to be completely inappropriate. On the other hand, since in bosonic systems $Sl_1$ is the set of separable states, partial transposition provides here a necessary condition for a state to belong to $Sl_1$. For bosonic systems it is thus reasonable to ask questions of the sort: Do bosonic entangled states with positive partial transpose (PPTES) exist?

For the case of $K = 2$ a necessary and sufficient condition for a mixed state to have a Slater number one is given either by the Peres–Horodecki criterion, i.e., by the positivity of the partial transpose, or by the Wootters approach as discussed in Section 3. The latter result we state again in the following theorem:

THEOREM 5.1′.  *Let the bosonic mixed state acting in $\mathcal{S}(\mathcal{C}^2 \otimes \mathcal{C}^2)$ have a spectral decomposition $\rho = \sum_{i=1}^r |\Psi_i\rangle\langle\Psi_i|$, where $r$ is the rank of $\rho$, and the eigenvectors $|\Psi_i\rangle$ belonging to nonzero eigenvalues $\lambda_i$ are normalized as $\langle\Psi_i|\Psi_j\rangle = \lambda_i \delta_{ij}$. Let $|\Psi_i\rangle = \sum_{a,b} v_{ab}^i b_a^\dagger b_b^\dagger |\Omega\rangle$ in some basis and define the complex symmetric $r \times r$ matrix $C$ by*

$$C_{ij} = \sum_{abcd} \varepsilon^{ac} \varepsilon^{bd} v_{ab}^i v_{cd}^j, \tag{83}$$

*($\varepsilon^{01} = -\varepsilon^{10} = 1$, and $\varepsilon^{aa} = 0$ otherwise) which can be represented using a unitary matrix as $C = UC_dU^T$, with $C_d = \text{diag}[c_1, c_2, \ldots, c_r]$ diagonal and $|c_1| \geq |c_2| \geq \cdots \geq |c_r|$. The state $\rho$ has Slater*

*number* 1 *if and only if*

$$|c_1| \le \sum_{i=2}^{r} |c_i|. \tag{84}$$

### 6.2. Bosonic Slater Witnesses

We now turn to the more difficult case of $K > 2$ where as for fermions no complete characterization of pure and mixed state quantum correlations can be given. Again the concept of witnesses turns out to be useful here and we can directly translate most of the fermionic results from Section 5.2. We will only list the theorems here and skip the proofs which are discussed in detail in [43].

PROPOSITION 5.1′. *Any bosonic state of class* $k$, $\rho_k$, *can be written as a convex combination of a density matrix of class* $k - 1$ *and a so-called bosonic* $k$-*edge state* $\delta$,

$$\rho_k = (1 - p)\rho_{k-1} + p\delta, \qquad 1 \ge p > 0, \tag{85}$$

*where the edge state* $\delta$ *has Slater number* $\ge k$.

This again follows from the convexity and compactness of the sets $Sl_k$. As in the case of fermions, there is an optimal decomposition of the form (85) with $p$ minimal. Alternatively, restricting ourselves to decompositions $\rho_k = \sum_i p_i |\psi\rangle_i^{r_i} \langle\psi|_i^{r_i}$ with all $r_i \le k$, we can always find a decomposition of the form (85) with $\delta \in Sl_k$. This allows us to define $k$-edge states and $k$-Slater witnesses as in the fermionic case.

DEFINITION 5.2′. *A bosonic* $k$-*edge state* $\delta$ *is a bosonic state such that* $\delta - \varepsilon|\psi^{<k}\rangle\langle\psi^{<k}|$ *is not positive, for any* $\varepsilon > 0$ *and* $|\psi^{<k}\rangle$.

CRITERION 5.1′. *A bosonic mixed state* $\delta$ *is a bosonic* $k$-*edge state if and only if there exists no* $|\psi^{<k}\rangle$ *such that* $|\psi^{<k}\rangle \in R(\delta)$.

DEFINITION 5.3′. *A hermitian operator* $W$ *is a bosonic Slater witness of class* $k$ ($k$-*SlW*, $k \ge 2$) *if and only if* $\mathrm{Tr}(W\sigma) \ge 0$ *for all* $\sigma \in Sl_{k-1}$, *and there exists at least one bosonic* $\rho \in Sl_k$ *such that* $\mathrm{Tr}(W\rho) < 0$.

With the same definitions as in the paragraph before Lemma 5.1 in Section 5.2 (but now all the operators act in the symmetric space $\mathcal{S}(\mathcal{C}^K \otimes \mathcal{C}^K)$) we have

LEMMA 5.1′. *Given a bosonic* $k$-*edge state* $\delta$, *then*

$$W = P - \frac{\varepsilon}{c}C \tag{86}$$

*is a bosonic* $k$-*SlW which detects* $\delta$.

Similarly as in Section 5.2, the simplest choice of $P$ and $C$ consists in taking projections onto $K(\delta)$ and the identity operator on the symmetric space $\mathbb{1}_s$, respectively.

PROPOSITION 5.2′. *Any bosonic Slater witness can be written in the canonical form,*

$$W = \tilde{W} - \varepsilon\mathbb{1}_s, \tag{87}$$

*such that* $R(\tilde{W}) = K(\delta)$, *where* $\delta$ *is a bosonic* $k$-*edge state and* $0 < \varepsilon \le \inf_{|\psi^{<k}\rangle}\langle\psi|\tilde{W}|\psi\rangle$.

### 6.2.1. *Optimal Bosonic Slater Witnesses*

We will now discuss the optimization of bosonic Slater witnesses, applying the same definitions of finer and optimal as for fermions. Again we have that if the set $T_W$ of pure tangent states of Slater rank $<k$,

$$T_W = \{|\psi\rangle \text{ such that } \langle\psi|W|\psi\rangle = 0\}, \tag{88}$$

spans the complete Hilbert space $\mathcal{S}(\mathcal{C}^K \otimes \mathcal{C}^K)$, then $W$ is an optimal $k$-SlW. Otherwise we can optimize the witness by subtracting from it a positive operator $P$, such that $P T_W = 0$. For example, for Slater witnesses of class 2 this is possible provided that $\inf_{|e\rangle \in \mathcal{C}^K} [P_e^{-1/2} W_e P_e^{-1/2}]_{\min} > 0$. Here for any $X$ acting on $\mathcal{S}(\mathcal{C}^K \otimes \mathcal{C}^K)$ we define

$$X_e = [\langle e, .|X|e, .\rangle + \langle e, .|X|., e\rangle + \langle ., e|X|e, .\rangle + \langle ., e|X|., e\rangle], \tag{89}$$

as an operator acting in $\mathcal{C}^K$, and $[X]_{\min}$ denotes its minimal eigenvalue (compare [63]). An example of an optimal bosonic witness of Slater number $k$ in $\mathcal{S}(\mathcal{C}^K \otimes \mathcal{C}^K)$ is given by

$$W = \mathbb{I}_s - \frac{K}{k-1}\mathcal{P}, \tag{90}$$

where $\mathcal{P}$ is a projector onto a "maximally correlated state," $|\Psi\rangle = (1/\sqrt{K}) \sum_{a=1}^{K} b_a^\dagger b_a^\dagger |\Omega\rangle$. That this witness is optimal can be seen as in Section 5.2.1.

Finally we only want to mention that it is again possible to relate positive maps to bosonic Slater witnesses, leading to another interesting class of necessary separability conditions. As for fermions (cf. Section 5.2.1) the map associated with the witness (90) is decomposable.

### 6.3. Bosonic Entangled States and Positive Partial Transpose

In the case of distinguishable particles there are strong indications that the Schmidt rank of entangled states with the PPT property is not maximal, and rather low. This has been conjectured for the states in a $3 \times 3$-dimensional space in Ref. [60], and for the states in a $N \times N$-dimensional space in Ref. [66]. We expect that similar situations take place for the Slater rank of bosonic states. In fact we have not been able to find a two-boson mixed state that would have the PPT property and would be nevertheless entangled; i.e., it would have Slater rank strictly greater than 1. For bosonic 3-qubit states as well as for bosonic $N$-qubit states of rank $\leq N$ we were even able to prove that such states do not exist.

Our findings are summarized in the following two theorems. The first one deals with the case of $K = 3$, i.e., three-dimensional single-particle space, but can be easily generalized to arbitrary $K$. The second one deals with bosonic systems of $N$ qubits, i.e., $N$ bosons in a two-dimensional single particle space.

THEOREM 6.1.    *Let a bosonic mixed state $\rho$ acting in $\mathcal{S}(\mathcal{C}^3 \otimes \mathcal{C}^3)$, which we treat as a symmetrized space of Alice and Bob, have a positive partial transpose with respect to, say, Alice. Then*

(I)    *If the rank of $\rho$, $r(\rho) = 3$, then the Slater rank of $\rho$, $Sl(\rho) = 1$; i.e., $\rho$ is separable.*

(II)    *If the rank of $\rho$, $r(\rho) = 4$, then generically there exist exactly 4 product vectors of the form $|e_i, e_i\rangle$ in the range of $\rho$, and the Slater rank of $\rho$, $Sl(\rho) = 1$, i.e., $\rho$ is separable, provided $\langle e_i, e_i|\rho^{-1}|e_j, e_j\rangle = p_i \delta_{ij}$, where the inverse is taken on the range. In such case $\rho \sum_{i=1}^{4} p_i |e_i, e_i\rangle \langle e_i, e_i|$.*

*Proof.* This theorem is a simple generalization of the result of Ref. [67]. In particular from Theorem 1 of that paper it follows that any (symmetric or not) PPT state of rank 3 is separable, which proves (I). To prove (II), we observe that the vector $|e, e\rangle$ is in the range of $\rho$ if it is orthogonal to vectors which span the kernel of $\rho$. There are two such vectors $|\phi_j\rangle$, $j = 1, 2$, since the whole space $\mathcal{S}(\mathcal{C}^3 \otimes \mathcal{C}^3)$ is 6 dimensional. Since in a convenient basis up to normalization we can write $|e\rangle = (1, z_1, z_2)$, the equations $\langle \phi_j | e, e \rangle = 0$ constitute a system of two quadratic polynomials in $z_1$ and $z_2$. Such a system of equations has generically 4 solutions $|e_i, e_i\rangle$, $i = 1, \ldots, 4$. From that it follows that $\rho$ is separable if and only if $\rho = \sum_{i=1}^{4} p_i |e_i, e_i\rangle \langle e_i, e_i|$. Using this equation, we observe that if $\rho^{-1}|e_i, e_i\rangle = |v\rangle$, then $|e_i, e_i\rangle = \rho|v\rangle$ and from the linear independence of $|e_i, e_i\rangle$ we get that $\langle e_j, e_j | v \rangle = 0$ for $j \neq i$, and $\langle e_i, e_i | v \rangle = 1$. This implies that $\langle e_i, e_i | \rho^{-1} | e_j, e_j \rangle = p_i \delta_{ij}$. ∎

THEOREM 6.2. *Let a bosonic mixed state $\rho$ acting in the symmetric $N$-qubit space $\mathcal{S}(\mathcal{C}^2 \otimes \cdots \otimes \mathcal{C}^2)$, which we treat as a symmetrized space of Alice, Bob, Charlie, etc., have a positive partial transpose with respect to, say, Alice. For $N > 3$ let $r(\rho) \leq N$. Then $\rho$ is separable.*

*Proof.* Let us consider first the case $N = 3$. The state $\rho$ is bosonic, i.e., has a maximal rank 4, which is the dimension of the space of totally symmetric vectors. Suppose that the state $\rho$ is, however, also a PPT state with respect to Alice. We can treat it then as a PPT state in a $2 \times 4$ dimensional space of Alice and Bob and Charlie grouped together. Such a state of rank 4 is necessarily separable and can be represented as $\rho = \sum_{i=1}^{4} p_i |e_i, \Psi_i\rangle \langle e_i, \Psi_i|$, where the projectors onto the vectors $|\Psi_i\rangle$ are in general entangled pure states of Bob and Charlie [68]. Since they belong to the range of the reduced density matrix $\text{Tr}_A \rho$, they must belong to $\mathcal{S}(\mathcal{C}^2 \otimes \mathcal{C}^2)$. Obviously, the vectors $|e_i, \Psi_i\rangle$ belong to the range of $\rho$, and thus to the symmetric space $\mathcal{S}(\mathcal{C}^2 \otimes \mathcal{C}^2 \otimes \mathcal{C}^2)$. Direct inspection shows that the only vectors of this from are $|e_i, e_i, e_i\rangle$: writing the Schmidt decomposition $|\Psi_i\rangle = a|00\rangle + b|11\rangle$, and expanding $|e_i\rangle = \alpha|0\rangle + \beta|1\rangle$ in the same basis, we immediately see that both $\alpha b$ and $\beta a$ must be equal to zero.

The proof for higher $N$ is analogous. We assume that $\rho$ has rank $\leq N$ and a positive partial transpose with respect to Alice. Since $\rho$, regarded as a matrix acting in a $2 \times 2^{N-1}$-dimensional space, is supported in reality in $\mathcal{C}^2 \otimes \mathcal{S}((\mathcal{C}^2)^{\otimes N-1})$, i.e., in a $2 \times N$-dimensional space, the results of Ref. [68] hold and $\rho$ must be separable with respect to the partition Alice − the rest, and therefore have a form $\rho = \sum_{i=1}^{N} p_i |e_i, \Psi_i\rangle \langle e_i, \Psi_i|$. But then, using the analogous argumentation as above, we see that $|e_i, \Psi_i\rangle = |e_i, e_i, \ldots, e_i\rangle$.

# 7. CONCLUSIONS

In conclusion, we have studied and characterized quantum correlations in systems of (i) two distinguishable particles, (ii) two fermions, and (iii) two bosons. As an equivalent to the well-known Schmidt decomposition and rank for distinguishable particles we introduced the concepts of Slater decomposition and rank, i.e., writing fermionic and bosonic pure states as sums of orthogonal Slater determinants or permanents, respectively.

For the case of the smallest non-trivial Hilbert space we were able to identify interesting properties shared by all these systems: an appropriate time reversal operator allows us to define a *correlation measure*, the *concurrence*, which can also be expressed through the coefficients of a state in the so-called *magic basis*. This also allows for perfect analogues of Wootters' formula [27] for the correlation measure of mixed two-qubit states. As we noted, these analogies follow directly if the system of two fermions in a four-dimensional single-particle space is considered as the most general one from which the other two can be derived.

Subsequently we analyzed systems of fermions or bosons in higher-dimensional single-particle spaces and systems of more than two indistinguishable particles. There is no straightforward extension of the results obtained for low-dimensional Hilbert spaces. We gave necessary and sufficient criteria to

identify the Slater rank of pure two-particles states by contractions of the $\varepsilon$-tensor with its coefficient matrix. These results are sufficient to classify quantum correlations of pure states in arbitrary-dimensional single-particle spaces. For the case of three or more indistinguishable particles it was first established that a general state cannot be written as a sum of orthogonal Slater determinants, which demonstrates yet another analogy to distinguishable particles. We showed that non-correlated pure states can be identified through projections of the multi-particle state onto states of two fermions.

For general two-fermion mixed states we reviewed the concept of witnesses of Slater number $k$ and introduced a similar concept for bosons. In both cases we showed how to optimize these witnesses and gave an example of an optimal witness.

Finally we explored the role of the PPT criterion in bosonic systems. We gave separability criteria for low-rank two-boson mixed states in a three-dimensional single-particle space having a positive partial transpose. We also showed that there are no bosonic three-qubit states that have a positive partial transpose and nevertheless contain quantum correlations. The same is true for bosonic $N$-qubit states of rank $\leq N$.

## APPENDIXES

### A. Mode Correlations

Here we discuss briefly the rather complementary concept to deal with fermionic correlations introduced by Zanardi [41]. Again consider the quantum dot example and suppose the system evolves to a state (here we neglect interaction of the particles)

$$|\tilde{\psi}'\rangle = \frac{1}{2}[|\phi\rangle|\uparrow\rangle \otimes |\phi\rangle|\downarrow\rangle + |\chi\rangle|\uparrow\rangle \otimes |\chi\rangle|\downarrow\rangle + |\phi\rangle|\downarrow\rangle \otimes |\phi\rangle|\uparrow\rangle + |\chi\rangle|\downarrow\rangle \otimes |\chi\rangle|\uparrow\rangle] \tag{91}$$

$$= \frac{1}{\sqrt{2}}[f_{\phi,\uparrow}^{\dagger} f_{\phi,\downarrow}^{\dagger} + f_{\chi,\uparrow}^{\dagger} f_{\chi,\downarrow}^{\dagger}]|0\rangle. \tag{92}$$

If the tunneling barrier is raised in this state then either Alice or Bob finds two electrons in their dot; i.e., there is no particle entanglement present here. But if we forget about the spin and map the two particle basis state $f_i^{\dagger} f_j^{\dagger}|0\rangle$ onto $|n_\phi\rangle \otimes |n_\chi\rangle$, where $n_\phi$ and $n_\chi$ are the occupation numbers of the left and the right dot, respectively, then the result is a state $\propto |2\rangle \otimes |0\rangle + |0\rangle \otimes |2\rangle$. This is an entangled state, but now the entangled entities are not the particles themselves but "modes." Each mode is associated with (in this case more than one) creation operator $f_i^{\dagger}$.

This is the concept of mode entanglement. In [41, 42] correlations are analyzed not by looking at the particles themselves but by partitioning the state space into different modes. In the simplest case these modes are associated with the $2K$ single particle basis states such that the occupation number is either 0 or 1 in the case of fermions. These $2K$ modes are then mapped onto the space of $2K$ qubits such that the $k$th qubit is in state $|1\rangle$ (state $|0\rangle$) if the $k$th mode is occupied (not occupied).

More formally this mapping is describe for the basis states of $N$ fermions as [41]

$$\Lambda : \mathcal{H}_{2K}^F(N) \rightarrow (\mathcal{C}^2)^{\otimes 2K} \tag{93}$$

$$f_{i_1}^{\dagger} \ldots f_{i_N}^{\dagger}|0\rangle \rightarrow \otimes_{k=1}^{2K}|\chi(k; i_1, \ldots, i_N)\rangle \tag{94}$$

(for $i_1 < \cdots < i_N$) and linearly extended to the complete Hilbert space. The characteristic function $\chi$ is defined as

$$\chi(k; i_1, \ldots, i_N) = \begin{cases} 1, & k \in \{i_1, \ldots, i_N\} \\ 0, & k \notin \{i_1, \ldots, i_N\}. \end{cases} \tag{95}$$

The mapping is not bijective in this form as not all possible $K$-qubit states are realized, i.e., $\mathcal{H}_{2K}^F(N)$ is not isomorphic to this space. An isomorphism can be formed by not fixing the number of fermions in the system, i.e., by considering

$$\Lambda : \mathcal{H}_{2K}^F \to (\mathcal{C}^2)^{\otimes 2K}, \tag{96}$$

where $\mathcal{H}_{2K}^F = \otimes_{N=1}^{2K} \mathcal{H}_{2K}^F(N)$ is the total Fock space of $0, \ldots, 2K$ fermions. Notice that this point might raise problems in concrete applications as it requires sources and drains to adjust the number of particles.

### B. Proofs (Quantum Correlations of Pure Fermionic and Bosonic States in Higher-Dimensional Hilbert Spaces)

Here we give proofs of some of the lemmas on indistinguishable particles in higher-dimensional Hilbert spaces from Section 4.

### B.1. *Fermionic States*

First notice that according to Eq. (6) for any complex antisymmetric $2K \times 2K$ coefficient matrix $w$ there is a unitary transformation $\mathcal{U}$ such that

$$w'_{ij} = (UwU^T)_{ij} = z_1 \varepsilon^{ij34\ldots(2K)} + z_2 \varepsilon^{12ij56\ldots(2K)} + \cdots + z_K \varepsilon^{12\ldots ij}, \tag{97}$$

where $\varepsilon^{i_1,\ldots i_{2K}}$ is the totally antisymmetric unit tensor in $2K \times \cdots \times 2K$ and $z_k \geq 0$.

*Proof of Lemma 4.1.* [$\Rightarrow$] Consider the case $\alpha = 5$, $\beta = 6$. In the sum all terms with at least one $i, j, k, l \in \{5, 6\}$ vanish, and thus

$$\sum_{i,j,k,l}^{6} w_{ij} w_{kl} \varepsilon^{ijkl56} = \sum_{i,j,k,l}^{4} w_{ij} w_{kl} \varepsilon^{ijkl} = C(|v\rangle), \tag{98}$$

where $|v\rangle = v_{ij} f_i^\dagger f_j^\dagger |0\rangle \in \mathcal{A}(\mathcal{H}_4 \otimes \mathcal{H}_4)$ and $v_{ij}$ is constructed from $w_{ij}$ by deleting the last two columns and rows.

Because by assumptions $|w\rangle$ has Slater rank 1 also $|v\rangle$ has to have Slater rank 1 unless $|v\rangle = 0$. In both cases $C(|v\rangle)$ has to vanish. The same argument can be repeated for every combination of $\alpha$ and $\beta$ (only deleting different rows and columns from the coefficient matrix $w$).

[$\Leftarrow$] We will show the negated claim: there is at least one sum that does not vanish if $|w\rangle$ has Slater rank $> 1$. The two possible cases to be distinguished are Slater rank three or Slater rank two. If the Slater rank is three then $w$ has full rank and thus $\det(w) \neq 0$. Using the expression for the determinant of an antisymmetric matrix from Eq. (18) it holds

$$48 \det(w) = \sum_{\alpha,\beta=1}^{6} w_{\alpha\beta} \underbrace{\sum_{i,j,k,l=1}^{6} w_{ij} w_{kl} \varepsilon^{ijkl\alpha\beta}}_{x^{\alpha\beta}} \neq 0, \tag{99}$$

implying that at least one $x^{\alpha\beta} \neq 0$.

If $|w\rangle$ has Slater rank 2 then $r\{w\} = 4$ and we can find a unitary transformation $\mathcal{U}$ such that

$$w'_{i'j'} = \sum_{i,j=1}^{6} U_{i'i} w_{ij} U_{j'j} \tag{100}$$

contains only zeros in the last two rows and columns. $|w\rangle$ has Slater rank 2 if and only if $|w'\rangle = \sum_{i,j} w'_{ij}(f')_i^\dagger (f')_j^\dagger |0\rangle$ has Slater rank 2 and it follows ($w'$ is a $4 \times 4$ matrix only and thus it is possible to use the concurrence from Section 3 which does not vanish if and only if $|w'\rangle$ has Slater rank 2)

$$0 \neq C(|w'\rangle) = \sum_{i,j,m,n=1}^{4} w'_{ij} w'_{mn} \varepsilon^{ijmn} \tag{101}$$

$$= \sum_{i,j,m,n=1}^{6} w'_{ij} w'_{mn} \varepsilon^{ijmn56} \tag{102}$$

$$= \sum_{\substack{i,j,m,n=1 \\ i',j',m',n'=1}}^{6} U_{ii'} w_{i'j'} U_{jj'} U_{mm'} w_{m'n'} U_{nn'} \varepsilon^{ijmn56} \tag{103}$$

$$= \sum_{\substack{i,j,m,n=1 \\ i',j',m',n'=1}}^{6} w_{i'j'} w_{m'n'} \underbrace{U_{ii'} U_{jj'} U_{mm'} U_{nn'} \varepsilon^{ijmn56}}_{\tilde{\varepsilon}^{i'j'm'n'}}. \tag{104}$$

It is easy to verify that $\tilde{\varepsilon}^{i'j'm'n'}$ is also antisymmetric in all indices so it has to have the form

$$\tilde{\varepsilon}^{i'j'm'n'} = \xi_{56} \varepsilon^{i'j'm'n'56} + \xi_{46} \varepsilon^{i'j'm'n'46} + \cdots + \xi_{12} \varepsilon^{i'j'm'n'12} \tag{105}$$

(where some but not all $\xi_{\alpha\beta}$ may be zero) and then

$$0 \neq \sum_{i',j',m',n'=1}^{6} w_{i'j'} w_{m'n'} (\xi_{56} \varepsilon^{i'j'm'n'56} + \xi_{46} \varepsilon^{i'j'm'n'46} + \cdots + \xi_{12} \varepsilon^{i'j'm'n'12}) \tag{106}$$

$$0 \neq \sum_{\alpha\beta=1}^{6} \xi_{\alpha\beta} \underbrace{\sum_{i',j',k',l'=1}^{6} \varepsilon^{i'j'k'l'\alpha\beta} w_{i'j'} w_{k'l'}}_{x^{\alpha\beta}} \tag{107}$$

such that again at least one $x^{\alpha\beta} \neq 0$.

*Proof of Lemma 4.2.* If $N = K$ then the claim is that $|w\rangle$ does not have maximal Slater rank if and only if

$$\sum_{i_1,\ldots,i_{2K}=1}^{2K} w_{i_1 i_2} \cdots w_{i_{2K-1} i_{2K}} \varepsilon^{i_1 \ldots i_{2K}} = 0. \tag{108}$$

This is the statement of Eq. (18) so Lemma 4.2 surely holds for all cases $[K = N, N]$. This is the starting point for giving the proof by induction. For a combination $[K, N](N < K)$ the assumption will be that the lemma holds for $[K, N+1]$, $[K-1, N]$ and $[N, N]$ (Fig. 5 illustrates the induction process).
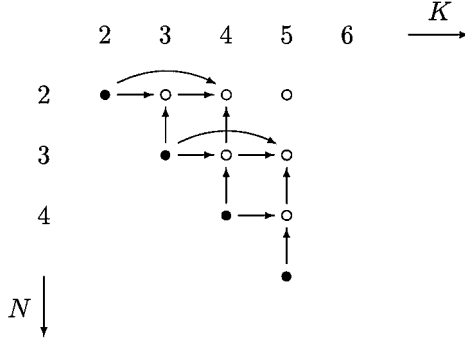
**FIG. 5.** Construction of the proof of Lemma 4.2 by induction. Black dots mark the combinations $[K = N, N]$ where Eq. (18) can be applied.

[$\Rightarrow$]   Introduce a two-fermion state $|v\rangle \in \mathcal{A}(\mathcal{H}_{2K-2} \otimes \mathcal{H}_{2K-2})$ by constructing its coefficient matrix $v$ from $w$ by deleting the rows and columns $\alpha_{2(K-N)}$ and $\alpha_{2(K-N)-1}$. Since $|w\rangle$ is assumed to have Slater rank $<N$ also $|v\rangle$ has to have Slater rank $<N$ (because its mathematical rank cannot raise when some rows and columns are deleted). Then it follows

$$\sum_{i_1,\ldots,i_{2N}=1}^{2K} w_{i_1 i_2} \ldots w_{i_{2N-1} i_{2N}} \varepsilon^{i_1 \ldots i_{2N} \alpha_1 \ldots \alpha_{2(K-N)}} \tag{109}$$

$$= \sum_{i_1,\ldots,i_{2N}=1}^{2(K-1)} v_{i_1 i_2} \ldots v_{i_{2N-1} i_{2N}} \varepsilon^{i_1 \ldots i_{2N} \alpha_1 \ldots \alpha_{2(K-1-N)}} = 0, \tag{110}$$

because by assumption the lemma holds for $K - 1$ and $N$.

[$\Leftarrow$]   We will show that there is at least one non-vanishing sum if the Slater rank is $\geq N$. Then if all terms vanish the Slater rank has to be $<N$. Again there are two cases to be distinguished:

*Case 1.*   $|w\rangle$ has Slater rank $>N$. By assumption the lemma holds for $[K, N+1]$ and thus

$$0 \neq \sum_{i_1,\ldots,i_{2N+2}=1}^{2K} w_{i_1 i_2} \ldots w_{i_{2N+1} i_{2N+2}} \varepsilon^{i_1 \ldots i_{2N+2} \alpha_1 \ldots \alpha_{2(K-N-1)}} \tag{111}$$

for at least one combination of $\alpha_1, \ldots, \alpha_{2(K-N-1)}$. But then

$$0 \neq \sum_{i_{2N+1}, i_{2N+2}}^{2K} w_{i_{2N+1} i_{2N+2}} \underbrace{\sum_{i_1,\ldots,i_{2N}}^{2K} w_{i_1 i_2} \ldots w_{i_{2N-1} i_{2N}} \varepsilon^{i_1 \ldots i_{2N} i_{2N+1} i_{2N+2} \alpha_1 \ldots \alpha_{2(K-N-1)}}}_{x^{i_{2N+1} i_{2N+2} \alpha_1 \ldots \alpha_{2(K-N-1)}}} \tag{112}$$

such that at least one $x^{i_{2N+1} i_{2N+2} \alpha_1 \ldots \alpha_{2(K-N-1)}} \neq 0$.

*Case 2.*   $|w\rangle$ has Slater rank $N$. Then $r\{w\} = 2N$ and there is a unitary transformation $U \in SU(2K)$ such that

$$w'_{i' j'} = \sum_{i,j=1}^{2K} U_{i'i} w_{ij} U_{j'j} \tag{113}$$

contains zeros in the last $(2K - 2N)$ columns and rows. $|w'\rangle$ also has to have Slater rank N and because the lemma is assumed to be valid for $[K = N, N]$ it holds

$$0 \neq \sum_{i_1,\ldots,i_{2N}=1}^{2N} w'_{i_1 i_2} \ldots w'_{i_{2N-1} i_{2N}} \varepsilon^{i_1 \ldots i_{2N}} \tag{114}$$

$$= \sum_{i_1,\ldots,i_{2N}=1}^{2K} w'_{i_1 i_2} \ldots w'_{i_{2N-1} i_{2N}} \varepsilon^{i_1 \ldots i_{2N}(2N+1)\ldots(2K)} \tag{115}$$

$$= \sum_{\substack{i_1 \ldots i_{2N}=1 \\ j'_1 \ldots j'_{2N}=1}}^{2K} U_{i_1 j'_1} w'_{j'_1 j'_2} U_{i_2 j'_2} \ldots U_{i_{2N-1} j'_{2N-1}} w'_{j'_{2N-1} j'_{2N}} U_{i_{2N} j'_{2N}} \varepsilon^{i_1 \ldots i_{2N}(2N+1)\ldots(2K)} \tag{116}$$

$$= \sum_{j'_1 \ldots j'_{2N}=1}^{2K} w_{j'_1 j'_2} \ldots w_{j'_{2N-1} j'_{2N}} \underbrace{\sum_{i_1 \ldots i_{2N}=1}^{2K} U_{i_1 j'_1} \ldots U_{i_{2N} j'_{2N}} \varepsilon^{i_1 \ldots i_{2N}(2N+1)\ldots(2K)}}_{\tilde{\varepsilon}^{j'_1 \ldots j'_{2N}(2N+1)\ldots(2K)}}. \tag{117}$$

$\tilde{\varepsilon}^{j'_1 \ldots j'_{2N}(2N+1)\ldots(2K)}$ has to be antisymmetric in all indices so it has the form

$$\tilde{\varepsilon}^{j'_1 \ldots j'_{2N}(2N+1)\ldots(2K)} = \sum_{\alpha_1,\ldots,\alpha_{2(K-N)}=1}^{2K} \xi_{\alpha_1 \ldots \alpha_{2(K-N)}} \varepsilon^{j'_1 \ldots j'_{2N} \alpha_1 \ldots \alpha_{2(K-N)}} \tag{118}$$

(some but not all $\xi$ might be zero) and then

$$0 \neq \sum_{\alpha_1 \ldots \alpha_{2(K-N)}=1}^{2K} \xi_{\alpha_1 \ldots \alpha_{2(K-N)}} \underbrace{\sum_{j'_1 \ldots j'_{2N}=1}^{2K} w_{j'_1 j'_2} \ldots w_{j'_{2N-1} j'_{2N}} \varepsilon^{j'_1 \ldots j'_{2N} \alpha_1 \ldots \alpha_{2(K-N)}}}_{x^{\alpha_1 \ldots \alpha_{2(K-N)}}}, \tag{119}$$

where at least one $x^{\alpha_1 \ldots \alpha_{2(K-N)}} \neq 0$ is necessary.

*Proof of Lemma 4.3.* [$\Rightarrow$] $|w\rangle$ has Slater rank one so there exists $U$, $UU^\dagger = 1$, such that

$$w'_{ijk} = w_{lmn} U_{li} U_{mj} U_{nk} = z \varepsilon^{ijk456\ldots2K}. \tag{120}$$

Then, for arbitrary $|a\rangle$ and writing $|a'\rangle = U^\dagger |a\rangle$, we have

$$|v'\rangle = R_{|a'\rangle} |w'\rangle \quad \text{with } v'_{ij} = 3 \sum_{k=1}^{2k} w'_{ijk} a'_k = \sum_{k,l=1}^{2K} z \varepsilon^{ijk456\ldots2K} a_l U^*_{kl} = (A \oplus 0)_{ij} \tag{121}$$

with the $3 \times 3$ antisymmetric matrix $A$ and 0 as the $(2K - 3) \times (2K - 3)$-dimensional zero. $A$ has rank zero or two and thus there exists unitary $V$ such that

$$(V v' V^T)_{ij} = \beta \varepsilon^{ij345\ldots(2K)} \tag{122}$$

for some $\beta$. Inserting Eqs. (120) and (121) shows that $|v\rangle = R_{|a\rangle}|w\rangle$ indeed has Slater rank one (if $\beta \neq 0$):

$$\beta \varepsilon^{ij345...(2K)} = \sum_{l,m,n,o,p,q=1}^{2K} V_{im} w_{opq} U_{mo} U_{np} U_{kq} a_l U_{kl}^* V_{jn} \tag{123}$$

$$= \sum_{o,p,q=1}^{2K} (U^T V)_{oi} w_{opq} a_q (U^T V)_{pj}. \tag{124}$$

[$\Leftarrow$]  Here we make use of the fact that an $N$-fermion state $|w\rangle$ (coefficient matrix $w$) in a $2K$-dimensional single-particle space has Slater rank one (it can, after some transformation of the single-particle basis, be written as a single Slater determinant) if and only if there exists a set of orthonormal vectors $\{\vec{e}^\alpha\}_{\alpha=1,...,K}$ with $\vec{e}^\alpha \cdot \vec{e}^\beta = \delta^{\alpha\beta}$, such that for $\alpha_1, \ldots, \alpha_N \in \{1, \ldots, 2K\}$

$$w_{ijk} e_i^{\alpha_1} \ldots e_k^{\alpha_N} = z e^{\alpha_1 ... \alpha_N(N+1)...(2K)}. \tag{125}$$

These vectors are the columns of the matrix $U$ that transforms the single particle space.

Choose an arbitrary $\vec{e}^1$, $|\vec{e}^1| = 1$, such that $v_{jk} = \sum_i w_{ijk} e_i^1$ is not the $2K \times 2K$-dimensional zero. The resulting two fermion state $|v\rangle$ by assumptions has Slater rank 1 and thus there exist $\vec{e}^2, \vec{e}^3, \ldots,$ $\vec{e}^{2K}$ such that $\vec{e}^\alpha \vec{e}^\beta = \delta^{\alpha\beta}$ and

$$\sum_{j,k=1}^{2K} v_{jk} e_j^\alpha e_k^\beta = \sum_{i,j,k=1}^{2K} w_{ijk} e_i^1 e_j^\beta e_k^\gamma = z\varepsilon^{1\beta\gamma 4...(2K)}. \tag{126}$$

But we furthermore claim that $|w\rangle$ has Slater rank one:

$$\sum_{i,j,k=1}^{2K} w_{ijk} e_i^\alpha e_j^\beta e_k^\gamma = z\varepsilon^{\alpha\beta\gamma 4...(2K)} \qquad \text{for } \alpha, \beta, \gamma \in \{1 \ldots 2K\}. \tag{127}$$

Because of Eq. (126) this is obvious if $(\alpha, \beta, \gamma)$ is a permutation of $(1, 2, 3)$ and otherwise if $\alpha = 1$. So further attention has only to be paid to the cases where $1 < \alpha < \beta < \gamma$.

Consider $|v^\alpha\rangle$ with $v_{jk}^\alpha = \sum w_{ijk} e_k^\alpha$ for $1 < \alpha \leq 3$. By assumption the two-fermion state $|v^\alpha\rangle$ has Slater rank one (or is zero) and thus there is at most a two-dimensional subspace $\mathcal{M}$ such that for any two $\vec{a} \in \mathcal{M}$ and $\vec{b} \in \mathcal{M}$, $\vec{a} \neq \vec{b}$, $\sum w_{ijk} e_i^\alpha a_j b_k \neq 0$. Because of Eq. (126), $\mathcal{M}$ is spanned by $\vec{e}^\beta, \vec{e}^\gamma$ where $\{\beta, \gamma\} = \{1, 2, 3\} \setminus \{\alpha\}$. The $\vec{e}$'s are orthogonal and thus $w_{ijk} e_i^\alpha e_j^{\beta'} e_k^{\gamma'} = 0$ if $1 < \alpha < 4$ and $\alpha < \beta' < \gamma'$.

For $3 < \alpha < \beta < \gamma$ fixed suppose $\sum w_{ijk} e_i^\alpha e_j^\beta e_k^\gamma \neq 0$. Then there exist a two-dimensional subspace $\mathcal{M}$ spanned by $\vec{e}^2$ and $\vec{e}^3$ and an orthogonal subspace $\mathcal{N}$ spanned by $\vec{e}^\beta$ and $\vec{e}^\gamma$ such that $\sum w_{ijk} [e_i^1 + e_i^\alpha] a_j b_k \neq 0$ for $\vec{a}$ and $\vec{b}$ both in $\mathcal{M}$ or both in $\mathcal{N}$ and $\vec{a} \neq \vec{b}$. This contradicts the assumption that $R_{|e^1\rangle+|e^\alpha\rangle}|w\rangle$ has Slater rank one.

*Proof of Lemma 4.5.*  [$\Rightarrow$] $|w\rangle$ has Slater rank one; i.e., we can find $\vec{e}^1, \ldots, \vec{e}^{2K}$ such that

$$\sum_{i_1,...,i_N=1}^{2K} w_{i_1...i_N} e_{i_1}^{\alpha_1} \ldots e_{i_N}^{\alpha_N} = z\varepsilon^{\alpha_1...\alpha_N(N+1)...(2k)}. \tag{128}$$

Now consider $v_{i_1...i_{N-1}} = \sum w_{i_1...i_N} x_{i_N}$ for arbitrary $\vec{x}$. If $\vec{x} = \vec{e}^\alpha$ then $|v\rangle$ has Slater rank 1 if $\alpha \leq N$

or is zero if $\alpha > N$. Otherwise it holds that

$$\sum_{i_{N-1}=1}^{2K} v_{i_1 \dots i_{N-1}} e_{i_{N-1}}^{\alpha} = 0 \quad \text{for } \alpha > N \qquad \text{and} \qquad \sum_{i_{N-1}=1}^{2K} v_{i_1 \dots i_{N-1}} x_{i_{N-1}} = 0 \tag{129}$$

and we can choose $\vec{b}^{\alpha} = \vec{e}^{\alpha}$ for $\alpha > N$, $\vec{b}^N = \vec{x}$, and the remaining $\vec{b}^{\alpha}$ for $\alpha < N$ such that $\vec{b}^{\alpha_1} \vec{b}^{\alpha_2} = \delta^{\alpha_1 \alpha_2}$ to get

$$\sum_{i_1, \dots, i_{N-1}=1}^{2K} v_{i_1 \dots i_{N-1}} b_{i_1}^{\alpha_1} \dots b_{i_{N-1}}^{\alpha_{N-1}} = \tilde{z} \varepsilon^{\alpha_1 \dots \alpha_{N-1} N \dots (2K)} \tag{130}$$

which means that $|v\rangle$ has Slater rank one if $\tilde{z} \neq 0$ and is zero otherwise.

[$\Leftarrow$]   This is similar to the three-fermion case.

## B.2. *Bosonic States*

*Proof of Lemma 4.1.*   [$\Rightarrow$] Let $|v\rangle$ have Slater rank one and for any $1 \leq \alpha \leq 3$ let $v'$ be the $2 \times 2$-matrix that results from deleting the row and column $\alpha$. If $|v\rangle$ has Slater rank one then also $|v'\rangle = \sum_{i,j=1}^{2} v'_{ij} b_i^{\dagger} b_j^{\dagger} |0\rangle$ has Slater rank one (unless it is zero) and the claim follows from Eq. (30).

[$\Leftarrow$]   We will show that at least one sum in Eq. (67) does not vanish if $|v\rangle$ has Slater rank larger than one. The two possible cases are Slater rank three and Slater rank two. If the Slater rank is three then $v$ has full rank and $\det v \neq 0$. There exists a unitary transformation $U$ of the single particle space such that

$$v'_{i'j'} = \sum_{i,j=1}^{3} U_{ii'} v_{i'j'} U_{jj'} \tag{131}$$

is diagonal. In this basis

$$0 \neq 3! \det v' = \sum_{i=1}^{3} v'_{ii} \sum_{k,m=1}^{3} v'_{kk} v'_{mm} \varepsilon^{ikm} \varepsilon^{ikm} \tag{132}$$

$$= \sum_{i=1}^{3} v'_{ii} \sum_{\substack{k,m=1 \\ k',l',m',n'=1}}^{3} U_{kk'} v_{k'l'} U_{kl'} U_{mm'} v_{m'n'} U_{mn'} \varepsilon^{ikm} \varepsilon^{ikm} \tag{133}$$

$$= \sum_{i=1}^{3} v'_{ii} \sum_{\alpha,\beta=1}^{3} \xi_{\alpha}^{i} \xi_{\beta}^{i} \underbrace{\sum_{k',l',m',n'=1}^{3} v_{k'l'} v_{m'n'} \varepsilon^{\alpha k'm'} \varepsilon^{\beta l'n'}}_{x^{\alpha\beta}} \neq 0 \tag{134}$$

and thus at least one $x^{\alpha\beta} \neq 0$. To show that this implies that at least one $x^{\alpha\alpha} \neq 0$, let $\{\alpha, \beta\} \in \{1, 2, 3\}$ and let $\gamma$ be the remaining index. Then

$$|x^{\alpha\beta}| = 2|\varepsilon^{\alpha\beta\gamma} \varepsilon^{\beta\alpha\gamma} v_{\beta\alpha} v_{\gamma\gamma} + e^{\alpha\beta\gamma} \varepsilon^{\beta\gamma\alpha} v_{\beta\gamma} v_{\gamma\alpha}| \tag{135}$$

$$= 2|\varepsilon^{\alpha\beta\gamma} \varepsilon^{\beta\alpha\gamma} v_{\beta\alpha} v_{\gamma\gamma} - e^{\alpha\beta\gamma} \varepsilon^{\beta\alpha\gamma} v_{\beta\gamma} v_{\gamma\alpha}| \tag{136}$$

$$= 2|v_{\beta\alpha} v_{\gamma\gamma} - v_{\beta\gamma} v_{\gamma\alpha}| \stackrel{!}{=} 0 \Leftrightarrow 1 = v_{\gamma\gamma}^2 \frac{v_{\beta\alpha}^2}{v_{\gamma\alpha}^2 v_{\beta\gamma}^2}. \tag{137}$$

On the other hand if $\alpha \in 1, 2, 3$ and $\beta, \gamma$ are the remaining two indices, then

$$|x^{\alpha\alpha}| = 2\left|\varepsilon^{\alpha\beta\gamma}\varepsilon^{\alpha\beta\gamma}v_{\beta\beta}v_{\gamma\gamma} + \varepsilon^{\alpha\beta\gamma}\varepsilon^{\alpha\gamma\beta}v_{\beta\gamma}^2\right| \tag{138}$$

$$= \left|2v_{\beta\beta}v_{\gamma\gamma} - v_{\beta\gamma}^2\right| \overset{!}{=} 0 \Leftrightarrow v_{\beta\gamma}^2 = v_{\beta\beta}v_{\gamma\gamma} \tag{139}$$

and thus if $x^{11} = 0$, $x^{22} = 0$, and $x^{33} = 0$ then $v_{23}^2 = v_{22}v_{33}$, $v_{13}^2 = v_{11}v_{33}$, and $v_{12}^2 = v_{11}v_{22}$. Then Eq. (137) is fulfilled and $x^{\alpha\beta} = 0$ for all choices of $\alpha$ and $\beta$. Thus at least one $x^{\alpha\beta} \neq 0$ implies that at least one $x^{\alpha\alpha} \neq 0$.

If the Slater rank is two then there exists a unitary transformation $U$ such that

$$v'_{i'j'} = \sum_{i,j=1}^{3} U_{ii'}v_{i'j'}U_{jj'} = \text{diag}(v'_{11}, v'_{22}, 0), \tag{140}$$

and thus

$$0 \neq \sum_{k,m=1}^{2} v'_{kk}v'_{mm}\varepsilon^{3km}\varepsilon^{3km} \tag{141}$$

$$= \sum_{\substack{k,m=1 \\ k',l',m',n'=1}}^{3} U_{kk'}v_{k'l'}U_{kl'}U_{mm'}v_{m'n'}U_{mn'}\varepsilon^{3km}\varepsilon^{3km}, \tag{142}$$

such that the above arguments can be repeated. Using this, Lemma 4.2 can then be proven by induction.

*Proof of Lemma 4.3.* We will give the proof for the case $N = 3$. [$\Rightarrow$] $|v\rangle$ has Slater rank one and, following Definition 4.1, there exists a unitary transformation $U$ such that

$$v'_{ijk} = \sum_{l,m,n=1}^{K} v_{lmn}U_{il}U_{jm}U_{kn} = z\delta_{i1}\delta_{j1}\delta_{k1}. \tag{143}$$

Then for arbitrary $|a\rangle$ it is obvious that $R_{|a\rangle}|v\rangle$ has Slater rank one (unless it is zero), because (here $a'_k = U_{kl}a_l$)

$$3\sum_{k=1}^{K} v'_{ijk}a'_k = 3a_1z\delta_{i1}\delta_{j1}. \tag{144}$$

[$\Leftarrow$] Notice that if a $K \times K$-matrix $v$ has rank one and (normalized) eigenvector $\vec{e}$, then if the normalized vector $\vec{x}$ maximizes $\|v\vec{x}\|$ then $\vec{x} = \vec{e}$. Now let $\vec{x}$ and $\vec{y}$ be normalized vectors varying over the unit sphere and maximize $\|\sum_{ijk}v_{ijk}x_iy_j\|$. A maximum exists because the product of two unit spheres is a compact space and $\|\cdot\|$ is a continuous function. Let the maximum occur at $\vec{x} = \vec{e}^{(1)}$ and $\vec{y}$. Now $\vec{y}$ is the eigenvector of $\sum_i v_{ijk}e_i^{(1)}$, which by assumption has rank one, because $\vec{y}$ maximizes $\|\sum_{i,j}v_{ijk}e_i^{(1)}y_j\|$. Similarly $\vec{e}^{(1)}$ is the eigenvector of $\sum_i v_{ijk}y_i$. Then we have

$$\sum_{i,j}^{3} v_{ijk}e_i^{(1)}y_j = \lambda_1 y_k \qquad \text{and} \qquad \sum_{i,j}^{3} v_{ijk}y_ie_j^{(1)} = \tilde{\lambda}_1 e_k^{(1)} \tag{145}$$

and by comparing both equations

$$\vec{y} \equiv \vec{e}^{(1)}, \qquad \tilde{\lambda}_1 \equiv \lambda_1, \qquad \sum_{i,j,k}^{3} v_{ijk} e_i^{(1)} e_j^{(1)} e_k^{(1)} = \lambda_1, \tag{146}$$

where $\lambda_1$ can be chosen real and positive by adjusting the phase of $\vec{e}^{(1)}$. Furthermore $\sum_{i,j} v_{ijk} e_i^{(1)} z_j = 0$ for any $\vec{z} \perp \vec{e}^{(1)}$.

Now repeat this maximization, but this time restrict $\vec{x}$ and $\vec{y}$ to the space perpendicular to $\vec{e}^{(1)}$. If the result is called $\vec{e}^{(2)}$, then $\sum_{i,j,k} v_{ijk} e_i^{(2)} e_j^{(2)} e_k^{(2)} = \lambda_2$ and $\lambda_2 \leq \lambda_1$. In this way a complete basis is constructed. If $v$ is written in this basis then

$$v' = v \frac{1}{\sqrt{K}} \left( \vec{e}^{(1)} + \cdots + \vec{e}^{(K)} \right) = \frac{1}{\sqrt{K}} \text{diag}[\lambda_1, \ldots, \lambda_K], \qquad \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_K \geq 0. \tag{147}$$

By assumption $|v'\rangle$ has to have Slater rank one; i.e., $v'$ has to have rank one, and it follows that $\lambda_2 = \cdots = \lambda_K = 0$. Thus

$$\sum_{i,j,k} v_{ijk} e_i^{(\alpha)} e_j^{(\beta)} e_k^{(\gamma)} = \lambda_1 \delta_{1\alpha} \delta_{1\beta} \delta_{1\gamma} \tag{148}$$

and $|v\rangle$ has indeed Slater Rank 1.

## ACKNOWLEDGMENTS

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