We characterize and classify quantum correlations in two-fermion systems having \( 2K \) single-particle states. For pure states we introduce the Slater decomposition and rank (in analogy to Schmidt decomposition and rank), i.e. we decompose the state into a combination of elementary Slater determinants formed by mutually orthogonal single-particle states. Mixed states can be characterized by their Slater number which is the minimal Slater rank required to generate them. For \( K = 2 \) we give a necessary and sufficient condition for a state to have a Slater number of 1. We introduce a correlation measure for mixed states which can be evaluated analytically for \( K = 2 \). For higher \( K \), we provide a method of constructing and optimizing Slater number witnesses, i.e. operators that detect Slater number for some states.

\( 03.67 \text{-} a, 03.65 \text{-} Bz, 89.70 \text{-} +c \)

I. INTRODUCTION

In the recent years a lot of effort \([1,2]\) in Quantum Information Theory (QIT) has been devoted to the characterization of entanglement, which is one of the key features of quantum mechanics \([3]\). The resources needed to implement a particular protocol of quantum information processing (see e.g. \([4]\)) are closely linked to the entanglement properties of the states used in the protocol. In particular, entanglement lies at heart of quantum computing \([3]\). The most fundamental question with regard to entanglement is: given a state of a multiparty system, is it entangled, or not (i.e. is it separable \([5]\))? If the answer is yes, then the next question is how entangled it is. For pure states in bipartite systems the latter question can be answered by looking at the Schmidt decomposition \([6]\), i.e. decomposition of the vector in a product basis of the Hilbert space with a minimal number of terms. For mixed states already the first question is not answered. There exist, however, many separability criteria, such as the Peres-Horodecki criterion \([7,8]\), and more recent methods of construction of entanglement witnesses and the corresponding “entanglement revealing” positive maps \([9,10]\).

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. In this case the indistinguishable character of the particles involved (electrons, photons,...) has to be taken into account. Thus, a quantum state must be formulated in terms of Slater determinants, or Slater permanents for fermions and bosons, respectively. Slater determinants and permanents are the natural analogs of pure product states of separated systems, which so far have mainly been studied in Quantum Information Theory. Generically, a Slater determinant contains correlations due to the exchange statistics of the indistinguishable particles. As a simplest possible example consider a wavefunction of two (spinless) fermions,

\[
\Psi(\vec{r}_1, \vec{r}_2) = \frac{1}{\sqrt{2}} \left[ \phi(\vec{r}_1) \chi(\vec{r}_2) - \phi(\vec{r}_2) \chi(\vec{r}_1) \right] \quad (1)
\]

with two orthonormalized single-particle wavefunctions \( \phi(\vec{r}) \), \( \chi(\vec{r}) \). Operator matrix elements between such elementary Slater determinants contain terms due to the antisymmetrization of coordinates (“exchange contributions” in the language of Hartree-Fock theory). However, if the moduli of \( \phi(\vec{r}) \), \( \chi(\vec{r}) \) have only vanishingly small overlap, these exchange correlations will also tend to zero for any physically meaningful operator. This situation is generically realised 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 present in Eq. (1) has no physical effect. As a another example where such exchange correlations vanish at long distances consider the groundstate of the free electron gas. This state has spatial density correlations which fall off algebraically with the distance, and are accompanied by oscillations with a periodicity of half the Fermi wavelength. Therefore, correlations of this type are negligible for sufficiently large distances, even though the decay is only algebraic and therefore not particularly rapid. Here the single-particle wavefunctions are plane waves having constant modulus in space, and the decay of exchange correlations is a many-particle interference effect.

In any case, 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.
The situation is different if the particles constituting, say, qubits are close together and possibly coupled in some computational process. This the case for all proposals of quantum information processing based on quantum dots technology [11–13]. Here qubits are realized by the spins of electrons living in a system of quantum dots. The electrons have the possibility of tunneling eventually from one dot to the other with a probability which can be modified by varying external parameters such as gate voltages and magnetic field. In such a situation the fermionic statistics of electrons is clearly essential.

Additional correlations in many-body-systems of indistinguishable particles arise if more than one Slater determinant or permanent is involved, i.e. if there is no single-particle basis such that a given state of distinguishable particles can be formulated as an elementary Slater determinant, or permanent (i.e. fully antisymmetric, or symmetric combination of single particle states). These correlations are the analog of quantum entanglement in separated systems and are essential for quantum information processing in non-separated systems. As an example consider a “swap” process exchanging the spin states of electrons on coupled quantum dots by gating the tunneling amplitude between them [12,13]. During such a process the system is temporarily in a highly “entangled” state, while the initial and final state are essentially elementary Slater determinants. Moreover, by adjusting the gating time appropriately one can also perform a “square root of a swap” which turns an elementary Slater determinant into a “maximally entangled” state in much the same way [13].

It is the purpose of the present paper to analyse the above type of “entanglement”, or better to say quantum correlations between indistinguishable fermions, in more detail. However, to avoid confusion with the existing literature we shall reserve in the following the term “entanglement” for separated systems and characterize the analogous quantum correlation phenomenon in non-separated fermionic systems by the notions of Slater rank and Slater number to be defined below.

We are going to formulate analogies with the theory of entanglement, and translate several very recent results [10,14,15] concerning standard systems of distinguishable parties (Alice ≠ Bob) to the case of indistinguishable fermions. In general we will deal with a system of two fermions living in a 2K-dimensional single-particle space. The plan of the paper is as follows: In section II we discuss pure states, and formulate the analog of Schmidt decomposition and rank – Slater decomposition and rank. We discuss then an easy operational criterion to determine if a given state is of Slater rank 1 for the case of two electrons in a system of two neighboring quantum dots (K = 2), first derived in Ref. [13]. In section III we define the concept of Slater number for mixed states. We present necessary and sufficient condition for a mixed state to have the Slater number 1 for K = 2. This is an analog of the Peres-Horodecki criterion [7,8] in the Wootters formulation [16]. In section IV we extend the results of section III and define a Slater correlation measure which is an analog of the entanglement formation measure [17], and which can be calculated exactly for the case K = 2, in analogy to the Wootters result [16]. In section V we turn to the case K > 2 and introduce Slater number witnesses of canonical form (defined in analogy to entanglement [9,14] and Schmidt number [18,15] witnesses). We construct examples of such k-Slater witnesses, which provide necessary conditions for a state to have the Slater number smaller than k; we discuss here also optimization of Slater witnesses. Finally, we present the associated [20] positive maps. We close by giving an outlook on further analogies, but also differences, concerning entanglement in separated systems as opposed to non-separated systems of indistinguishable particles.

II. SLATER RANK OF PURE STATES

We consider two indistinguishable fermions having the single particle Hilbert space C2K. This situation is given, e. g., in a system of two electrons in K neighboring quantum dots where only the orbital ground state of each dot is taken into account. Alternatively one may think of, say, two quantum dots with an appropriate number of orbital states available for the two fermions.

The states (density matrices) in such a system are positive self-adjoint operators acting on the asymmetric space A(C2K ⊗ C2K). Let us first consider pure states, i.e. projectors on a vector |Ψ⟩ ∈ A(C2K ⊗ C2K). Let f_a, f^†_b denote the fermionic annihilation and creation operators of the single-particle states enumerated by a = 1,...,2K, and forming an orthonormal basis in C2K. Let |Ω⟩ denotes the vacuum state. Each vector in two electron space can be represented as |Ψ⟩ = ∑_{a,b} w_{ab} f^†_a f_b |Ω⟩, where w_{ab} = −w_{ba} is an antisymmetric matrix. We have the following generalization of the Theorem 4.3.15 from Ref. [19], which allows then to define the Slater decomposition

Lemma 1 For any antisymmetric N × N matrix A ≠ 0 there exist an unitary transformation U, such that A = U^T Z U, where the matrix Z has blocks on the diagonal,

Z = diag [Z_0, Z_1, ..., Z_M], Z_0 = 0, Z_i = \begin{bmatrix} 0 & z_i \\ -z_i & 0 \end{bmatrix},

(2)

and Z_0 is a (N − 2M) × (N − 2M) null matrix.

Proof: Let A be a N × N, complex, antisymmetric matrix acting on C^N, A = −A^T, hence A^1 = −A^*. Let us define: B := AA^* = −AA^†. B is hermitian, B = B^†, hence diagonalizable by an unitary transformation: B = U D U^†, UU^† = I, U - diagonal. Let us define: C := U^† A U^*, It is easy to check that C is antisymmetric, C^T = −C, and normal CC^† = C^† C. Let us decompose C

2
where \( Y \) implies that in the new basis \( W \) of \( \mathbb{C}^4 \times \mathbb{C}^4 \times \mathbb{C}^4 \times \mathbb{C}^4 \).

**Remark:** The quantity \( \eta(\Psi) \) can be constructed from the dual state
\[
|\tilde{\Psi}\rangle = \sum_{a,b} \tilde{w}_{ab} f_a \dagger f_b \dagger |\Omega\rangle
\]
defined by the dual matrix
\[
\tilde{w}_{ab} = \sum_{c,d} \epsilon^{abcd} w_{cd}^* .
\]

With these definitions we have
\[
\eta(\Psi) = \left| \langle \tilde{\Psi} | \tilde{\Psi} \rangle \right|^\frac{1}{2} ,
\]

where \( w \) is the antisymmetric 4x4-matrix defining \( |\Psi\rangle \).

In the Appendix we list some further useful properties of \( \eta(\Psi) \) and the relation of the dualisation operation to an antiunitary implementation of particle-hole-transformation. It is worth noticing that the Lemma 3 can be generalized to the case of \( K \) fermions having a single particle space \( \mathbb{C}^{2K} \).

### III. Slater Number of Mixed States

Let us now generalize the concepts introduced above to the case of mixed states. To this aim we define, in analogy to Schmidt number of mixed states [18,15], the Slater number:

**Definition 1** Consider a density matrix \( \rho \) of a two fermion system, and all its possible convex decompositions in terms of pure states, namely \( \rho = \sum_i p_i |\psi_i^r\rangle \langle \psi_i^r| \), where \( r_i \) denotes the Slater rank of \( |\psi_i^r\rangle \); the Slater number of \( \rho \), \( k \), is defined as \( k = \inf \{ r_{\max} \} \) where \( r_{\max} \) is the maximum Slater rank within a decomposition, and the infimum is taken over all decompositions.

In other words, \( k \) is the minimal Slater rank of the pure states that are needed in order to construct \( \rho \), and there is a construction of \( \rho \) that uses pure states with Slater rank not exceeding \( k \).

Many of the results concerning Schmidt numbers can be directly translated to the Slater number. For instance, let us denote the whole space of density matrices
in \( \mathcal{A}(\mathbb{C}^{2K} \otimes \mathbb{C}^{2K}) \) 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. \( SL_1 \subset SL_2 \subset \ldots \subset SL_k \subset \ldots \subset SL_K \). 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.

Determination of the Slater number in general is a very difficult task. Similarly, however, as in the case of separability of mixed states of two qubits (i.e. states in \( \mathbb{C}^2 \otimes \mathbb{C}^2 \)), and one qubit–one qutrit (i.e. states in \( \mathbb{C}^2 \otimes \mathbb{C}^3 \)) [8], the situation is particularly simple in the case of small \( K \). For \( K = 1 \) there exist only one state (a singlet). For \( K = 2 \), necessary and sufficient condition for a given mixed state to have the Slater number 1 can be found. One should note, however, that in the considered case of fermionic states there exist no simple analogy of the partial transposition, which is essential for the theory of entangled states. In fact, the Peres–Horodecki criterion [7,8] in 2 \( \times \) 2 and 2 \( \times \) 3 spaces says that a state is separable iff its partial transpose is positively defined. It is known, however, that the Peres-Horodecki criterion is equivalent to the Wootters [16] criterion, that relates separability to the quantity called concurrence, which is then related to the Wootters [16] criterion, that relates separability to the quantity called concurrence, which is then related to eigenvalues of a certain matrix. This latter approach can be used to characterized fermionic states in \( \mathcal{A}(\mathbb{C}^4 \otimes \mathbb{C}^4) \).

We have the following Theorem:

**Theorem 1** Let the mixed state acting in \( \mathcal{A}(\mathbb{C}^4 \otimes \mathbb{C}^4) \) has a spectral decomposition \( \rho = \sum_{i=1}^{r} |\Psi_i\rangle \langle \Psi_i| \), where \( \rho \) is the rank of \( \rho \), and the eigenvectors \( |\Psi_i\rangle \) belonging to nonzero eigenvalues \( \lambda_i \) are normalized as \( \langle \Psi_i | \Psi_j \rangle = \delta_{ij} \).

Let \( |\Psi_j\rangle = \sum_{a,b} w_{ab,j}^i |\Omega\rangle \) in some basis, and let \( C \) denotes the complex symmetric \( r \times r \) matrix

\[
C_{ij} = \sum_{abcd} c_{abcd} w_{ab,i}^j w_{cd,i}^j,
\]

which can be represented using an unitary matrix as \( C = U C_d U^T \) with a diagonal \( C_d = \text{diag}(c_1, c_2, \ldots, c_r) \), and \( |c_1| \geq |c_2| \geq \ldots \geq |c_r| \). The state \( \rho \) has Slater number 1 iff

\[
|c_1| \leq \sum_{i=2}^{r} |c_i|.
\]

**Proof:** Let us assume that a state \( \rho \) acting in \( \mathcal{A}(\mathbb{C}^4 \otimes \mathbb{C}^4) \) has the Slater number 1, i.e.,

\[
\rho = \sum_{i=1}^{r} |\Psi_i\rangle \langle \Psi_i| = \sum_{k=1}^{r'} |\phi_k\rangle \langle \phi_k|,
\]

where all \( |\phi_k\rangle \) have Slater rank 1, whereas \( r' \) can be an arbitrary integer \( \geq r \). But, \( |\phi_k\rangle \) can be represented as

\[
|\phi_k\rangle = \sum_{i=1}^{r} U_{ki} |\Psi_i\rangle = \sum_{i=1}^{r} \sum_{a,b} U_{ki} w_{ab}^i f_{1}^{a} f_{1}^{b} |\Omega\rangle.
\]

From the Lemma (3) we obtain that for each \( k \), \( \eta(w'(k)) = 0 \), where \( w'(k)_{ab} = \sum_{i=1}^{r} U_{ki} w_{ab}^i \). The matrices \( U_{ki} \) must therefore for every \( k \) fulfill

\[
\sum_{abcd} c_{abcd} w_{ab,i}^j w_{cd,i}^j U_{ki} U_{kj} = \sum_{i,j=1}^{r} C_{ij} U_{ki} U_{kj} = 0. \tag{14}
\]

At the same time from Eq. (13) we obtain that

\[
\sum_{k=1}^{r'} U_{ki} U_{kj} = \delta_{ij}. \tag{15}
\]

The Slater rank 1 is thus equivalent to the existence of the \( r' \times r \) matrix \( U_{ki} \) that fulfills Eqs. (14) and (15).

It is convenient to represent the rows of the matrix \( U_{ki} \) as vectors in a \( r \) dimensional Hilbert space \( \mathcal{H}_{aux} \). Eqs. (14) and (15) reduce then to \( \sum_{k=1}^{r'} |R_{ki}\rangle \langle R_{k}| = \mathbb{I} \), and \( \langle R_{ki}^*|C|R_{k}\rangle = 0 \) for all \( k \). One can always change a basis in \( \mathcal{H}_{aux} \), i.e. replace \( |R_{ki}\rangle \rightarrow U|R_{ki}\rangle \). Such transformation does not affect Eq. (15), and transforms \( C \rightarrow U^T C U \).

Since \( C \) is symmetric, \( U \) can be chosen in such a way that \( C \) in the chosen basis is diagonal. Eqs. (14) reduce then to \( \sum_{k=1}^{r} c_1 U_{ki}^2 = 0 \). In this new basis the construction of \( U_{ki} \) using the method of Wootters [16] can be carried over. One can always assume that \( c_1 U_{k1}^2 \) is real and positive, by choosing the phases of \( |R_{k}\rangle \). Then, one observes that if Eq. (14) is fulfilled, then

\[
0 = \sum_{i=1}^{r} c_1 U_{ki}^2 \geq |c_1| |U_{k1}^2| - \sum_{i=2}^{r} |c_i| |U_{ki}^2| \tag{16}
\]

Summing the above inequality over \( k \) and using Eq. (15), we obtain the necessary condition

\[
|c_1| \leq \sum_{i=2}^{r} |c_i|. \tag{17}
\]

To show that it is also the sufficient condition, we take

\[
r' = 2 \text{ if } r = 2, \quad r' = 4 \text{ if } r = 3, 4, \quad r' = 8 \text{ if } r = 5, 6,
\]

and \( U_{ki} = \pm 1_{ki} \exp(i\theta_i) / \sqrt{r} \). Eqs. (14) are then all equivalent to

\[
|c_1| = \sum_{i=2}^{r} c_i \exp(2i\theta_i), \tag{18}
\]

and the angles \( \theta_i \) can indeed be chosen to assure that Eq. (18) is fulfilled, provided the condition (17) holds. The \( \pm 1_{ki} \) signs are designed in such a way that Eq. (15) is fulfilled. Thus for \( r' = 2 \) we take \( (+,+), (+,-) \) for \( i = 1, 2 \), for \( r' = 4 \) we take \( (+++), (+-+-), (+-++), (+---) \) for \( i = 1, \ldots, 4 \) (or any 3 of them for \( i = 1, \ldots, 3 \)), and finally for \( r' = 8, (++++) \) (or any 5 of them for \( i = 1, \ldots, 5 \)), and finally for \( r' = 8, (++++) \) (or any 5 of them for \( i = 1, \ldots, 5 \)). In the latter case we take again as many vectors as we need, i.e. \( i = 1, \ldots, 5 \leq r \leq 6 \).
The above Theorem is an analog of the Peres-Horodecki-Wooters result for the two-fermion systems having the single particle space of dimension $2K \leq 4$. The situation is much more complicated, when we go to $K > 2$; similarly as in the case of separability problem in $\mathbb{C}^M \otimes \mathbb{C}^N$ with $MN > 6$. These issues are investigated in section V. In the following section, however, we shall concentrate on the case $K = 2$.

IV. SLATER CORRELATION MEASURE

The similarity of our approach to that of Wooters [16] can be pushed further, and in particular allows us to define and calculate, for the case of $K = 2$, the “Slater formation measure” (in analogy to entanglement formation measure [17]).

To this aim we first consider a pure (normalized) state $|\tilde{\psi}\rangle = \sum \sum_{a,b} w_{ab} f^i_a f^j_b |\Omega\rangle$, and define the Slater correlation measure of $|\tilde{\psi}\rangle$ as in Lemma 3 (cf. Ref. [13]),

$$\eta(|\tilde{\psi}\rangle) = \langle \tilde{\psi} | \tilde{\psi} \rangle,$$

with $|\tilde{\psi}\rangle$ being the dual of $|\tilde{\psi}\rangle$. Obviously, dual states, as well as the function $\eta(.)$ of Eq. (19) can be also defined for unnormalized states, which in the following will be denoted as in previous sections, without the bar.

The measure (19) has all desired properties [17,21], such that it vanishes iff $|\tilde{\psi}\rangle$ has Slater rank 1, it is invariant with respect to local bilateral unitary operations, or, in another words, with respect to changes of the basis in the single particle space.

Having defined the measure for the pure states, we can consider the following definition:

**Definition 2** Consider a density matrix $\rho$ of a two fermion system acting in $\mathcal{A}(\mathbb{C}^4 \otimes \mathbb{C}^4)$, and all its possible convex decompositions in terms of pure states, namely $\rho = \sum_i |\psi_i\rangle \langle \psi_i| = \sum_i p_i |\tilde{\psi}_i\rangle \langle \tilde{\psi}_i|$, where the unnormalized states $|\tilde{\psi}_i\rangle = \sqrt{p_i} |\psi_i\rangle$; the Slater formation measure of $\rho$, $Sl(\rho)$ is defined as

$$Sl(\rho) = \inf \left\{ \sum_i p_i \eta(|\tilde{\psi}_i\rangle) \right\},$$

where the infimum is taken over all decompositions.

In other words, $Sl(\rho)$ is the minimal amount of Slater correlations of the pure states that are needed in order to construct $\rho$, and there is a construction of $\rho$ that uses pure states with “averaged” Slater correlation $E(\rho)$.

Note that $\sum_i p_i \eta(|\tilde{\psi}_i\rangle) = \sum_i \eta(|\tilde{\psi}_i\rangle)$. The measure $Sl(\rho)$ can be directly related to the matrix $C_{ij}$ of Eq. (11), and to its “concurrence”, as we shall see below. It is invariant not only with respect to local bilateral unitary operations, but it cannot increase under local bilateral LOCC, i.e. trace preserving maps of the form $\rho \rightarrow M(\rho) = \sum_j A_j \otimes A_j \rho A_j^\dagger \otimes A_j^\dagger$, where each $A_j$ acts in $\mathbb{C}^4$, and $\sum_j A_j^\dagger A_j = I$. Such transformations correspond to mixtures of density matrices obtained after nonunitary changes of the basis in the single particle space. It is easy to see that

$$Sl(M(\rho)) = \left( \sum_j |\text{det} A_j| Sl(\rho) \right) \leq Sl(\rho).$$

We have the following theorem:

**Theorem 2** For any $\rho$ acting in $\mathcal{A}(\mathbb{C}^4 \otimes \mathbb{C}^4)$

$$Sl(\rho) = |c_1| - \sum_{i=2}^{r'} |c_i|,

(20)$$

where $c_i$ are the diagonal elements of $C$ (Eq. (11)) in the basis that diagonalizes it.

**Proof:** The proof is essentially the same as the one in the previous section. We consider arbitrary expansion, $\rho = \sum_{k=1}^{r'} |\phi_k\rangle \langle \phi_k|$, where $|\phi_k\rangle = \sum_j U_{kj} |\Psi_j\rangle$, and $|\Psi_j\rangle$ are the unnormalized eigenvectors of $\rho$. It is easy to see that

$$Sl(|\phi_k\rangle \langle \phi_k|) = \left( \sum_{i,j=1}^{r'} C_{ij} U_{ki} U_{kj} \right)

(21)$$

and $\sum_{k=1}^{r'} U_{ki}^\dagger U_{kj} = \delta_{ij}$. By changing the basis to the one in which $C$ is diagonal we get (after choosing the phases of $U_{kj}$ such that $c_1 U_{k1}^2$ are real and positive):

$$\sum_{k=1}^{r'} Sl(|\phi_k\rangle \langle \phi_k|) = \sum_{k=1}^{r'} \left( \sum_j c_j U_{kj}^2 \right) \geq |c_1| - \sum_{i=2}^{r'} |c_i|.

(22)$$

This inequality becomes an inequality when we use the same construction of $U_{kj}$ as in previous section, namely $U_{kj} = \pm 1_{kj} \exp(i\theta_j)/\sqrt{r'}$, with $\theta_j$ selected in such a way that (independently of $k$),

$$\left( \sum_j c_j U_{kj}^2 \right) = \frac{1}{r'} \left( |c_1| - \sum_{i=2}^{r'} |c_i| \right).

(23)$$

The above construction provides a rare, to our knowledge, example of generalization of the formation measure that can be analytically evaluated. Obviously, since we have introduced the concept of Slater coefficients, we may define other Slater correlations measures for pure states as appropriately designed convex functions of the Slater coefficients (in analogy to entanglement monotones, [22]). For $K = 2$, and most probably only for $K = 2$, all these measures are equivalent and the corresponding induced measures for mixed states can be analytically evaluated.
V. SLATER WITNESSES

We now investigate fermion 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, follow here the lines of the papers that we have written on entanglement witnesses [10,14], and Schmidt number witnesses [15].

In order to determine the Slater number of a density matrix $\rho$ notice that due to the fact that the sets $Sl_k$ are convex and compact, any density matrix of class $k$ can be decomposed as a convex combination of a density matrix of class $k - 1$, and a remainder $\delta$ [23]:

**Proposition 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 $\delta$:

$$\rho_k = (1 - p)\rho_{k-1} + p\delta, \quad 1 \geq p > 0 \quad (24)$$

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

The decomposition (24) is obtained by subtracting projectors onto pure states of Slater rank inferior to $k$, $P = |\psi<k\rangle\langle\psi<k|$ 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 $\rho' \propto \rho - \lambda|\psi<k\rangle\langle\psi<k|$ is non negative iff $|\psi<k\rangle \in R(\rho)$ and $\lambda \leq (\langle\psi<k|\rho^{-1}|\psi<k\rangle)^{-1}$ (see [23]). 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 Schmidt number, there exists an optimal decomposition of the form (24) with $p$ minimal. Also restricting ourselves to decompositions $\rho_k = \sum_i p_i|\psi_i^+\rangle\langle\psi_i^+|$ with all $r_i \leq k$, we can always find a decomposition of the form (24) with $\delta \in Sl_k$. We define below more precisely what an edge state is.

**Definition 3** A $k$-edge state $\delta$ is a state such that $\delta - \epsilon|\psi<k\rangle\langle\psi<k|$ is not positive, for any $\epsilon > 0$ and $|\psi<k\rangle$.

**Criterion 1** A mixed state $\delta$ is a $k$-edge state iff there exists no $|\psi<k\rangle$ such that $|\psi<k\rangle \in R(\delta)$.

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

**Definition 4** A hermitian operator $W$ is a Slater witness of class $k$ if $Tr(W\sigma) \geq 0$ for all $\sigma \in Sl_{k-1}$, and there exists at least one $\rho \in Sl_k$ such that $Tr(W\rho) < 0$.

It is straightforward to see that every SIW that detects $\rho$ given by (24) also detects the edge state $\delta$, since if $Tr(W\rho) < 0$ then necessarily $Tr(W\delta) < 0$, too. Thus, the knowledge of all SIW’s of $k$-edge states fully characterizes all $\rho \in Sl_k$. Below, we show how to construct for any edge state a SIW which detects it. Most of the technical proofs used to construct and optimize Slater witnesses are very similar to those presented in Ref. [10] for entanglement witnesses.

All the operators we consider below act in $A(C^{2K} \otimes C^{2K})$. Let $\delta$ be a $k$-edge state, $C$ an arbitrary positive operator such that $Tr(C\delta) > 0$, and $P$ a positive operator whose range fulfills $R(P) = K(\delta)$. We define $\epsilon \equiv \inf_{|\psi<k\rangle}\langle\psi<k|P|\psi<k\rangle$ and $c \equiv \sup \langle\psi|C|\psi\rangle$.

Note that $c > 0$ by construction and $\epsilon > 0$, because $R(P) = K(\delta)$ and therefore, since $R(\delta)$ does not contain any $|\psi<k\rangle$ by the definition of edge state, $K(\delta)$ cannot contain any $|\psi<k\rangle$ either. This implies:

**Lemma 4** Given an $k$-edge state $\delta$, then

$$W = P - \epsilon C \quad (25)$$

is a $k$-SIW which detects $\delta$.

The simplest choice of $P$ and $C$ consists in taking projections onto $K(\delta)$ and the identity operator on the asymmetric space $I_a$, respectively. As we will see below, this choice provides us with a canonical form of a $k$-SIW.

**Proposition 2** Any Slater witness can be written it the canonical form:

$$W = \tilde{W} - \epsilon I_a, \quad (26)$$

such that $R(\tilde{W}) = K(\delta)$, where $\delta$ is a $k$-edge state and $0 < \epsilon \leq \inf_{|\psi|\in Sl_{k-1}}\langle\psi|\tilde{W}|\psi\rangle$.

**Proof**: Assume $W$ is an arbitrary $k$-SIW so that $Tr(W\sigma) \geq 0$ for all $\sigma \in Sl_{k-1}$, and there $\exists$ at least one $\rho$ such that $Tr(W\rho) < 0$. $W$ has at least one negative eigenvalue. Construct $W + \epsilon I_a = \tilde{W}$, so that $W$ is a positive operator on $A(C^{2K} \otimes C^{2K})$, but it does not have a full rank $K(\tilde{W}) \neq 0$ (by continuity this construction is always possible). But $\langle\psi<k|\tilde{W}|\psi<k\rangle \geq \epsilon > 0$ since $W$ is a $k$-SIW, ergo no $|\psi<k\rangle \in K(\tilde{W})$.□

**Definition 5** A $k$-Slater witness $W$ is tangent to $Sl_{k-1}$ at $\rho$ if $\exists$ a state $\rho \in Sl_{k-1}$ such that $Tr(W\rho) = 0$.

**Observation 1** The state $\rho$ is of Slater class $k - 1$ if for all $k$-SIW’s tangent to $Sl_{k-1}$, $Tr(W\rho) \geq 0$.

**Proof** (See [10]): (only if) Suppose that $\rho$ is of class $k$. From Hahn-Banach theorem, there exists a $k$-SIW, $W$, that detects it. We can subtract $\epsilon I_a$ from $W$, making $W - \epsilon I_a$ tangent to $Sl_{k-1}$ at some $\sigma$, but then $Tr(\rho(W - \epsilon I_a)) < 0$.□
We will now discuss the optimization of a Slater witness. As proposed in [10] and [15] an entanglement witness (Schmidt witness) $W$ is optimal if there exists no other EW that detects more states than it. The same definition can be applied to Slater witnesses. We say that a $k$–Slater witness $W_2$ is finer than a $k$–Slater witness $W_1$, if $W_2$ detects more 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 $|\psi^{<k}\rangle$ pure states of Slater rank $k-1$ for which the expectation value of the $k$-Slater witness $W$ vanishes:

$$T_W = \{|\psi^{<k}\rangle\ s.t. \langle\psi^{<k}|W|\psi^{<k}\rangle = 0\},$$

(27)
i.e. the set of tangent pure states of Slater rank $k-1$. $W$ is an optimal k-SIW iff $W - eP$ is not a k-SIW, for any positive operator $P$. If the set $T_W$ spans the whole Hilbert space $A(C^{2K} \otimes C^{2K})$, then $W$ is an optimal k-SIW. If $T_W$ does not span $A(C^{2K} \otimes C^{2K})$, 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 $\inf_{|\psi\rangle \in C^{2K}}[P_{e^{1/2}}W]\min > 0$, where for any $X$ acting on $A(C^{2K} \otimes C^{2K})$

$$X_e = \left[\langle e,|X|e,\rangle - \langle e,|X|e,\rangle \right],$$

(28)
is treated as an operator acting in $C^{2K}$, and $[X]\min$ denotes its minimal eigenvalue (see [10]). An example of an optimal witness of Slater number $k$ in $A(C^{2K} \otimes C^{2K})$ is given by

$$W = 1_n - \frac{K}{k-1}p,$$

(29)
where $p$ is a projector onto a “maximally correlated state”, state $|\Psi\rangle = \frac{1}{\sqrt{K}} \sum_{i=1}^{K} f_{a_1(i)}^{\dagger} f_{a_2(i)}^{\dagger}|\Omega\rangle$ (cf. Eq. 5).

The reader can easily check that the above witness operator has mean value zero in the states $f_{a_1(i)}^{\dagger} f_{a_2(i)}^{\dagger}|\Omega\rangle$ for $i = 1, 2$, but also for all states of the form $g_1^{\dagger} g_2^{\dagger}|\Omega\rangle$ where

$$g_1^{\dagger} = f_{a_1(1)}^{\dagger} e^{i\varphi_{11}} + f_{a_1(2)}^{\dagger} e^{i\varphi_{12}} + f_{a_2(1)}^{\dagger} e^{i\varphi_{21}} + f_{a_2(2)}^{\dagger} e^{i\varphi_{22}},$$

(30)
$$g_2^{\dagger} = -f_{a_1(1)}^{\dagger} e^{-i\varphi_{11}} + f_{a_1(2)}^{\dagger} e^{-i\varphi_{12}} - f_{a_2(1)}^{\dagger} e^{-i\varphi_{21}} + f_{a_2(2)}^{\dagger} e^{-i\varphi_{22}},$$

(31)
for arbitrary $\varphi_{ij}, i,j = 1,2$. The set $T_W$ spans in this case the whole Hilbert space $A(C^{2K} \otimes C^{2K})$, ergo $W$ is optimal.

VI. CONCLUSIONS AND OUTLOOK

It is interesting to consider linear maps associated with Slater witnesses via the Jamiołkowski isomorphism [20]. Such maps employ $W$ acting in $H_A \otimes H_B = C^{2K} \otimes C^{2K}$, and transform a state $\rho$ acting in $H_A \otimes H_C = C^{2K} \otimes C^{2K}$ into another state acting in $H_B \otimes H_C = C^{2K} \otimes C^{2K}$, $M(\rho) = Tr_A(W \rho^T)$. Obviously, such map are positive on separable states: When $\rho$ is separable, then for any $|\Psi\rangle \in H_B \otimes H_C$, the mean value of $\langle \Psi|M(\rho)|\Psi\rangle$, becomes a convex sum of mean values of $W$ in some product states $|e,f\rangle \in H_A \otimes H_B$. Since $W$ act in fact in the antisymmetric space, we can antisymmetrize those $|e,f\rangle \rightarrow (|e,f| - |f,e\rangle)$. Such antisymmetric states have, however, Slater rank 1, and all SIW 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. [10,14]; they provide thus an interesting class of necessary separability conditions. The map associated to the witness (29) is, however, decomposable, i.e. is a sum of completely positive map, and another completely positive map composed with transposition. This follows from the fact that the witness operator has a positive partial transpose, i.e. it itself can be presented as a partial transpose of a positive operator.

B. Slater witnesses and positive maps

Summarizing, we have presented a general characterization of quantum correlated states in two-fermion systems with $2K$-dimensional single-particle space. This aim has been achieved by introducing the concepts of Slater decomposition and rank for pure states, and Slater number for mixed states. In particular, for the important case $K = 2$ the quantum correlations in mixed states can be characterized completely in analogy to Wootters’ result for separated qubits [16], and using the findings of Ref. [13] for pure states. Similarly to the case of separated systems, the situation for $K > 2$ is more complicated. Therefore, we have also introduced witnesses of Slater number $k$, and presented the methods of optimizing them.

Possible directions for future work include generalizations of the present results to more than two fermions, and the development of an analogous theory for indistinguishable bosons. For this purpose a lot of the concepts developed so far are expected to be useful there as well. However, there are certainly also fundamental differences between quantum correlations in bosonic and fermionic systems. As an example consider the notion of unextendible product bases introduced recently in separated systems [24]. These are sets of product states spanning a subspace of the Hilbert space whose orthogonal complement does not contain any product state. All such unextendible product bases constructed so far involve product states of the form $|\psi\rangle \otimes |\chi\rangle$ with $|\psi\rangle$ and $|\chi\rangle$
we get the dualisation operator \( \hat{\Phi} \) as a special case.\( ^{8} \) The dualisation of a state is invariant under a unitary single-particle transformation, and refer explicitly to a certain single-particle transformation. The dualisation operator is similar to Wootters' construction for the single-qubit system. The correlation measure \( \eta(\langle \Psi \rangle) = |\langle \Psi | \Psi \rangle|, \langle \Psi | = \mathcal{D} \langle \Psi \rangle \), remains invariant under such an operation. Eq. A3 implies that \( \mathcal{D} \) is unchanged by unitary single-particle operations, \[ \mathcal{U} \mathcal{D} \mathcal{U}^+ = \mathcal{D} \Leftrightarrow [\mathcal{U}, \mathcal{D}] = 0 \] which can also be expressed as \[ \mathcal{U} \mathcal{U}_{p-h} \mathcal{U}^T = \mathcal{U}_{p-h} \] for any unitary single-particle transformation \( \mathcal{U} \).

The dualisation operator \( \mathcal{D} \) is the antunitary implementation of the particle-hole-transformation. We note that the complex conjugation involved there is necessary for \( \mathcal{D} \) being compatible with single-particle transformations \( \mathcal{U} \),

\[ \mathcal{D} \mathcal{U} f_a^+ \mathcal{D}^{-1} = \sum_b U_{ba}^* f_b \]

\[ = \mathcal{U} \mathcal{D} f_a^+ \mathcal{D}^{-1} \mathcal{U}^+ . \]

If the complex conjugation would be left out, \( \mathcal{U} \) and \( \mathcal{D} \) would not commute.

The correlation measure \( \eta \) to an antiunitary operator is similar to Wootters' construction for a separate system of two qubits [16]. The correlation measure there ("concurrence") relies on the time inversion operation. The operator of time inversion in the two-qubit system is invariant under local unitary transformations in each qubit space. This property is similar to the invariance of the dualisation operator under unitary transformations in the single-particle space.

\[ \mathcal{K}(a|\alpha \rangle + b|\beta \rangle) = a^* \mathcal{K}|\alpha \rangle + b^* \mathcal{K}|\beta \rangle . \]

Its action on the single-particle basis states and the fermionic vacuum is given by

\[ \mathcal{K} f_a^+ \mathcal{K} = f_a^+ , \quad \mathcal{K} f_a \mathcal{K} = f_a , \quad \mathcal{K}|\Omega \rangle = |\Omega \rangle . \] The relations (A7) are to be seen as a part of the definition of \( \mathcal{K} \) and refer explicitly to a certain single-particle basis defined by the operators \( f_a, f_a^+ \). However, switching to a different complex conjugation operator \( \mathcal{K} \)'s, fulfilling the relations (A7) in a different basis, has only trivial effects without any physical significance. In particular, as one can see from the properties given above, the correlation measure \( \eta(\langle \Psi \rangle) = |\langle \Psi | \Psi \rangle|, \langle \Psi | = \mathcal{D} \langle \Psi \rangle \), remains invariant under such an operation.

APPENDIX A

We now list further properties of the correlation measure \( \eta \) for pure states \( |\Psi\rangle = \sum_{a,b=1}^4 w_{ab} f_a^+ f_b |\Omega \rangle \) of two fermions in a four-dimensional single-particle space [13], and add some further remarks.

The matrix \( w \) transforms under a unitary transformation of the one-particle space,

\[ f_a^+ \to \mathcal{U} f_a^+ \mathcal{U}^+ = \sum_b U_{ba} f_b^+ , \quad (A1) \]
as

\[ w \to U w U^T , \quad (A2) \]

where \( U^T \) is the transpose (not the adjoint) of \( U \). Under such a transformation, \( |\Psi \rangle \to |\Phi \rangle = \mathcal{U}|\Psi \rangle \), scalar products of the form \( \langle \Phi_1 | \Phi_2 \rangle \) remain unchanged up to a phase,

\[ \langle \Phi_1 | \Phi_2 \rangle = \det U \langle \Phi_1 | \Phi_2 \rangle . \quad (A3) \]

Therefore, in particular, \( \eta(\langle \Psi \rangle) \) in invariant under arbitrary single-particle transformations.

The dualisation of a state \( |\Psi\rangle \) can be identified as a particle-hole-transformation,

\[ \mathcal{U}_{p-h} f_a^+ \mathcal{U}_{p-h} = f_a , \quad \mathcal{U}_{p-h} |\Omega \rangle = f_1^+ f_2^+ f_3^+ f_4^+ |\Omega \rangle , \quad (A4) \]

along with a complex conjugation. In fact, the operator of dualisation \( \mathcal{D} \),\( |\Psi \rangle \to |\tilde{\Psi} \rangle = \mathcal{D}|\Psi \rangle \), can be written as

\[ \mathcal{D} = -\mathcal{U}_{p-h} \mathcal{K} , \quad (A5) \]

where \( \mathcal{K} \) is the usual operator of complex conjugation which acts on a general state vector as

\[ \mathcal{K}(a|\alpha \rangle + b|\beta \rangle) = a^* \mathcal{K}|\alpha \rangle + b^* \mathcal{K}|\beta \rangle . \]

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