Computable measures for the entanglement of indistinguishable particles

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We discuss particle entanglement in systems of indistinguishable bosons and fermions, in finite Hilbert spaces, with focus on operational measures of the entanglement of particles. We show how to use von Neumann entropy, negativity, and entanglement witnesses in these cases, proving interesting relations.We obtain analytic expressions to quantify the entanglement of particles in homogeneous *D*-dimensional Hamiltonians with certain symmetries.

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I. INTRODUCTION

The notion of entanglement, first noted by Einstein, Podolsky, and Rosen [\[1\]](#page-6-0), is considered one of the main features of quantum mechanics, and became a subject of great interest in the last few years due to its primordial role in quantum computation and quantum information [\[2–5\]](#page-6-0). Despite being widely studied in systems of distinguishable particles, entanglement been given less attention in the case of indistinguishable ones. In this case the space of quantum states is restricted to symmetric (S) or antisymmetric (A) subspaces, depending on the bosonic or fermionic nature of the system.

Entanglement of indistinguishable systems is much subtler than that of distinguishable ones, and there has been distinct approaches to its treatment, which consist essentially in the analysis of the correlations under two different aspects: the correlations genuinely arising from the entanglement between the *particles* (which we will call hereafter as "*entanglement of particles*") [\[6–8\]](#page-6-0), and the correlations arising from the entanglement between the *modes* of the system ("*entanglement of modes*") [\[9–11\]](#page-6-0). These two notions of entanglement are complementary, and the use of one or the other depends on the particular situation under scrutiny. For example, the correlations in eigenstates of a many-body Hamiltonian could be more naturally described by particle entanglement, whereas certain quantum information protocols could prompt a description in terms of entanglement of modes.

Zanardi [\[9\]](#page-6-0) as well as Wiseman and Vaccaro [\[10\]](#page-6-0) associate a Fock space to the the several distinguishable modes of a system of indistinguishable particles, which allows one to employ all the tools commonly used in distinguishable quantum systems. This notion is formalized in terms of commuting subalgebras of observables by Benatti *et al.* [\[11\]](#page-6-0). In this work we will deal with the notion of entanglement of particles [\[6–8\]](#page-6-0), which calls for different tools. Several notions for the entanglement of particles have been proposed in the literature, which agree in some respects, but differ in others. According to Eckert *et al.* [\[6\]](#page-6-0), who base their analysis in the characterization of the *useful* correlations in systems of indistinguishable particles as opposed to correlations arising purely from their statistics, the pure states with no "quantum

correlations" (in agreement with the authors, who use this term instead of entanglement of particles) are those described by a single Slater determinant for fermions, or a single Slater permanent formed out of a single one-particle state in the bosonic case. Li *et al.* [\[8\]](#page-6-0) base their analysis on the resolution of the state in a direct sum of single-particle states. Gihardi and Marinatto [\[7\]](#page-6-0) relate the notion of entanglement of quantum systems composed of two identical constituents to the impossibility of attributing a complete set of properties to both particles. It is important to note that these different definitions agree in the fermionic case, showing that the correlations generated by mere antisymmetrization of the state due to indistinguishability of their particles do not truly constitute entanglement; or equivalently, states described by a single Slater determinant, which are eigenstates of the free fermions Hamiltonian (single-particle Hamiltonian), have no entanglement between their particles. On the other hand, such definitions may disagree with each other in the bosonic case. Entanglement of indistinguishable fermions is far simpler than that of indistinguishable bosons. The definitions by Li *et al.* [\[8\]](#page-6-0) and Gihardi and Marinatto [\[7\]](#page-6-0), although distinct, result in the same set of pure bosonic states without entanglement, which is greater than that defined by Eckert *et al.* [\[6\]](#page-6-0). Interestingly, as in the fermionic case, the former set corresponds to the eigenstates of the free-boson Hamiltonian, which is expected not to possess entanglement.

Once one has opted for a certain notion for the entanglement of particles, the next step is to devise a method to calculate it. There are some interesting operational measures such as the Slater concurrence [\[6\]](#page-6-0) for two fermions or bosons of dimensions $\mathcal{A}(\mathcal{H}^4 \otimes \mathcal{H}^4)$ and $\mathcal{S}(\mathcal{H}^2 \otimes \mathcal{H}^2)$; the von Neumann entropy of the single-particle reduced state for pure states of two particles [\[8,12\]](#page-6-0); and the linear entropy of the single-particle reduced state of *N*-fermion pure states [\[13\]](#page-6-0). In a previous work [\[14\]](#page-6-0), we showed how to calculate optimal entanglement witnesses for indistinguishable fermions, and introduced a new operational measure. With our witnesses we can calculate the generalized robustness of entanglement for systems with arbitrary number of fermions, with single-particle Hilbert space of arbitrary dimension. Interestingly, in the case of two fermions with a four-dimensional single-particle Hilbert space, the generalized robustness coincides with the Slater concurrence. All these measures have limitations, either conceptual or computational, and should be considered complementary. The quantification of entanglement of particles for general states, fermionic or bosonic, remains an open problem.

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In this work, as a natural extension of $[14]$, we will show how to calculate entanglement witnesses for the bosonic case, but they will not be optimal due to some subtleties of the unentangled bosonic states. We will show that functions of the purity of the single-particle reduced state quantify entanglement for pure states, with the caveat that for some special known values, the quantifier is inconclusive for bosons. This extends previous results by Paskauskas and You [\[12\]](#page-6-0) and Plastino *et al.* [\[13\]](#page-6-0). We will also see that a simple shift in the well-known negativity $[Neg(\rho) = ||\rho^{T_i}||_1 - \text{const.}]$ [\[15\]](#page-6-0) results in a quantifier for the entanglement of particles in bosons and fermions. Finally, in the context of entanglement in many-body systems [\[4,5,16\]](#page-6-0), we will analyze homogeneous *D*dimensional Hamiltonians with certain symmetries by means of the von Neumann entropy of the single-particle reduced state.

This paper is organized as follows. In Sec. II we consider the entanglement of particles in fermionic states, showing how the purity of the single-particle reduced state can be used as a measure for pure states, and the negativity for the general case. In Sec. [III](#page-2-0) the same analysis is made for bosons. In Sec. [IV](#page-2-0) we discuss entanglement witnesses in bosonic systems. In Sec. [V](#page-3-0) we make some remarks about the different measures for the entanglement of particles, and discuss how they compare for pure states with single-particle Hilbert space with the smallest dimension, proving some relations. In Sec. [VI](#page-4-0) we show how to use the tools presented in the previous sections in the context of entanglement in many-body systems. In the Appendix, we prove the expressions for the negativity of bosons and fermions. We conclude in Sec. [VII.](#page-5-0)

II. FERMIONS

Systems of indistinguishable particles have a more concise description in the second quantization formalism. Therefore we introduce operators with the following anticommutation relations:

$$
\{f_i^{\dagger}, f_j^{\dagger}\} = \{f_i, f_j\} = 0, \quad \{f_i, f_j^{\dagger}\} = \delta_{ij}.
$$
 (1)

 f_i^{\dagger} and f_i are the fermionic creation and annihilation operators, respectively, such that their application on the vacuum state $(|0\rangle)$ creates or annihilates a fermion in state *i*. The vacuum state is defined such that that $f_i|0\rangle = 0$. As mentioned in the Introduction, the different definitions for the entanglement of particles agree with each other in the fermionic case, in the sense that the set of unentangled states can be defined as follows.

Fermionic state without particle entanglement: A fermionic state $\sigma \in \mathcal{B}(\mathcal{A}(\mathcal{H}_1^d \otimes \cdots \otimes \mathcal{H}_N^d))$ has no particle entanglement if it can be decomposed as a convex combination of Slater determinants, namely,

$$
\sigma = \sum_{i} p_i \ a_1^{i^{\dagger}} \cdots a_N^{i^{\dagger}} |0\rangle\langle 0| a_N^{i} \cdots a_1^{i}, \quad \sum_{i} p_i = 1, \tag{2}
$$

where a_k^i ^T = $\sum_{l=1}^d u_{kl}^i f_l^{\dagger}$ ($\{a_k^i\}$ ^T) is a set of orthonormal operators in the index k), U^i is a unitary matrix of dimension dN , and $\{f_l^{\dagger}\}\$ is an orthonormal basis of fermionic creation operators for the space of a single fermion (\mathcal{H}^d) . Note that unentangled pure states are single Slater determinants. The single-particle reduced states ($\sigma_{r(s|_1)}$) of a single Slater determinant have a particularly interesting form and stand for the pure states in the "*N*-representable" reduced space (single-particle reduced space respective to the antisymmetric space of *N* fermions) [\[17\]](#page-6-0).

Single-particle reduced fermionic state without particle entanglement: Given a pure fermionic state without particle entanglement, i.e., a single Slater determinant, $|\psi\rangle$ = $a_{\phi_1}^{\dagger} a_{\phi_2}^{\dagger} \cdots a_{\phi_N}^{\dagger}$ |0), where $\{a_{\phi_i}^{\dagger}\}\$ are orthonormal, we have the equivalence

$$
\sigma_{r_{(\text{SI}_1)}} \equiv \frac{1}{N} \sum_{i=1}^N a_{\phi_i}^\dagger |0\rangle\langle 0| a_{\phi_i} \iff |\psi\rangle = a_{\phi_1}^\dagger a_{\phi_2}^\dagger \cdots a_{\phi_N}^\dagger |0\rangle, \tag{3}
$$

where $\sigma_{r_{(Sl_1)}} = \text{Tr}_1 \cdots \text{Tr}_{N-1}(|\psi\rangle \langle \psi|)$ is the single-particle reduced state (Tr*ⁱ* is the partial trace over particle *i*). Therefore, if σ is a mixed unentangled state, its single-particle reduced state in the *N*-representable reduced space is

$$
\sigma_r \equiv \text{Tr}_1 \cdots \text{Tr}_{N-1}(\sigma) = \sum_i p_i \sigma_{r_{(\text{SI}_1)}}^i.
$$
 (4)

Now, aware of Eq. (3) , it is straightforward to conclude that shifted positive semidefinite functions of the purity of the single-particle reduced state can be used to measure the entanglement of particles of a pure fermionic state, a result similar to that obtained by Paskauskas and You [\[12\]](#page-6-0) or Plastino *et al.* [\[13\]](#page-6-0). Using, for example, the von Neumann entropy $S(\rho) = \text{Tr}(-\rho \ln \rho)$, we see that $S(\rho_r =$ $Tr_1 \cdots Tr_{N-1}(|\psi\rangle \langle \psi|) \ge S(\sigma_{r(s_{1})}) = \ln N$, and thus a measure *E* for the entanglement of particles of a pure fermionic state can be defined as a shifted von Neumann entropy of the single-particle reduced state.

Shifted von Neumann entropy of entanglement for pure states:

$$
E(|\psi\rangle\langle\psi|) = S(\rho_r) - \ln N. \tag{5}
$$

The case of pure states is easy due to the unique form of the unentangled single-particle reduced states [Eq. (3)], which is no longer the case for mixed states [Eq. (4)]. Though not obvious, but straightforward to prove as we show in the Appendix, we can measure the entanglement of particles of mixed fermionic states by the following shifted negativity.

Shifted negativity:

$$
Neg(\rho) = \begin{cases} \|\rho^{T_i}\|_1 - N & \text{if } \|\rho^{T_i}\|_1 > N, \\ 0 & \text{otherwise,} \end{cases}
$$
 (6)

where T_i is the partial transpose over the *i*th particle, and $\|\cdot\|_1$ is the trace norm. If ρ is a single Slater determinant, its trace norm is *N*, and it is smaller in the case of an unentangled mixed state, as shown in the Appendix. Note, however, that we do not know if there are entangled fermionic states whose negativity is null. It is easy to check that as expected, the particle entanglement is nonincreasing under one-particle symmetric operations (local symmetric operations), as shown in our previous work [\[14\]](#page-6-0).

III. BOSONS

As in the previous section, we introduce operators to describe the bosonic system in the second quantization formalism. The operators satisfy the usual commutation relations

$$
[b_i^{\dagger}, b_j^{\dagger}] = [b_i, b_j] = 0, \quad [b_i, b_j^{\dagger}] = \delta_{ij}, \tag{7}
$$

where b_i^{\dagger} and b_i are the bosonic creation and annihilation operators, respectively, such that their application on the vacuum state (|0) creates or annihilates a boson in state *i*. The vacuum state is defined such that $b_i |0\rangle = 0$. The different notions of particle entanglement in bosons diverge from each other, resulting in two distinct sets of unentangled states.

Bosonic pure state with no particle entanglement: A bosonic pure state $|\psi\rangle \in \mathcal{S}(\mathcal{H}_1^d \otimes \cdots \otimes \mathcal{H}_N^d)$ without particle entanglement can be written as

Definition 1.
$$
|\psi\rangle = \prod_{i=1}^{N_o} \frac{(b_{\phi_i}^{\dagger})^{n_{\phi_i}}|0\rangle}{\sqrt{(n_{\phi_i}!)}},
$$
 (8)

Definition 2.
$$
|\psi\rangle = \frac{1}{\sqrt{N!}} (b_{\phi}^{\dagger})^N |0\rangle,
$$
 (9)

where $b_{\phi_i}^{\dagger} = \sum_{k=1}^d u_{ik} b_k^{\dagger} (\{ b_{\phi_i}^{\dagger} \})$ is a set of orthonormal operators in the index *i*), *U* is a unitary matrix of dimension dN_o , N_o is the number of distinct occupied states, and n_{ϕ_i} is the number of bosons in the state *φi*. Unentangled mixed states are those that can be written as convex combinations of unentangled pure states. We clearly see that the set of states without particle entanglement according to definition 1 includes the set derived from definition 2, since the latter is a particular case of the former, with $N_o = 1$.

On the one hand, definition 2 mirrors the case of distinguishable particles. Therefore one can use the entropy of the one-particle reduced state $S(\rho_r)$ and the usual negativity $\|\rho^{T_i}\|_1 - 1$ to quantify the entanglement. On the other hand, the problem is delicate for definition 1, since the equivalence between pure states without particle entanglement and the single-particle reduced states is no longer uniquely defined by the analog of Eq. (3) . The shifted negativity given by Eq. (6) is still valid, but now we do know that there are entangled states with $\|\rho^{T_i}\|_1 < N$. The entropy of the one-particle reduced state gives information about particle entanglement, but as a quantifier it must be better understood. We know that an unentangled bosonic pure state, according to Eq. (8) , has the following one-particle reduced state:

$$
\sigma_r(\phi_i, \phi_j) = \frac{1}{N} \text{Tr} \left(b_{\phi_j}^{\dagger} b_{\phi_i} | \psi \rangle \langle \psi | \right) = \begin{cases} \frac{1}{N} n_{\phi_i}, \text{ if } \phi_i = \phi_j \\ 0, \text{ otherwise,} \end{cases}
$$

\n
$$
\sigma_r = \frac{1}{N} \sum_{i=1}^{N_o} n_{\phi_i} b_{\phi_i}^{\dagger} |0\rangle \langle 0| b_{\phi_i}, \tag{10}
$$

where $\sigma_r(\phi_i, \phi_j)$ is a matrix element of σ_r . The entropy of the one-particle reduced state assumes the special values

$$
S(\sigma_r) = -\sum_{i=1}^{N_o} \left(\frac{n_{\phi_i}}{N}\right) \ln\left(\frac{n_{\phi_i}}{N}\right). \tag{11}
$$

Note that $0 \le S(\sigma_r) \le \ln N$, and therefore when $S(\rho_r) > \ln N$, the pure state *ρ* is *entangled*. The pure state is also *entangled* if $S(\rho_r)$ is not one of the values given by Eq. (11). Take for example the case of two bosons: we have either $N_o = 1, n_{\phi_i} = 2$ and thus $S(\sigma_r) = 0$, or $N_o = 2$, $n_{\phi_i} = 1$ and $S(\sigma_r) = \ln 2$. Given an arbitrary pure state ρ of two bosons, if $S(\rho_r) = 0$ we can say with certainty that the state has no particle entanglement, but if $S(\rho_r) = \ln 2$ we cannot conclude anything, because either a state with no particle entanglement, e.g., $|\psi\rangle = b_{\phi_i}^{\dagger} b_{\phi_j}^{\dagger} |0\rangle$, or an entangled one, e.g., $|\psi\rangle = \frac{1}{\sqrt{3}} (c_i b_{\phi_i}^{\dagger} b_{\phi_i}^{\dagger} + c_j b_{\phi_j}^{\dagger} b_{\phi_j}^{\dagger} +$ $c_k b_{\phi_k}^{\dagger} b_{\phi_k}^{\dagger}$ |0), with $c_{i,j,k} \in \mathcal{R}$, and $S(\rho_r) \subset (0, \ln 3]$, could have the same von Neumann entropy for the one-particle reduced state.

IV. WITNESSED ENTANGLEMENT

In this section we present a bosonic entanglement witness. Although it is analogous to the fermionic entanglement witness we introduced in a previous work [\[14\]](#page-6-0), it is not optimal due to the complicated structure of the unentangled bosonic states.

A Hermitian operator *W* is an entanglement witness for a given entangled quantum state ρ [\[18\]](#page-6-0) if its expectation value is negative for the particular entangled quantum state $[Tr(W\rho) < 0]$, while it is non-negative on the set of nonentangled states *S* [$\forall \sigma \in S$, Tr($W\sigma$) ≥ 0]. We say that W_{opt} is the optimal entanglement witnesses (OEW) for ρ , if

$$
Tr(W_{\text{opt}}\rho) = \min_{W \in \mathcal{M}} Tr(W\rho), \tag{12}
$$

where M represents a compact subset of the set of entanglement witnesses W . With OEWs we can quantify entanglement $E(\rho)$ by means of an appropriate choice of the set M [\[19\]](#page-6-0):

$$
E(\rho) = \max[0, -\min_{W \in \mathcal{M}} \text{Tr}(W\rho)].
$$
 (13)

In the fermionic case $[14]$, restricting the witness operators to the antisymmetric space $\{W = A W A^{\dagger}\}\$, the constraint $\{W \leq$ A} defines the fermionic generalized robustness $R_g^{\mathcal{F}}$; while the constraint $\{Tr(W) = D_a\}$, where D_a is the antisymmetric *N*-particle Hilbert space dimension, defines the fermionic random robustness $R_r^{\mathcal{F}}$; and the constraint $\{Tr(W) \leq 1\}$ defines the fermionic robustness of entanglement $R_e^{\mathcal{F}}$. These quantifiers correspond to the minimum value of s ($s \ge 0$), such that

$$
\sigma = \frac{\rho + s\varphi}{1 + s} \tag{14}
$$

is an unentangled state [according to Eq. (2)], where φ can be entangled or not in the case of $R_g^{\mathcal{F}}$, is unentangled in the case of R^2 , and is the maximally mixed state A/D_a in the case of $R_r^{\mathcal{F}}$.

The method for obtaining the OEW in the fermionic case is based on semidefinite programs (SDPs) [\[20\]](#page-6-0), which can be solved efficiently with arbitrary accuracy. Now we will mimic the procedure for constructing *W* presented in [\[14\]](#page-6-0), and try to obtain the generalized robustness for bosonic states. Consider the following SDP:

minimize Tr(*W*
$$
\rho
$$
)
\nminimize Tr(*W* ρ)
\nsubject to
\n
$$
\begin{cases}\n\sum_{i_{N-1}=1}^{d} \cdots \sum_{i_{1}=1}^{d} \sum_{j_{1}=1}^{d} \cdots \sum_{j_{N-1}=1}^{d} \left(c_{i_{N-1}}^{N-1*} \cdots c_{i_{1}}^{1*} c_{j_{1}}^{1} \cdots c_{j_{N-1}}^{N-1} W_{i_{N-1} \cdots i_{1}} j_{1} \cdots j_{N-1} \right) \ge 0, \\
& \forall c_{i}^{k} \in C, 1 \le k \le (N-1), 1 \le i \le d, \\
& \mathcal{S} W \mathcal{S}^{\dagger} = W, \\
& W \le \mathcal{S},\n\end{cases}
$$
\n(15)

where *d* is the dimension of the single-particle Hilbert space, S is the symmetrization operator, $W_{i_{N-1}\cdots i_1 j_1\cdots j_{N-1}} =$ *b*_{*iN−1}* \cdots *b_i*₁</sub> *W b*^{\dagger}_{*j*}¹ \cdots *b*^{\dagger}_{*jN−1*} \in *B*(*H^d*) is an operator acting on the space of one boson, and $\{b_l^{\dagger}\}\$ is an orthonormal basis of bosonic creation operators. The notation $W \leq S$ means that $(S - W) \ge 0$ is a positive semidefinite operator. The optimal *W* obtained by this program is an entanglement witness, but it cannot be optimal, as we now discuss.

For an arbitrary bosonic unentangled state σ , the semipositivity condition $\text{Tr}(W\sigma) \geq 0$ is equivalent to

$$
\langle 0| b_N b_{N-1} \cdots b_1 W b_1^{\dagger} \cdots b_{N-1}^{\dagger} b_N^{\dagger} |0\rangle \geq 0, \qquad (16)
$$

for all orthonormal sets of creation operators ${b_k^{\dagger}}$. This condition is taken into account in the second and third lines of Eq. (15) by means of the semipositivity of the operator $b_{N-1} \cdots b_1 W b_1^{\dagger} \cdots b_{N-1}^{\dagger}$. Therefore, the entanglement witness *W* will not detect bosonic entangled states of the form $b_1^\dagger \cdots b_{N-1}^\dagger \tilde{b}_N^\dagger |0\rangle$, where \tilde{b}_N^\dagger is not orthogonal to b_k^\dagger , a problem which does not arise in the fermionic case due to the Pauli exclusion principle. In numerical tests, we noticed that the quality of *W* improves with the increase of the single-particle Hilbert space dimension.

V. MEASURES INTERRELATIONS

In this section we highlight the relationship among the measures of particle entanglement for fermionic and bosonic pure states in the smallest dimension, $\mathcal{A}(\mathcal{H}^4 \otimes \mathcal{H}^4)$ and $S(\mathcal{H}^2 \otimes \mathcal{H}^2)$, respectively. While the fermionic case resembles that of distinguishable qubits, the bosonic case is more intricate due to the structure of the unentangled states.

For pure states of distinguishable qubits, $\rho = |\psi\rangle \langle \psi|$ $\mathcal{B}(\mathcal{H}^2\otimes\mathcal{H}^2)$, the following equivalence is well known for generalized robustness $\mathcal{R}_g(\rho)$, robustness of entanglement $\mathcal{R}_e(\rho)$, random robustness $\mathcal{R}_r(\rho)$, Wooters concurrence $C_W(\rho)$, negativity Neg(ρ), and entropy of entanglement $E(\rho)$ [\[21–](#page-6-0)[24\]](#page-7-0):

$$
\mathcal{R}_{g}(\rho) = \mathcal{R}_{e}(\rho) = \frac{1}{2}\mathcal{R}_{r}(\rho) = C_{W}(\rho) = \text{Neg}(\rho) \propto E(\rho).
$$
\n(17)

Recall that $E(\rho)$ is the Shannon entropy of the eigenvalues $(\lambda, 1 - \lambda)$ of the reduced one-qubit state, and $C_W =$ $\frac{2\sqrt{\lambda(1-\lambda)}}{2}$.

For pure two-fermion states, $\rho = |\psi\rangle \langle \psi| \in \mathcal{B}(\mathcal{A}(\mathcal{H}^4 \otimes$ \mathcal{H}^4)), we have found similar relations:

$$
\mathcal{R}_g^{\mathcal{F}}(\rho) = \mathcal{R}_e^{\mathcal{F}}(\rho) = \frac{2}{3}\mathcal{R}_r^{\mathcal{F}}(\rho) = C_S^{\mathcal{F}}(\rho) = \frac{1}{2}\text{Neg}(\rho) \propto E(\rho).
$$
\n(18)

Note that $Neg(\rho)$ and $E(\rho)$ are the shifted measures. The relations between robustness and Slater concurrence were observed numerically by means of optimal entanglement witnesses [\[14\]](#page-6-0), and now we prove them. Based on the Slater decomposition $|\psi\rangle = \sum_i z_i a_{2i-1}^{\dagger} a_{2i}^{\dagger} |0\rangle$, where $a_i^{\dagger} =$ $\sum_{k} U_{ik} f_{k}^{\dagger}$, we can write the following optimal decomposition [viz. Eq. [\(14\)\]](#page-2-0):

$$
\sigma_{\text{opt}} = \frac{1}{1+t} (\rho + t\phi_{\text{opt}}),\tag{19}
$$

$$
\phi_{\text{opt}} = \frac{1}{2} (a_1^{\dagger} a_3^{\dagger} |0\rangle \langle 0| a_3 a_1 + a_2^{\dagger} a_4^{\dagger} |0\rangle \langle 0| a_4 a_2).
$$
 (20)

Now we show that when $t = C_s^{\mathcal{F}}(\rho)$, σ_{opt} is unentangled and in the border of the uncorrelated states. We know that the Slater concurrence of the state is invariant under unitary local symmetric maps Φ . We can always choose Φ so that the singleparticle modes $\{a_i^{\dagger}\}\$ are mapped into the canonical modes ${f_i^{\dagger}}$ [\[25\]](#page-7-0). Therefore $\Phi \sigma_{opt} \rightarrow \sigma'_{opt} = \frac{1}{1+t} (|\psi'\rangle \langle \psi'| + t \phi'_{opt}),$ where $|\psi'\rangle = \sum_i z_i f_{2i-1}^{\dagger} f_{2i}^{\dagger}$, and $\phi_{opt}' = \frac{1}{2} (f_1^{\dagger} f_3^{\dagger} | 0 \rangle \langle 0 | f_3 f_1 +$ $f_2^{\dagger} f_4^{\dagger} |0\rangle \langle 0| f_4 f_2$.

The Slater concurrence of σ'_{opt} is given by $C_S^{\mathcal{F}}(\sigma'_{opt}) =$ $\max(0, \lambda_4 - \lambda_3 - \lambda_2 - \lambda_1)$, where $\{\lambda_i\}_{i=1}^4$ are the eigenvalmax(0,λ₄ − λ₃ − λ₂ − λ₁), where {λ_{i }_{i=1} are the eigenvalues, in nondecreasing order, of the matrix $\sqrt{\sigma'_{\text{op}}\sigma'_{\text{op}}},$ with $\tilde{\sigma}' = (K\mathcal{U} \cdot \sigma' \cdot (K\mathcal{U} \cdot)^\dagger$ *K* being the complex conjugation} $\widetilde{\sigma}_{opt}' = (\mathcal{KU}_{ph}) \sigma_{opt}' (\mathcal{KU}_{ph})^{\dagger}$, K being the complex conjugation
operator, and U₁, the particle-hole transformation. Consider operator, and \mathcal{U}_{ph} the particle-hole transformation. Consider the following matrix:

$$
\sqrt{\sigma_{\text{opt}}'\widetilde{\sigma}_{\text{opt}}'}
$$
\n
$$
= \sqrt{\frac{1}{(1+t)^2} [\rho'\widetilde{\rho'} + t(\rho'\widetilde{\phi}_{\text{opt}}' + \phi_{\text{opt}}'\widetilde{\rho'}) + t^2 \phi_{\text{opt}}'\widetilde{\phi}_{\text{opt}}'}.
$$
\n(21)

Note that $\sigma'_{\text{opt}}, \rho', \phi'_{\text{opt}}$ and their pairs are all real matrices. With the aid of Eqs. (19) and (20), it is easy to see that $\rho' \widetilde{\phi}'_{opt} =$ $\phi'_{opt}\tilde{\rho}' = 0$, and $\phi'_{opt}\tilde{\phi}'_{opt} = \frac{1}{2}\phi'_{opt}$, and that $\rho'\tilde{\rho}'$ is orthogonal to $\phi_{opt}' \tilde{\phi}_{opt}'$. Thus Eq. (21) reduces to

$$
\sqrt{\sigma_{\text{opt}}'\widetilde{\sigma}_{\text{opt}}'} = \frac{1}{(1+t)} \bigg(\sqrt{\rho'\widetilde{\rho}'} + \frac{t}{\sqrt{2}} \sqrt{\phi_{\text{opt}}'} \bigg). \tag{22}
$$

The eigenvalues of $\sqrt{\rho' \tilde{\rho}'}$ are easily obtained by means of the Slater decomposition, and the only non-null eigenvalue is its Slater decomposition, and the only non-null eigenvalue is given by $C_S^{\mathcal{F}}(\rho')$. $\sqrt{\phi_{\text{opt}}'}$ has just two non-null eigenvalues, which are equal, given by $\frac{1}{\sqrt{2}}$ [viz. Eq. [\(20\)\]](#page-3-0). Therefore the eigenvalues of the Eq. [\(21\)](#page-3-0) are $\frac{1}{(1+t)}(C_S^{\mathcal{F}}(\rho'), \frac{t}{2}, \frac{t}{2}, 0)$, and according to the definition of the Slater concurrence it follows directly that $C_S^{\mathcal{F}}(\sigma'_{opt}) = 0$ if and only if $t \geq C_S^{\mathcal{F}}(\rho')$.

We end this section by considering pure two-boson states, $\rho = |\psi\rangle\langle\psi| \in \mathcal{B}(\mathcal{S}(\mathcal{H}^2 \otimes \mathcal{H}^2))$. We have the following relations, which can be easily verified:

$$
C_S^{\mathcal{B}}(\rho) = \text{Neg}(\rho)_{\text{def.2}} \propto E(\rho)_{\text{def.2}}.\tag{23}
$$

In considering the measures corresponding to definition 1 of unentangled states [Eq. (8)], we see that they are related differently, since the negativity will always be zero for such states ($\|\rho^{T_i}\|_1 \leq 2$). This is due to the use of the upper limit in Eq. [\(A10\)](#page-6-0) (viz. Appendix). We could, however, instead of using this upper limit, obtain analytically the values of $\|\rho^{T_i}\|_1$ corresponding to the unentangled pure states, which would be equal to $\|\rho^{T_i}\|_1 = 1$ or 2, and perform a similar analysis to that made for the $S(\rho_r)_{\text{def.1}}$ in Eq. [\(11\).](#page-2-0) Thus it would be possible to relate the negativity and the entropy of entanglement according to definition 1. We see therefore that the relations between the distinct measures are similar to the distinguishable case when we consider definition 2 [Eq. [\(9\)\]](#page-2-0) of particle entanglement, possessing some discrepancies when we consider definition 1.

VI. HOMOGENEOUS *D***-DIMENSIONAL HAMILTONIAN**

Given the easy computability of the entanglement measures presented above, in particular the negativity and functions of the purity of the single-particle reduced state, in this section we employ them to quantify entanglement of particles in manybody systems, described by homogeneous Hamiltonians with certain symmetries.

Consider the Hamiltonian of a *D*-dimensional lattice, with *N* indistinguishable particles of spin Σ , L^D sites (with the closure boundary condition, $L + 1 = 1$), and the orthonormal basis $\{c_{\vec{i}\sigma}^{\dagger}, c_{\vec{i}\sigma}^{\dagger}\}$ of creation and annihilation operators for the particles in that lattice, where $\vec{i} = (i_1, \dots, i_D)$ is the spatial position vector, and $\sigma = -\Sigma$, $(-\Sigma + 1)$, \dots , $(\Sigma - 1)$, Σ is the spin in the direction \hat{S}_z . If the eigenstates are degenerate, we can use the negativity to quantify their entanglement, and if the eigenstates are nondegenerate, we can also use any function of the purity of their reduced state as a quantifier. For example, the purity function, i.e., $\text{Tr}(\rho_r^2)$, is lower than 1*/N* if (if and only if, in the case of fermions) the state is entangled. Thus we can define the measure *E* based on the purity function as $E(|\psi\rangle \langle \psi|) = \max\{0, \frac{1}{N} - \text{Tr}(\rho_r^2)\}\$. If, however, the Hamiltonian has some symmetries, it is possible to obtain an analytic expression for the particle entanglement of their eigenstates according to the von Neumann entropy of its single-particle reduced state. Let the Hamiltonian be *homogeneous*, and with the properties (1) their eigenstates are nondegenerate and (2) the Hamiltonian commutes with the spin operator S_z (thus S_z and the Hamiltonian share the same

eigenstates), if ρ is one of its eigenstates, we have then

$$
\text{Tr}\left(c_{\vec{i}\sigma}^{\dagger}c_{\vec{j}\bar{\sigma}}\,\rho\right) = \text{Tr}\left(c_{(\vec{i}+\vec{\delta})\sigma}^{\dagger}c_{(\vec{j}+\vec{\delta})\bar{\sigma}}\,\rho\right),\tag{24}
$$

$$
\operatorname{Tr}\left(c_{\overline{j}\sigma}^{\dagger}c_{\overline{j}\bar{\sigma}}\ \rho\right) = 0, \quad \forall \ i, j,
$$
\n⁽²⁵⁾

where Eq. (24) follows from the translational invariance property of the quantum state due to the homogeneity of the Hamiltonian, while Eq. (25) follows directly from condition (2). By condition (1) of nondegeneracy and the results of the previous sections, we know that the von Neumann entropy of the single-particle reduced state can be used as a quantifier of the particle entanglement. Let us calculate it.

We know that matrix elements of the reduced state are given by $\rho_r(\vec{i}\sigma, \vec{j}\bar{\sigma}) = \frac{1}{N} \text{Tr}(c_{\vec{j}\bar{\sigma}}^{\dagger} c_{\vec{i}\sigma} | \psi \rangle \langle \psi |)$ and, according to Eq. (25), subspaces of the reduced state with different spin *σ* are disjoint. We can therefore diagonalize the reduced state in these subspaces separately. Equation (24) together with the boundary condition fix the reduced state to a circulant matrix. More precisely, for the unidimensional case $(D = 1)$, given the subspace with spin σ and $\{c_{i\sigma}^{\dagger}\}_{i=1}^L$, the reduced state is given by the following $L \times L$ matrix:

$$
\rho_r^{\sigma} = \frac{1}{N} \begin{pmatrix} x_0 & x_1 & \cdots & x_{L-2} & x_{L-1} \\ x_{L-1} & x_0 & x_1 & & x_{L-2} \\ \vdots & x_{L-1} & x_0 & \ddots & \vdots \\ x_2 & \ddots & \ddots & x_1 \\ x_1 & x_2 & \cdots & x_{L-1} & x_0 \end{pmatrix}, \quad (26)
$$

$$
x_{\delta} = \langle c^{\dagger}_{(k+\delta)\sigma} c_{k\sigma} \rangle, \tag{27}
$$

$$
x_0 = \langle c_{k\sigma}^\dagger c_{k\sigma} \rangle = n_{k\sigma} \underbrace{=}_{\text{Eq.}(24)} n_{i\sigma} = \frac{N_\sigma}{L},\tag{28}
$$

where $N_{\sigma} = \sum_{j=1}^{L} n_{j\sigma}$. The terms x_{δ} can be obtained in several ways, $e.g.,$ directly from one-particle Green's function, by computational methods like quantum Monte Carlo, or by the Density Matrix Renormalization Group method (DMRG). The eigenvalues $\{\lambda_j^{\sigma}\}_{j=1}^L$ of the circulant matrix are given by $\lambda_j^{\sigma} = \sum_{k=0}^{L-1} x_k w_j^k$, where $w_j = \exp \frac{2\pi i j}{L}$. Thus the particle entanglement of that eigenstate can be calculated from $S(\rho_r)$ = $-\sum_{j,\sigma}\lambda_j^{\sigma}$ ln λ_j^{σ} .

For higher dimensions, given the subspace of a single particle with spin σ and $\{c_{i\sigma}^{\dagger}\}_{i=1}^{L^D}$, the characteristic vector of its circulant matrix (e.g., the matrix first line) is given by

 $[D = 2]$:

$$
\vec{v}_c = ([x_{00} \cdots x_{(L-1)0}] [x_{01} \cdots x_{(L-1)1}]
$$

$$
\cdots [x_{0(L-1)} \cdots x_{(L-1)(L-1)}]), \qquad (29)
$$

$$
\vec{v}_c = \left(v_{z=0}^{2D} \ v_{z=1}^{2D} \ \cdots \ v_{z=(L-1)}^{2D}\right),\tag{30}
$$

 ${\rm where} \quad v_{z=l}^{2D} = (\left[x_{00l} \cdots x_{(L-1)0l}\right]\left[x_{01l} \cdots x_{(L-1)1l}\right] \cdots \left[x_{0(L-1)l}\right]$ $\cdots x_{(L-1)(L-1)l}$]) is the characteristic vector of the plane $z = l$, and $x_{\delta_x \delta_y \delta_z} = \langle c_{(l+\delta_x)(m+\delta_y)(n+\delta_z)\sigma}^{\dagger} c_{(lmn)\sigma} \rangle$. Thus, the eigenvalues $\{\lambda_j^{\sigma}\}_{j=1}^{L^D}$ of the reduced state are given by

$$
[D = 2] : \lambda_j^{\sigma} = \sum_{l,m=0}^{L-1} x_{lm} w_j^{l+m}.
$$
 (31)

$$
[D = 3] : \lambda_j^{\sigma} = \sum_{l,m,n=0}^{L-1} x_{lmn} w_j^{l+mL+nL^2}, \qquad (32)
$$

where $w_j = \exp \frac{2\pi i j}{L^D}$. If we wished to obtain the particle entanglement according to the purity function, as presented in the beginning of this section, we would easily obtain the following expression:

$$
E(|\psi\rangle\langle\psi|) = \max\left\{0, \frac{1}{N} - \frac{L^D}{N^2} \sum_{\vec{\delta},\sigma} \left| \langle c_{(\vec{i}+\vec{\delta})\sigma}^{\dagger} c_{\vec{i}\sigma} \rangle \right|^2 \right\}
$$
(33)

for any fixed spatial position vector \vec{i} . Note, however, that although the calculation of the purity function is simple even for the case of a general Hamiltonian, since it is just the sum over the one-particle Green's function $\langle c_{i\sigma}^{\dagger} c_{k\sigma} \rangle$ [note that $\text{Tr}(\rho_r^2) = \frac{1}{N^2} \sum_{\vec{i}, \vec{k}, \sigma, \widetilde{\sigma}} |\langle c_{\vec{i}\widetilde{\sigma}}^{\dagger} c_{\vec{k}\sigma} \rangle|^2$] and thus does not require the diagonalization of the single-particle reduced state, the measure according to the von Neumann entropy can be more interesting, given its wide application in quantum information theory.

VII. CONCLUSION

Entanglement of distinguishable particles is related to the notion of separability, i.e., the possibility of describing the system by a simple tensor product of individual states. In systems of indistinguishable particles, the symmetrization or antisymmetrization of the many-particle state eliminates the notion of separability, and the concept of entanglement becomes subtler. If one is interested in the different modes (or configurations) the system of indistinguishable particles can assume, it is possible to use the same tools employed in systems of distinguishable particles to calculate the entanglement of modes. On the other hand, if one is interested in the genuine entanglement between the particles, as discussed in the present work, one needs new tools. In this case, we have seen that entanglement of particles in fermionic systems is simple, in the sense that the necessary tools are obtained by simply antisymmetrizing the distinguishable case, and one is led to the conclusion that unentangled fermionic systems are represented by convex combinations of Slater determinants. The bosonic case, however, does not follow straightforwardly by symmetrization of the distinguishable case. The possibility of multiple occupation implies that a many-particle state of Slater rank one in one basis can be of higher rank in another basis. This ambiguity reflects on the possibility of multiple values of the von Neumann entropy for the one-particle reduced state of a pure many-particle state. Aware of the subtleties of the bosonic case, we have proven that a *shifted* von Neumann entropy and a *shifted* negativity can be used to quantify entanglement of particles. Motivated by previous results with fermionic optimal entanglement witnesses, we have proven relations for robustness of entanglement and Slater concurrence for two-fermion systems with a four-dimensional single-particle Hilbert space, in particular showing that the generalized robustness and the Slater concurrence coincide for pure states. We have shown that the bosonic entanglement witness analogous to the fermionic entanglement witness is not optimal, due to the possibility of multiple occupation in the former case. Nonetheless, numerical calculations have shown that the bosonic witness improves with the increase of the single-particle Hilbert space dimension. Finally, we have illustrated how the tools presented in this article could be useful in analyzing the properties of entanglement in many-body systems, obtaining in particular analytic expressions for the entanglement of particles according to the von Neumann entropy of the single-particle reduced state in homogeneous *D*-dimensional Hamiltonians.

Though we have not studied quantum correlations beyond entanglement, we mention that the *quantumness* or *nonclassicality* of states of indistinguishable particles can be reduced to the calculation of bipartite entanglement between the main system and an ancilla, following the *activation protocol* introduced by Piani *et al.* [\[26\]](#page-7-0). In this case, besides the usual symmetrization of operations to preserve indistinguishability, one must be more careful with the phraseology, because a *system of indistinguishable particles* cannot be classical. We will defer this discussion to a future work.

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APPENDIX: NEGATIVITY IN FERMIONIC AND BOSONIC STATES

In this appendix we calculate the trace norm of the partial transpose of an uncorrelated fermionic or bosonic state, i.e., $\|\sigma^{T_i}\|_1 = \text{Tr}[(\sigma^{T_i}, \sigma^{T_i^{\dagger}})^{\frac{1}{2}}]$, thus proving the *shifted negativity* [Eq. (6)]. We do so by the explicit diagonalization of the operator ($\sigma^{T_i} \sigma^{T_i^T}$). Consider first the case of a fermionic or bosonic pure state $\sigma = |\psi\rangle \langle \psi|$, as given by Eqs. [\(2\)](#page-1-0) and [\(8\),](#page-2-0) which can be rewritten as

$$
\sigma = C \sum_{\pi\pi'} \epsilon_{\pi} \epsilon_{\pi'} P_{\pi} \, |\phi_1 \phi_2 \cdots \phi_N\rangle \, \langle \phi_N \cdots \phi_2 \phi_1 | P_{\pi'}, \quad (A1)
$$

with $|\psi\rangle = \sqrt{C} \sum_{\pi} \epsilon_{\pi} P_{\pi} |\phi_1 \phi_2 \cdots \phi_N\rangle$, where ϕ_i, ϕ_j are either equal or orthonormal, P_{π} are the permutation operators, ϵ_{π} is the permutation parity ($\epsilon = \pm 1$ for fermions, $\epsilon = 1$ for bosons), and $C = (N!)^{-1}$ for fermions or $C =$ $[N! \prod_{i=1}^{N_o} (n_{\phi_i}!)]^{-1}$ for bosons. From now on we omit the normalization *C* and introduce the following notation:

$$
P_{\pi} |\phi_1 \cdots \phi_N\rangle = |\pi(\phi_1 \cdots \phi_N)\rangle = |\pi(\phi_1)\pi(\phi_2) \cdots \pi(\phi_N)\rangle.
$$
\n(A2)

Now we make the partial transpose on the first particle explicit:

$$
\sigma^{T_1} = \sum_{\pi\pi'} \epsilon_{\pi} \epsilon_{\pi'} \left| \pi'(\phi_1)\pi(\phi_2 \cdots \phi_N) \right\rangle \langle \pi'(\phi_N \cdots \phi_2)\pi(\phi_1) |,
$$
\n(A3)

$$
(\sigma^{T_1})^{\dagger} = \sigma^{T_1},\tag{A4}
$$

$$
\sigma^{T_1} \sigma^{T_1} = \sum_{\pi, \pi', \tilde{\pi}, \tilde{\pi}'} \epsilon_{\pi} \epsilon_{\pi'} \epsilon_{\tilde{\pi}} \epsilon_{\tilde{\pi}'} |\pi'(\phi_1) \pi(\phi_2 \cdots \phi_N) \rangle \times \langle \pi'(\phi_N \cdots \phi_2) \pi(\phi_1) | \tilde{\pi}'(\phi_1) \tilde{\pi}(\phi_2 \cdots \phi_N) \rangle \times \langle \tilde{\pi}'(\phi_N \cdots \phi_2) \tilde{\pi}(\phi_1) |, \tag{A5}
$$

$$
\sigma^{T_1} \sigma^{T_1} = \sum_{\pi', \tilde{\pi}} \epsilon_{\pi'} \epsilon_{\tilde{\pi}} \langle \pi'(\phi_N \cdots \phi_2) | \tilde{\pi}(\phi_2 \cdots \phi_N) \rangle | \pi'(\phi_1) \rangle
$$

$$
\times \langle \tilde{\pi}(\phi_1) | \otimes \sum_{\pi, \tilde{\pi}'} \epsilon_{\pi} \epsilon_{\tilde{\pi}'} \langle \pi(\phi_1) | \tilde{\pi}'(\phi_1) \rangle
$$

$$
\times | \pi(\phi_2 \cdots \phi_N) \rangle \langle \tilde{\pi}'(\phi_N \cdots \phi_2) |.
$$
 (A6)

We analyze only the bosonic case, and the fermions follow by setting $N_o = N$ and $n_{\phi_i} = 1$.

Consider the first line of Eq. $(A6)$. As states ϕ_i are not necessarily orthogonal and may be the same, we have contributions when the permutations π' , $\tilde{\pi}$ are equal and in some cases even when they are different. It can be seen that there are $n_k[(N-1)!]$ permutations such that $\pi'(\phi_1) = \phi_k$, and for each of these there are $\prod_{i=1}^{N_o} (n_{\phi_i}!)$ permutations $\tilde{\pi}$ such that $\tilde{\pi}(\phi_1) = \phi_k$, resulting in non-null contributions $\langle \pi'(\phi_N \cdots \phi_2) | \tilde{\pi}(\phi_2 \cdots \phi_N) \rangle \neq 0$. If $\tilde{\pi}(\phi_1) \neq \phi_k$ then the contribution is null $\langle \pi'(\phi_N \cdots \phi_2) | \tilde{\pi}(\phi_2 \cdots \phi_N) \rangle = 0$ [simply note that the set ${\lbrace \tilde{\pi}(\phi_2 \cdots \phi_N) \rbrace}$ always has n_k states ϕ_k , whereas ${\pi'(\phi_N \cdots \phi_2)}$ has only $n_k - 1$. The first line of Eq. (A6) thus reduces to

$$
\sum_{k=1}^{N_o} n_k [(N-1)!] \left[\prod_{i=1}^{N_o} (n_{\phi_i}!) \right] |\phi_k\rangle \langle \phi_k|. \tag{A7}
$$

Now we analyze the second line of Eq. (A6). This term has non-null contributions only if $\pi(\phi_1)$ = *π*^{$\tilde{\pi}$ ['](ϕ ₁). For permutations of the type π (ϕ ₁) = $\tilde{\pi}$ ['](ϕ ₁) =} ϕ_k , the matrix $|\pi(\phi_2 \cdots \phi_N)\rangle \langle \tilde{\pi}'(\phi_N \cdots \phi_2)|$ can assume

 $\frac{(N-1)!}{(n_{k}-1)!\prod_{i=1, (i\neq k)}^{N_0} (n_{\theta_i}!)} = \frac{n_{\phi_k}(N-1)!}{\prod_{i=1}^{N_0} (n_{\phi_i}!)}$ distinct combinations from the elements of the set ${\lbrace \pi(\phi_2 \cdots \phi_N) \rbrace}$. Note that there are

 $\prod_{i=1}^{N_o} (n_{\phi_i})$ permutations of type $\pi(\phi_1) = \phi_k$ generating the same "ket" $|\pi(\phi_2 \cdots \phi_N)\rangle$ [or "bra" $\langle \tilde{\pi}'(\phi_N \cdots \phi_2)\rangle$]. Thus we have

$$
\sum_{\pi,\tilde{\pi}'} \epsilon_{\pi} \epsilon_{\tilde{\pi}'} \langle \pi(\phi_1) | \tilde{\pi}'(\phi_1) \rangle | \pi(\phi_2 \cdots \phi_N) \rangle \langle \tilde{\pi}'(\phi_N \cdots \phi_2) |
$$
\n
$$
= \left[\prod_{i=1}^{N_o} (n_{\phi_i}!) \right]^2 | \psi_k \rangle \langle \psi_k |,
$$
\n(A8)

where $|\psi_k\rangle = \sum_i |\pi_k^i(\phi_2 \cdots \phi_N)\rangle$, with $\pi_k^i(\phi_2 \cdots \phi_N)$ being all the possible permutations such that $\pi_k^i(\phi_1) = \phi_k$, and $\langle \pi_k^i(\phi_2 \cdots \phi_N)|\pi_k^j$ $\langle \pi_k^i(\phi_2 \cdots \phi_N)|\pi_k^j(\phi_2 \cdots \phi_N)\rangle = \delta_{ij}$. We have then $\langle \psi_k|\psi_{k'}\rangle = n_{\phi_k}(N-1)!$ s. ... and finally the second line of Eq. (46) is $\prod_{i=1}^{n_{\theta_k}(N-1)!} \delta_{kk'}$, and finally the second line of Eq. (A6) is reduced to

$$
\sum_{k=1}^{N_o} \left[\prod_{i=1}^{N_o} (n_{\phi_i}!) \right]^2 |\psi_k\rangle \langle \psi_k|
$$
\n
$$
= \left[\prod_{i=1}^{N_o} (n_{\phi_i}!) \right] (N-1)! \sum_{k=1}^{N_o} n_{\phi_k} \frac{|\psi_k\rangle \langle \psi_k|}{\langle \psi_k | \psi_k \rangle}. \quad (A9)
$$

From Eqs. (A7) and (A9) and remembering to reintroduce the normalization constant *C*, we obtain

$$
\left\| |\psi\rangle\langle\psi|^{T_A} \right\|_1 = \frac{\left(\sum_{k=1}^{N_o} \sqrt{n_{\phi_k}} \right)^2}{N} \le N. \tag{A10}
$$

The last step follows by noting that $\sum_{k=1}^{N_o} n_k = N$, and thus $\sum_{k=1}^{N_o} \sqrt{n_k} \le N$. Because the trace norm is a convex function, we can write for uncorrelated mixed states $\|\sum_j p_j \sigma_j^{T_i}\|_1 \leq$ $\sum_j p_j$ $\|\sigma_j^{T_i}\|_1$, and we are done.

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as follows: $f_k^{\dagger} \mapsto \sum_j v_{kj} f_j^{\dagger}$, where v_{kj} is a unitary matrix. The basis $\{a_i^{\dagger}\}\$ is given, after such transformation, by $a_k^{\dagger} \mapsto \sum_{j,l} u_{kj}(v_{jl} f_l^{\dagger})$. We can always choose Φ such that $v = u^{\dagger}$, and thereby we have $\{a_i^{\dagger}\}\mapsto \{f_i^{\dagger}\}.$

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