One-body entanglement as a quantum resource in fermionic systems

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We show that one-body entanglement, which quantifies the mixedness of the eigenvalues of the single particle density matrix (SPDM) of a fermionic system, can be considered as a quantum resource. We define the free states and operations for this resource through majorization, and show that pure state conversion via these operations will in general imply a decrease in one-body entanglement. It is then demonstrated that fermion linear optics operations, which include one-body unitary transformations and measurements of the occupancy of single particle modes, are free operations implying a majorization relation between the initial and postmeasurement SPDMs. Finally, it is shown that the ensuing resource is consistent with a model of fermionic quantum computation. A general bipartite-like formulation of one-body entanglement is also discussed.

Quantum entanglement and identical particles are two fundamental concepts in quantum mechanics. Entanglement in systems of distinguishable components is particularly valuable in the field of quantum information theory [1] because it can be considered as a resource within the Local Operations and Classical Communication (LOCC) paradigm [1,2]. Extending the notion of entanglement to the realm of indistinguishable particles is, however, not straightforward because the constituents of the system cannot be individually accessed. Different approaches have been considered, like mode entanglement [3,5], where subsystems correspond to a set of single particle (SP) states in a given basis, extensions based on correlations between observables [6–10] and entanglement beyond symmetrization [11–21], which is independent of the choice of SP basis. Several studies on the relation between these types of entanglement [5,16,20,22–27] and on whether exchange correlations can be associated with entanglement [28,32] have been recently made. In this letter we will focus on entanglement beyond antisymmetrization in fermionic systems and analyze its consideration as a quantum resource.

Quantum resource theories (QRT) [33,34] have recently become a topic of great interest since they essentially describe quantum information processing under a restricted set of operations. Standard entanglement theory in systems of distinguishable components is just one of these theories, amongst which we may include others like quantum reference frames and asymmetry [35], quantum thermodynamics [36,37], coherence [38,39], non-locality [40] and non-Gaussianity [41].

In the usual entanglement theory a multipartite quantum system shared by distant parties is considered. These parties can operate each on their own subsystem and are allowed to communicate via classical channels [2]. From these physical restrictions the LOCC set arises naturally as the set of free operations of the resource theory, and the set of free (separable) states is then derived so that free operations map this set onto itself. In our case the situation is reversed: Ignoring antisymmetrization correlations defines Slater Determinants (SDs) and their convex hull as the separable, i.e. “free” set of states, and we are looking for a set of free operations consistent with these free states, i.e., operations satisfying the so-called golden rule of QRT’s [33]. In order to accomplish this goal we first define a partial order relation on the Fock space $\mathcal{F}$ of the system which determines whether a given pure fermionic state can be considered more or less entangled than another state. We propose here to base it on the mixedness of their corresponding single particle density matrix (SPDM) $\rho^{(1)}$ (also denoted as one-particle or one-body DM), compared via majorization. The free operations that we look for, which we will denote as one-body free operations $\mathcal{O}$, are those that do not increase this mixedness. We will show that these operations include basic measurements such as those determining the occupation of a SP level. A bipartite-like formulation for this entanglement will be also considered.

We consider a SP space $\mathcal{H}$ of dimension $n$ and a set of fermionic creation and annihilation operators $c_i^\dagger, c_i$, $i = 1, \ldots, n$ associated with an orthogonal basis $\{|i\rangle = c_i^\dagger |0\rangle\}$ of $\mathcal{H}$, satisfying the anticommutation relations $\{c_i, c_j^\dagger\} = \delta_{ij}$, $\{c_i, c_j\} = 0 = \{c_i^\dagger, c_j^\dagger\}$. The elements of the SPDM in a general fermionic state $\rho$ are

$$\rho^{(1)}_{i\nu} = (c_i^\dagger c_i) = Tr c_i^\dagger c_i.$$

As is well known, $\rho^{(1)}$ is an hermitian matrix with eigenvalues $\lambda_{\nu} = (c_i^\dagger c_i) \in [0,1]$, where $c_i = \sum_i U_{i\nu} c_i^\dagger$, with $U$ the unitary matrix satisfying $\{c_i, c_{\nu}\} = (U^\dagger \rho^{(1)} U)_{i\nu} = \lambda_{\nu} \delta_{i\nu}$, are the fermion operators associated to the “natural” orbitals $|\nu\rangle = c_\nu^\dagger |0\rangle$ diagonalizing $\rho^{(1)}$. Hence, for pure states $\rho = |\Psi\rangle \langle \Psi|$ the “mixedness” of $\rho^{(1)}$ reflects the deviation of $|\Psi\rangle$ from a SD, with $(\rho^{(1)})^2 = \rho^{(1)}$ iff $|\Psi\rangle$ is a SD, i.e. iff $\lambda_{\nu} = 0$ or 1 $\forall \nu$.

Such mixedness can be characterized through majorization [12,35]. Given two fermionic states $|\Psi\rangle$, $|\Phi\rangle$ with the same fermion number $N$ ($Tr \rho^{(1)}_{\Phi} = Tr \rho^{(1)}_{\Psi} = N$) we will say that $|\Phi\rangle$ is not more one-body entangled than $|\Psi\rangle$ if the eigenvalues of $\rho^{(1)}_{\Phi}$ majorize those of $\rho^{(1)}_{\Psi}$:

$$\lambda(\rho^{(1)}_{\Psi}) \prec \lambda(\rho^{(1)}_{\Phi}),$$
which means \(\sum_{i=1}^{m} \lambda_i(\rho_\Psi^{(1)}) \leq \sum_{i=1}^{m} \lambda_i(\rho_\Psi^{(1)})\) for \(m = 1, \ldots, n - 1\), with identity for \(m = n\) and the eigenvalues sorted in decreasing order. Thus, SDs are the least one-body entangled states. This definition is analogous to that imposed by LOCC operations in the standard entanglement theory for distinguishable subsystems, where a pure state \(|\Psi_{AB}\rangle\) of a bipartite system can be converted through LOCC operations to another pure state \(|\Phi_{AB}\rangle\) iff \(\lambda(\rho_{\Phi}) < \lambda(\rho_{\Psi})\) \([13, 46]\). Here \(\rho_{\Phi}, \rho_{\Psi}\) are the reduced densities of either \(A\) or \(B\) (which have the same nonzero eigenvalues) determined by \(|\Psi_{AB}\rangle\) and \(|\Phi_{AB}\rangle\). Hence \(|\Phi_{AB}\rangle\) is not more entangled than \(|\Psi_{AB}\rangle\) if \(\lambda(\rho_{\Phi}) < \lambda(\rho_{\Psi})\). Local measurements reduce our ignorance about the state of the measured subsystem \([43]\), thus reducing the mixedness of the reduced densities and hence the bipartite entanglement. A similar result can be expected for one-body entanglement: operations that reduce our ignorance about the SPDVM should not increase one-body entanglement.

Before proving this statement, we notice that one-body entanglement also admits a bipartite-like formulation. A pure state \(|\Psi\rangle\) of \(N\) fermions can be written as

\[
|\Psi\rangle = \frac{1}{N} \sum_{i,j} \lambda_{ij} \hat{c}_{ij}^\dagger \hat{C}_{ij}^\dagger |0\rangle = \frac{1}{N} \sum_{\nu} \sqrt{\lambda_{\nu}} \hat{c}_{\nu}^\dagger \hat{C}_{\nu}^\dagger |0\rangle,
\]

where \(\hat{C}^\dagger = \hat{c}_{1}^\dagger \ldots \hat{c}_{N}^\dagger\), \(j = 1, \ldots, (N-1)\), are operators creating \(N-1\) fermions in specific states labelled by \(j\), satisfying \(|0\rangle \hat{C}_{ij}^\dagger |0\rangle = \delta_{ij} \delta_{j,1}\), and \(\Lambda\) is a \(n \times (N-1)\) matrix. Thus \(\rho^{(1)}(\Psi) = \sum_{\nu} \lambda_{\nu} \hat{c}_{\nu}^\dagger \hat{c}_{\nu} |0\rangle \) is the state of remaining \(N-1\) fermions when SP site \(i\) is occupied, whereas \(\hat{C}_{ij} |\Psi\rangle = (-1)^{N-1} \sum_{\nu} \lambda_{ij} \hat{c}_{\nu}^\dagger |0\rangle\) that of remaining fermion when the \(N-1\) SP states \(j\) are occupied. This implies

\[
\rho^{(1)}(\Psi) = (\Lambda^\dagger \Lambda)^{i,i'\nu}, \quad \rho^{(1)(N-1)}(\Psi) = (\Lambda^T \Lambda^*)^{j,j'\nu},
\]

where \(\rho^{(N-1)}\) is the \((N-1)\)-body DM. Hence, these two DM’s have the same nonzero eigenvalues \(\lambda_{\nu}\), which are the square of the singular values of the matrix \(\Lambda\), as in the distinguishable case \([11]\). They determine the averages of all one- and \((N-1)\)-body operators \(O^{(1)} = \sum_{i,i'} \langle i' | O^{(1)} | i \rangle \hat{c}_{i'}^\dagger \hat{c}_{ij}^\dagger \hat{O}^{(N-1)} = \sum_{j,j'} O^{(j,j')} \langle j, j' \rangle \hat{C}_{j'}^\dagger \hat{C}_{ij}^\dagger\) through

\[
\langle O^{(1)} \rangle = \text{Tr} \rho^{(1)}(\Psi), \quad \langle O^{(N-1)} \rangle = \text{Tr} \rho^{(N-1)}(\Psi).
\]

The final Schmidt-like representation in \([3]\) follows from the singular value decomposition \(\Lambda = UDV^\dagger\), with \(D_{\nu\nu'} = \sqrt{\lambda_{\nu}} \delta_{\nu\nu'}\), \(U, V\) unitary matrices and \(c_{\nu} = \sum_i U_{\nu i} \hat{c}_{i}^\dagger\), \(C_{\nu} = \sum_j V_{\nu j} \hat{C}_{j}^\dagger\), such that

\[
\langle c_{\nu}^\dagger c_{\nu'} \rangle = \lambda_{\nu} \delta_{\nu\nu'} = \langle C_{\nu}^\dagger C_{\nu'} \rangle,
\]

with \(|0\rangle \langle 0| \hat{c}_{\nu}^\dagger \hat{c}_{\nu'} |0\rangle = \delta_{\nu\nu'} |0\rangle \langle 0| \hat{C}_{\nu}^\dagger \hat{C}_{\nu'} |0\rangle\). Thus, \(C_{\nu} |\Psi\rangle = \sqrt{\lambda_{\nu}} C_{\nu}^\dagger |0\rangle\) and \(C_{\nu} |\Psi\rangle = (-1)^{N-1} \sqrt{\lambda_{\nu}} C_{\nu}^\dagger |0\rangle\), i.e. the orthogonal natural \(N-1\)-fermion states \(C_{\nu}^\dagger |0\rangle\) are those of remaining fermions when the natural SP orbital \(\nu\) is occupied, and vice versa. Notice, however, that \(c_{\nu}^\dagger\) will also appear in other \(C_{\nu}^\dagger\) with \(\nu' \neq \nu\), so that in general one-body entanglement describes that between one- and \((N-1)\)-body observables (rather than distinct modes).

If \(|\Psi\rangle\) is a SD, \(\lambda_{\nu} = 1\) for \(\nu \leq N\) and 0 otherwise, and the last expression in \([3]\) reduces to a single term \((C_{\nu}^\dagger \propto \prod_{\nu' \neq \nu} C_{\nu'}^\dagger \), with \(c_{\nu}^\dagger C_{\nu}^\dagger = c_{\nu'}^\dagger C_{\nu'}^\dagger\) for \(\nu, \nu' \leq N\). Otherwise \(|\Psi\rangle\) is one-body entangled.

We also remark that Eq. \(2\) implies

\[
E(|\Psi\rangle) \geq E(|\Psi\rangle)
\]

for any quantity of the form

\[
E(|\Psi\rangle) = S(\rho^{(1)}) = S(\rho^{(N-1)})
\]

where \(S\) is a Schur-concave \([44, 45]\) function of the argument such as any trace form entropy \([47]\) \(S_f(\rho^{(1)}) = \text{Tr} f(\rho^{(1)}) = \sum_{\nu} f(\lambda_{\nu})\) with \(f\) concave (and satisfying \(f(0) = f(1) = 0\) in order that it vanishes for a SD). Eq. \(9\) then plays the role of a one-body entanglement monotone. In particular, the von Neumann entropy of \(S(\rho^{(1)}) = -\sum_{\nu} \lambda_{\nu} \log_2 \lambda_{\nu}\), a quantity of interest in many-fermion systems and quantum chemistry \([48, 52]\) provides one of such monotones. Another example is the one-body entropy \([20, 25]\),

\[
S_1(\rho^{(1)}) = -\sum_{\nu} \lambda_{\nu} \log_2 \lambda_{\nu} + (1 - \lambda_{\nu}) \log_2 (1 - \lambda_{\nu})
\]

which represents the minimum relative entropy (in the grand canonical ensemble) between \(\rho = |\Psi\rangle \langle \Psi|\) and any fermionic gaussian state \(\rho_g\) \([25]\): \(\text{Min}_{\rho_g} S(\rho |\rho_g) = S_1(\rho^{(1)})\), where \(S(\rho |\rho') = -\text{Tr} \rho \log_2 \rho' - \log_2 \rho'\). It is also the minimum over all SP bases of the sum of all single mode entropies \(-\sum_{j} p_j \log_2 p_j + (1 - p_j) \log_2 (1 - p_j)\), where \(p_j = \langle c_{j}^\dagger c_{j} \rangle\) \([20]\). We finally mention that the SPDVM, and hence Eq. \(2\), can be experimentally accessed. Measurement of the fermionic SPDVM in optical lattices has been recently reported \([53]\). We now formulate the main results of this letter.

**Definition 1.** Let \(\varepsilon : \mathcal{F} \rightarrow \mathcal{F}\) be a quantum operation mapping the state \(\rho\) of a fermion system to

\[
\varepsilon(\rho) = \sum_j \mathcal{K}_j \rho \mathcal{K}_j^\dagger
\]

where \(\{\mathcal{K}_j, \sum_j \mathcal{K}_j^\dagger \mathcal{K}_j = 1\}\) are the Kraus operators associated to \(\varepsilon\) (assumed number conserving). Let \(\rho^{(1)}\) and \(\rho^{(1)}_j\) be the SPDVMs associated to \(\rho\) and \(p_j = \frac{\mathcal{K}_j \rho \mathcal{K}_j^\dagger}{\rho}\), with \(p_j = \text{Tr} \rho \mathcal{K}_j^\dagger \mathcal{K}_j\). We say that \(\varepsilon\) is a one-body free operation if the following relation is satisfied for all \(\rho\):

\[
\lambda(\rho^{(1)}) \leq \sum j p_j \lambda(\rho^{(1)}_j)
\]
Proposition 1. If $\varepsilon_1$ and $\varepsilon_2$ are one-body free operations, $\varepsilon_2 \circ \varepsilon_1$ is also a one-body free operation.

This is a minimal requirement that $\mathcal{O}$ should satisfy in order to ensure they can be applied any number of times in any order. It directly follows from Eqs. (11)-(12) ($\lambda(\rho^{(1)}) < \sum_{ij} p_{ij} \lambda(\rho_{ji}^{(1)})$ for $\mathcal{K}_j = \mathcal{K}_j^2 \mathcal{K}_i^1$). This property implies the following important result.

Proposition 2. The conversion of a pure state $|\Psi\rangle \in \mathcal{F}$ into another pure state $|\Phi\rangle \in \mathcal{F}$ by means of one-body free operations is possible only if Eq. (2) is satisfied.

Proof. The state conversion will consist in some sequence of one-body free operations, which can be resumed in just one of such operations due the closedness of $\mathcal{O}$ under composition. Let $\{\mathcal{K}_j\}$ be the associated Kraus operators. After this operation is performed, we should have $\mathcal{K}_j |\Psi\rangle = \sqrt{p_j} |\Phi\rangle \forall j$, with $p_j = \langle \Psi | \mathcal{K}_j^1 \mathcal{K}_i^1 |\Psi\rangle$, implying $\rho^{(1)}_j = \rho^{(1)}_{\Phi} \forall j$ and hence Eq. (2) when (12) is fulfilled. □

Eq. (12) also implies that any concave entropy $S(\rho^{(1)})$ (as $S_f(\rho^{(1)}) = Tr f(\rho^{(1)})$) will not increase on average after a one-body free operation: $S(\rho^{(1)}) \geq S(\sum p_j \rho_j^{(1)}) \geq \sum p_j S(\rho_j^{(1)})$. If $\rho = |\Psi\rangle \langle \Psi|$, then $\rho_j = |\Phi_j\rangle \langle \Phi_j|$ is pure $\forall j$, with $|\Phi_j\rangle \propto \mathcal{K}_j |\Psi\rangle$, and hence

$$E(|\Psi\rangle) \geq \sum p_j E(|\Phi_j\rangle),$$

indicating that one-body entanglement will not increase on average after such operation. In particular, if $|\Psi\rangle$ is a SD ($E(|\Psi\rangle) = 0$), all states $|\Phi_j\rangle$ must be SD’s ($E(|\Phi_j\rangle) = 0$) or zero ($p_j = 0$).

A first basic example of a one-body free operation is any measurement based on projectors onto SD’s $|\Phi_j\rangle$ ($\mathcal{K}_j \propto |\Phi_j\rangle \langle \Phi_j|$), where Eqs. (12)-(13) become trivial ($E(|\Phi_j\rangle) = 0 \forall j$). It is also obvious the inclusion in $\mathcal{O}$ of one-body unitary transformations $U' cU = \sum \alpha_c U'_c \alpha_c U$, where $U = \exp[-i \sum_{ij} H_{ij} \alpha_c^1 c_j^1 \alpha_c] \alpha_c$ with $H$ hermitian and $U = \exp[-i H]$. Such operators map the state $\rho$ of the system as $\rho \rightarrow U \rho^{(1)} U^\dagger$ and hence the SPDM as

$$\rho^{(1)} \rightarrow U \rho^{(1)} U^\dagger.$$ (14)

then leaving the eigenvalues of $\rho^{(1)}$ unchanged. They can always be implemented through composition of phase-shifting and beamsplitters unitaries $[53, 54]$, $U_{\phi}(\phi) = \exp[-i \phi c_i^1 c_i^1]$, $U_{\theta}(\theta) = \exp[-i \theta (c_i^1 c_j^1 + c_j^1 c_i^1)]$, which are the basic unitary elements of fermionic linear optics (FLO) operations $[53, 54]$.

FLO operations also include measurements of the occupancy of single-particle modes, described by projectors

$$\mathcal{P}_k = c_k^\dagger c_k, \quad \mathcal{P}^\perp_k = c_k c_k^\dagger,$$ (15)

satisfying $\mathcal{P}_k + \mathcal{P}^\perp_k = 1$. We will now show explicitly that they are one-body free operations.

![FIG. 1. Measurement of the occupancy of a single fermion mode $k$. It reduces (or does not increase) on average the mixedness of the SP density matrix $\rho^{(1)}$ ($\lambda$ denotes its spectrum) and hence the one-body entanglement.](image)

Theorem 1. The measurement of the occupancy of a single particle state $|k\rangle = c_k^\dagger |0\rangle \in \mathcal{H}$, described by the operators $[15] \lambda(\rho^{(1)} + \rho^{(1)}_k)$ constitutes a one-body free measurement.

Proof. Consider a general pure state $|\Psi\rangle$ of a fermionic system with SPDM $\rho^{(1)}$. Let $\rho_k^{(1)}$ and $\rho_k^{(1)}$ be the SPDM’s after sp mode $|k\rangle = c_k^\dagger |0\rangle$ is found to be occupied or empty, respectively, determined by the states $|\Psi_{k\perp}\rangle = \mathcal{P}^\perp_k |\Psi\rangle / \sqrt{\mathcal{P}_k |\Psi\rangle}$, with $p_k = \langle \Psi | \mathcal{P}_k |\Psi\rangle$ and $p_k = \langle \Psi | \mathcal{P}_k |\Psi\rangle = 1 - p_k$, such that

$$|\Psi\rangle = \sqrt{p_k} |\Psi_k\rangle + \sqrt{p_k^\perp} |\Psi_k^\perp\rangle.$$ (16)

We will prove relation (12).

$$\lambda(\rho^{(1)} + \rho_k^{(1)} + \rho_k^{(1)}) = p_k \lambda(\rho_k^{(1)} + \rho_k^{(1)}).$$ (17)

If the measured state $|k\rangle$ is a natural orbital such that $\langle c_i^\dagger c_j^\dagger |k\rangle = p_k \delta_{ik}$ with $p_k$ an eigenvalue of $\rho^{(1)}$, Eq. (17) is straightforward: In this case Eq. (16) leads to

$$\rho^{(1)} = p_k \rho_k^{(1)} + p_k \rho_k^{(1)},$$ (18)

since $\langle \Psi | c_i^\dagger c_j^\dagger |k\rangle = \delta_{ik} (1 - \delta_{ik}) (c_i^\dagger c_i^\dagger) = 0 \forall i, j$. Eq. (18) directly implies (17) since $\lambda(A + B) < \lambda(A) + \lambda(B)$ for any two hermitian $n \times n$ matrices $A, B [43, 57]$.

In the general case Eq. (18) no longer holds. Nevertheless, since $\langle \Psi | c_i^\dagger c_j^\dagger |k\rangle = 0$ for any two SP states $|i\rangle, |j\rangle$ orthogonal to $|k\rangle$, Eq. (16) implies, for any SP subspace $\mathcal{S}_\perp \subset \mathcal{H}$ orthogonal to the measured state $|k\rangle$,

$$\rho_{\mathcal{S}_\perp}^{(1)} = p_k \mathcal{P}_{\mathcal{S}_\perp} + p_k \mathcal{P}_k^{(1)} \mathcal{P}_{\mathcal{S}_\perp},$$ (19)

where $\rho_{\mathcal{S}_\perp}^{(1)} = \mathcal{P}_{\mathcal{S}_\perp} \rho^{(1)} \mathcal{P}_{\mathcal{S}_\perp}$ and $\mathcal{P}_k^{(1)} \mathcal{P}_{\mathcal{S}_\perp}$ are the restrictions of $\rho^{(1)}$ and $\rho_k^{(1)}$ to $\mathcal{S}_\perp$, and $\mathcal{P}_{\mathcal{S}_\perp}$ is the associated projector. This result is expected since the measurement is
orthogonal to $S$. And for any $S \subset \mathcal{H}$ containing the state $|k\rangle$, we have, as $\langle \Psi_c | c_k | \Psi_k \rangle = 0$,

$$\text{Tr} \rho_S^{(1)} = \text{Tr} \left[ p_k \rho_S^{(1)} + p_k' \rho_S^{(1)} \right] .$$

(20)

We can now prove the $m^{th}$ inequality in (17),

$$\sum_{\nu=1}^{m} \lambda_{\nu}(\rho_S^{(1)}) \leq \sum_{\nu=1}^{m} p_k \lambda_{\nu}(\rho_S^{(1)}) + p_k' \lambda_{\nu}(\rho_S^{(1)}) .$$

(21)

Let $S_m \subset \mathcal{H}$ be the subspace spanned by the first $m$ eigenstates of $\rho_S^{(1)}$, such that $\lambda_{\nu}(\rho_S^{(1)}) = \lambda_{\nu}(\rho_S^{(1)})$ for $\nu < m$. If $S_m$ is either orthogonal to $|k\rangle$ or fully contains $|k\rangle$ ($|k\rangle$ is a superposition of the first $m$ eigenstates), Eq. (21) is immediate since Eq. (19) or (20) holds for $S = S_m$, implying $\sum_{\nu=1}^{m} \lambda_{\nu}(\rho_S^{(1)}) = \text{Tr} \left[ p_k \rho_{kS_m}^{(1)} + p_k' \rho_{kS_m}^{(1)} \right]$, which leads to (21) as $\text{Tr} \rho_{k(kS_m)}^{(1)} \leq \sum_{\nu=1}^{m} \lambda_{\nu}(\rho_{kS_m}^{(1)})$.

Otherwise we add to $S_m$ the component $|k\rangle$ of $|k\rangle$ orthogonal to $S_m$, obtaining an $m + 1$ dimensional SP subspace $S'_m$, where $\text{Tr} (20)$ holds and still $\lambda_{\nu}(\rho_{S'_m}^{(1)}) = \lambda_{\nu}(\rho_S^{(1)})$ for $\nu < m$. We will prove that the remaining smallest eigenvalue satisfies

$$\lambda_{m+1}(\rho_{S'_m}^{(1)}) \geq p_k \lambda_{m+1}(\rho_{S_m}^{(1)}) + p_k' \lambda_{m+1}(\rho_{S_m}^{(1)}) ,$$

(22)

implying $\sum_{\nu=1}^{m+1} \lambda_{\nu}(\rho_S^{(1)}) \leq \sum_{\nu=1}^{m} p_k \lambda_{\nu}(\rho_{S_m}^{(1)}) + p_k' \lambda_{\nu}(\rho_{S_m}^{(1)})$ due to Eq. (20), and hence Eq. (21) [59]. To prove (22), we write the lowest eigenstate $|k\rangle$ of $\rho_S^{(1)}$ as $|k\rangle + \beta |k'\rangle$, with $|k'\rangle \in S'_m$ orthogonal to $|k\rangle$, such that $\lambda_{m+1}(\rho_{S'_m}^{(1)})$ is the smallest eigenvalue $\lambda_{-}$ of the matrix

$$\rho_{kk'}^{(1)} = \left( \begin{array}{ccc} \langle c_k' | c_k \rangle & \langle c_k' | c_k \rangle & \langle c_k' | c_k \rangle \\ \langle c_k' | c_k \rangle & \langle c_k' | c_k \rangle & \langle c_k' | c_k \rangle \\ \langle c_k' | c_k \rangle & \langle c_k' | c_k \rangle & \langle c_k' | c_k \rangle \end{array} \right) ,$$

(23)

whose eigenvalues are

$$\lambda_\pm = \frac{p_k + p_k'}{2} \pm \sqrt{\frac{(p_k - p_k')^2}{4} + |\langle c_k' | c_k \rangle|^2} .$$

(24)

Since $|\Psi\rangle = \sum_{\mu,\mu'} P_{\mu P_{\mu'}} |\Psi_{\mu}\rangle$, with $\mu = k, k', \mu' = k', k'$ and $P_{\mu P_{\mu'}} = \langle \mu P_{\mu'} | \mu P_{\mu'} \rangle$, we have

$$p_k = p_{kk'} + p_{kk'}, p_{kk'} = p_{kk} + p_{kk'}, \text{ and } \langle c_k' c_k \rangle = r \sqrt{p_{kk}p_{kk'}}$$

with $|r| = |\langle \Psi_{kk'} | \Psi_{kk'} \rangle| \leq 1$. Thus, using (24),

$$\lambda_- \geq p_{kk'} \geq p_k \lambda_{m+1}(\rho_{S_m}^{(1)}) + p_k' \lambda_{m+1}(\rho_{S_m}^{(1)}) ,$$

(25)

since $p_k \lambda_{m+1}(\rho_{S_m}^{(1)}) \leq p_{kk'}$ and $\lambda_{m+1}(\rho_{S_m}^{(1)}) = 0$. This proves the theorem for general pure states $|\Psi\rangle$ [30].

Previous proof actually shows the more general relation

$$\lambda(\rho_S^{(1)}) \sim p_k \lambda(\rho_{kS}^{(1)}) + p_k' \lambda(\rho_{k'S}^{(1)}) ,$$

(26)

valid for the restriction of $\rho^{(1)}$ to any subspace $S \subset \mathcal{H}$ either containing or orthogonal to the measured state $|k\rangle$ ($\langle P_S | k \rangle = 0$), as the argument of [59] remains valid.

Moreover $\rho_S^{(1)}$ will be determined by a mixed reduced state $\rho_S = \text{Tr}_{k\bar{k}} |\Psi\rangle \langle \Psi|$ satisfying $\langle \Psi | O_S | \Psi \rangle = \text{Tr} \rho_S O_S$ for any operator $O_S$ involving just creation and annihilation of SP states $|i\rangle \in S$ (commuting with the number parity $e^{i\pi N}$) [61]. Hence, Eq. (26) shows that (17) also holds for general mixed fermionic states $\rho$, since they can always be purified and seen as a reduced state $\rho_S$ of a pure fermionic state $|\Psi\rangle$ in an enlarged SP space [61].

It is actually also possible to extend previous proof to more general single-mode measurements:

**Corollary 1.** A general measurement on single-particle mode $k$ described by the operators

$$M_k = \alpha P_k + \beta P_k' , \quad M_{k'} = \gamma P_k + \delta P_k'$$

(27)

with $|\alpha|^2 + |\gamma|^2 = 1, |\beta|^2 + |\delta|^2 = 1$, is also a one-body free measurement. The proof is given in the Appendix.

We also notice that if $|\Psi\rangle$ is a SD, (17) entails that the states $|\Psi_k\rangle, \langle \Psi_k|$$ in (16) are both SD’s, as can be easily verified: Writing $c_k = \alpha c_k + \beta c_k$, with $\alpha |k\rangle$ the projection of $|k\rangle$ onto the SP subspace occupied in $|\Psi\rangle$ and $|k\rangle$ the orthogonal complement [62], we have

$$P_k |\Psi\rangle = \alpha^* c_k^\dagger c_k |\Psi\rangle, \quad P_{k'} |\Psi\rangle = \beta c_k^\dagger c_k |\Psi\rangle,$$

(28)

with $c_{k'}^d = \beta^* c_{k'} - \alpha^* c_k$, which are orthogonal SD’s. In the case (27), $\langle \Psi | M_{k(k')} |\Psi\rangle$ are then nonorthogonal SD’s.

It has been noted [63] that these features explain why the FLO computation model based on one-body unitaries and SD’s can be efficiently simulated in a classical computer, as the overlap $\langle \Psi | \Psi \rangle$ between any two SD’s can be evaluated through a determinant [54] that can be computed in polynomial time. Thus, matrix elements of free unitaries and probabilities of outcomes of free measurements (which are just overlaps between SD’s) can be efficiently simulated classically.

In Ref. [64] the simultaneous measurement of the occupancy of two single-particle modes $k, k'$, described by operators $\{ M_0 = P_k P_{k'}, M_1 = P_k P_{k'} + P_{k'} P_k, M_2 = P_{k'} P_{k'} \}$ associated to the possible results 0, 1 and 2 was also considered, showing that $M_1$ can map a SD into a state with Slater number 2, i.e., a one-body entangled state [65]. A measurement with $N$ such outcomes may return a state with an exponentially large $(2^N)$ Slater number, whose expectation values would be hard to evaluate classically. In [65] this operation is identified with a charge detection measurement in a system of free electrons, showing that it is possible to build a CNOT gate with just beamsplitters, spin rotations and charge detectors. The extended set of FLO + charge detection operations then enables quantum computation. These results, together with those derived here suggest that one-body entanglement might be the resource behind this model.

In summary, after providing a basis-independent bipartite-like formulation of one-body entanglement in
fermion systems, we have discussed its consideration as a quantum resource through majorization based relations. We have shown through a general proof suitable also for mixed states that FLO operations, including in particular direct (Eq. (15)) or generalized (Eq. (27)) measurements of the occupancy of a SP mode, are one-body free operations which cannot increase one-body entanglement. Present results can then provide the basis for a consistent resource theory associated to quantum correlations beyond antisymmetrization in fermionic systems.

**Appendix: Proof of Corollary 1.**

The post-measurement states determined by the operators (27), which satisfy $M_k^\dagger M_k + M_k^\dagger M_k = 1$, are

$$
\Phi_k = \frac{\alpha \sqrt{p_k} |\Psi_k\rangle + \beta \sqrt{p_k} |\Psi_k\rangle}{\sqrt{q_k},}
$$

$$
\Phi_k = \frac{\beta \sqrt{p_k} |\Psi_k\rangle + \alpha \sqrt{p_k} |\Psi_k\rangle}{\sqrt{q_k},}
$$

where $q_k = p_k |\alpha|^2 + p_k |\beta|^2$, $q_k = p_k |\alpha|^2 + p_k |\beta|^2$. We have to prove $\lambda(\rho^{(1)}) \leq q_k \lambda(\rho^{(1)}) + q_k \lambda(\rho^{(1)})$, where $\rho^{(1)}_k$ are now the SPDM’s determined by (29)–(30). Eq. (20), i.e.

$$
\rho^{(1)}_k = \frac{\lambda(\rho^{(1)}_k)}{\sqrt{q_k}} |\Psi_k\rangle \langle \Psi_k|,
$$

where $\rho^{(1)}_k = 0$ for $i = k$ or $i$ orthogonal to $k$. Proceeding similarly to Eq. (23), we see that $q_k \lambda_{m+1}(\rho^{(1)}_{k_S^m})$ is less or equal to the smallest eigenvalue $\lambda_{k_S^m}$ of

$$
\begin{pmatrix}
|\alpha|^2 |p_k |\sqrt{p_k} |\rho_{kk}'| r^* & |\alpha| |\beta| |\sqrt{p_k} \rho_{kk}^r| r^* \\
|\alpha| |\beta| |\sqrt{p_k} \rho_{kk}^r| r^* & |\beta|^2 |p_k |\rho_{kk}'| r^*
\end{pmatrix},
$$

while $q_k \lambda_{m+1}(\rho^{(1)}_{k_S^m})$ is less or equal to the smallest eigenvalue $\lambda_{k_S^m}$ of a similar matrix with $\alpha \rightarrow \gamma$, $\beta \rightarrow \delta$. It is then straightforward to prove from Eq. (24) that $\lambda_{m+1}(\rho^{(1)}_{k_S^m}) = \lambda_\gamma \geq \lambda_{k_{S^m}}$ (with equality for $|r| = 1$ or $|\alpha| = |\beta|$) from which Eq. (22) directly follows.

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[57] This includes the trivial case $p_k = 1$ or 0, where $|\Psi\rangle = |\Psi_k\rangle$ or $|\Psi_k\rangle$. In the following we consider $p_k \in (0, 1)$.
[58] If $[K_{ij}, O] = 0 \forall j \Rightarrow \text{Tr}[\rho O] \geq \text{Tr} \sum_j K_j p_j K_j O = \sum_j p_j \text{Tr}[\rho_j O]$.
[59] The largest $m$ eigenvalues $\lambda_\nu$ of an hermitian matrix $O$ satisfy $\sum_{\nu=1}^m \lambda_\nu \geq \text{Tr} P_m O = \sum_{\nu=1}^m \lambda_\nu$, for any rank $m$ orthogonal projector $P_m$, with $\lambda_\nu$ the sorted eigenvalues of $P_m O P_m$ (Kay Fan maximum principle [43]).
[60] As verification, by considering the largest eigenvalue $\lambda_+$ in (21) of a similar $2 \times 2$ block such that the first eigenstate of $\rho_{S_{i=1}}^{(1)}$ is spanned by $|k\rangle$ and $|k'\rangle$, we obtain $\lambda_1(\rho_{S_{i=1}}^{(1)}) = \lambda_+ \leq p_k + p_{k'} \leq p_k + p_k \lambda_1(\rho_{S_{i=1}}^{(1)})$, which is the first $(m = 1)$ inequality in (21).
[61] Writing $|\Psi\rangle = \sum_{\mu, \nu} \Gamma_{\mu\nu} A_\mu^c B_\nu^c |0\rangle$ with $A_\mu^c (B_\nu^c)$ containing creation operators just in $S (S_j)$ and satisfying $|0\rangle A_\mu^c B_\nu^c |0\rangle = \delta_{\mu, \nu'}$, $|0\rangle B_\nu^c B_\mu^c |0\rangle = \delta_{\nu, \mu'}$, then $\rho_{S} = \sum_{\mu, \nu} \Gamma_{\mu\nu} \Gamma_{\mu'\nu'} |\mu\rangle \langle \mu'| \langle \mu'| = A_\mu^c |0\rangle$. And given an arbitrary mixed state $\rho_{S}$, $|\Psi\rangle$ is a purification of $\rho_{S}$.
[62] If $|\Psi\rangle = (\prod_{i=1}^N c_{i}^c) |0\rangle$ with $c_i^c = \sum_{\alpha} U_{\alpha_i} c_i^\alpha$, then $\alpha c_{i}^c = \sum_{\alpha \leq \beta} \alpha c_{i}^\beta = \sum_{\alpha > \beta} \alpha c_{i}^\beta$, with $\alpha = \{c_{\mu}^\alpha, c_{\nu}^\alpha\}$ and $|\alpha|_1^2 = \sum_{\alpha \leq \beta} |\alpha|_1^2 = \sum_{\alpha \leq \beta} |\alpha|_1^2$. For $\alpha \neq 0$ the first $N c_{i}^c$’s can be chosen such that $c_{i}^c$ is one of them.
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[64] For example $(a_1^c a_1^c a_2^c a_2^c + a_1^c a_2^c a_2^c a_1^c) c_{2}^c |0\rangle = \frac{c_1^c - c_2^c}{\sqrt{2}} |0\rangle$ for $a_1^c(2) = \frac{c_1^c(2) + c_2^c(4)}{\sqrt{2}}$, which is a one-body entangled state of two fermions ($\lambda_\nu = 1/2$ for $\nu \leq 4$).
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