One-body information loss in fermion systems

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We propose an entropic measure of nonclassical correlations in general mixed states of fermion systems, based on the loss of information due to the unread measurement of the occupancy of single-particle states of a given basis. When minimized over all possible single-particle bases, the measure reduces to an entanglement entropy for pure states and vanishes only for states which are diagonal in a Slater determinant basis. The approach is also suitable for states having definite number parity yet not necessarily a fixed particle number, in which case the minimization can be extended to all bases related through a Bogoliubov transformation if quasiparticle mode measurements are also considered. General stationary conditions for determining the optimizing basis are derived. For a mixture of a general pure state with the maximally mixed state, a general analytic evaluation of the present measure and optimizing basis is provided, which shows that nonentangled mixed states may nonetheless exhibit a nonzero information loss.

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I. INTRODUCTION

Quantification of nonclassical correlations in quantum systems is one of the main topics in quantum information theory. Quantum entanglement is the most famous and best studied manifestation of such correlations, mainly because of its central role as a resource for quantum teleportation [1] and quantum computation [2–4]. Nevertheless, quantum entanglement is not the only type of nonclassical correlation. It is now well known that nonentangled mixed states can also exhibit nonclassical features, which may be relevant in mixed-state based algorithms such as that of Knill and Laflamme [5,6]. A great effort has therefore been devoted in recent years to understand and quantify the quantumness of correlations [7]. Various measures of these correlations beyond entanglement have then been proposed, which start with the quantum discord [8–11] and the one-way information deficit [12,13]. The latter has been extended to more general entropic forms [14], as a measure of the information loss due to a local measurement. Various other related measures have also been later introduced [7,15–21].

While these correlation measures have been intensively investigated in systems of distinguishable components, less attention has been given to their extension to systems of identical particles [22], and in particular to fermion systems. In these systems particles cannot be accessed individually because of indistinguishability, thus preventing the straightforward extension of the correlation measures defined for systems of distinguishable components, which are based on the tensor product structure of the state space. This property no longer holds for indistinguishable components, turning the characterization of correlations more complex. Various approaches for describing and quantifying entanglement in fermion systems have been introduced, based on quantum correlations and particlelike entanglement [23–31] and also on mode-type entanglement [32–35].

In a previous work [31] we analyzed the problem of quantifying entanglement in pure and mixed states of fermion systems having definite number parity, yet not necessarily a fixed particle number. The approach is based on a consistent definition of the measurement of the occupancy of a single-particle (sp) mode, and of the reduced state of such a mode and its orthogonal complement in the sp Hilbert space S. It leads to an entanglement entropy which is explicitly invariant under particle-hole (and also Bogoliubov) transformations, and which extends previous treatments for states with fixed particle number [23], providing at the same time a link between mode-based and particle-based approaches.

In this work we start by considering again the correlations between an sp mode and its orthogonal complement and define an entropic measure that quantifies the loss of information in the state of the system due to the measurement of the occupancy of that mode. Such loss is directly related to the entanglement generated between the system and the measurement device. We then consider the sum over all states on a given basis of S, minimized over all such bases, of this quantity as a measure of the minimum loss of information due to an unread measurement in this basis, extending the minimization to all bases related through a Bogoliubov transformation [36] if the occupancy measurement of quasiparticle modes is also allowed. It is then shown that this measure is a non-negative quantity which is zero if and only if the state of the system is a convex combination of Slater determinants in the same sp basis, reducing for pure states to the entanglement entropy defined in [31], in analogy with its counterpart [14] for systems of distinguishable constituents. General stationary conditions for the optimizing basis are also derived. An analytic evaluation of this measure for a mixture of a general pure state with the maximally mixed state is provided, which shows that in this case the optimizing quasiparticles are just those diagonalizing the generalized one-body density matrix, and that the present measure can be nonzero in nonentangled mixed states. Explicit comparison with the fermionic entanglement of formation in a specific case is also made. Two fermion states are as well discussed.

II. FORMALISM

A. Single-mode measurement and entanglement entropy

We first consider a pure state $|\psi\rangle$ of a fermion system with an *n*-dimensional single-particle (sp) Hilbert space S. The system is described by a set of operators $\{c_j, c_j^{\dagger}, \}$ satisfying the canonical anticommutation relations,

$$\{c_i, c_j\} = 0, \quad \{c_i, c_j^{\dagger}\} = \delta_{ij},$$
 (1)

such that $\{|j\rangle = c_j^{\dagger}|0\rangle$, $j = 1, ..., n\}$ is an orthonormal set of one-fermion states $(|0\rangle$ denotes the vacuum of the operators c_j). We will work within a grand canonical context, so the state $|\psi\rangle$ does not necessarily has a definite particle number $N = \sum_k c_k^{\dagger} c_k$. Nonetheless, we will always assume that $|\psi\rangle$ has a definite number parity,

$$P|\psi\rangle = \pm |\psi\rangle, \quad P = \exp[i\pi N] = \prod_{k} (1 - 2c_k^{\dagger}c_k), \quad (2)$$

in agreement with the standard superselection rule [37]. We will also denote by d the dimension of the Fock space of the system.

We now consider a partition (A, B) of a particular basis of S (see appendix), where A denotes the single mode or "level" k and B its orthogonal complement. Due to the anticommutation relations, the operators,

$$\Pi_k = c_k^{\dagger} c_k, \quad \Pi_{\bar{k}} = c_k c_k^{\dagger}, \quad \Pi_k + \Pi_{\bar{k}} = 1,$$
 (3)

constitute a basic set of orthogonal projectors, defining a standard projective measurement on the level *k*. The operator $\Pi_k (\Pi_{\bar{k}})$ projects the state onto the subspace of states with level *k* occupied (empty), so the set describes the measurement of the occupancy of this level. The ensuing post measurement states are $|\psi_k\rangle = \Pi_k |\psi\rangle / \sqrt{p_k}$ and $|\psi_{\bar{k}}\rangle = \Pi_{\bar{k}} |\psi\rangle / \sqrt{p_{\bar{k}}}$, with $p_k = \langle c_k^{\dagger} c_k \rangle = \langle \psi | c_k^{\dagger} c_k | \psi \rangle$ and $p_{\bar{k}} = \langle c_k c_k^{\dagger} \rangle = 1 - p_k$, such that

$$|\psi\rangle = \sqrt{p_k} |\psi_k\rangle + \sqrt{p_{\bar{k}}} |\psi_{\bar{k}}\rangle. \tag{4}$$

For any operator $O_A(O_B)$ that depends only on the operators c_k, c_k^{\dagger} ({ $c_j, c_j^{\dagger}, j \neq k$ }) we have, using (2),

$$\langle \psi | O_{A(B)} | \psi \rangle = p_k \langle \psi_k | O_{A(B)} | \psi_k \rangle + p_{\bar{k}} \langle \psi_{\bar{k}} | O_{A(B)} | \psi_{\bar{k}} \rangle$$

= Tr $\rho_{A(B)} O_{A(B)}$, (5)

where

$$\rho_A = p_k c_k^{\dagger} |0\rangle \langle 0| c_k + p_{\bar{k}} |0\rangle \langle 0|, \qquad (6)$$

$$\rho_B = p_k c_k |\psi_k\rangle \langle\psi_k| c_k^{\dagger} + p_{\bar{k}} |\psi_{\bar{k}}\rangle \langle\psi_{\bar{k}}|, \qquad (7)$$

play the role of reduced states for A and B.

As shown in [31], for pure states the mode measurement defined above allows one to define an entanglement entropy that quantifies the entanglement between the measured sp mode and its orthogonal complement in S. Indeed, the reduced states (6) and (7) have the same eigenvalues { p_k, p_k }, and hence the entanglement entropy for such bipartition is the Shannon entropy of that distribution:

$$E_{k}(|\psi\rangle) = -p_{k}\log_{2}(p_{k}) - p_{\bar{k}}\log_{2}(p_{\bar{k}}).$$
(8)

The sum of (8) over all states on a given basis of S, minimized over all sp bases, is the *one-body entanglement*

entropy [31],

$$S^{\rm sp}(|\psi\rangle) = \min_{\{c_k\}} \sum_k -p_k \log_2 p_k - p_{\bar{k}} \log_2 p_{\bar{k}}.$$
 (9)

The minimum in Eq. (9) is reached for those operators $\{c_k\}$ that diagonalize the one-body density matrix $\rho_{ij}^{\text{sp}} = \langle c_j^{\dagger} c_i \rangle$, i.e., for those satisfying $\langle c_i^{\dagger} c_i \rangle = \lambda_i \delta_{ij}$ [31]. Hence,

$$S^{\rm sp}(|\psi\rangle) = \operatorname{tr} h(\rho^{\rm sp}),\tag{10}$$

where $h(p) = -p \log_2 p - (1 - p) \log_2(1 - p)$ and tr the trace in the sp space. It is clear then that $S^{sp}(|\psi\rangle) = 0$ iff there is an sp basis in which the state is written as a Slater determinant, for in that case the eigenvalues of ρ^{sp} are either 0 or 1 ($(\rho^{sp})^2 = \rho^{sp}$). Then Slater determinants are considered here noncorrelated states, in agreement with [23].

If quasiparticle modes are to be allowed, then the minimization extends to all quasiparticle bases, i.e., sets of operators $\{a_i, a_i^{\dagger}\}$ related to the original fermion operators $\{c_i, c_i^{\dagger}\}$ through a Bogoliubov transformation [36]:

$$a_i = \sum_j \bar{U}_{ji} c_j + V_{ji} c_j^{\dagger}.$$
 (11)

Equation (11) can be written as

$$\begin{pmatrix} \boldsymbol{a} \\ \boldsymbol{a}^{\dagger} \end{pmatrix} = \mathcal{W}^{\dagger} \begin{pmatrix} \boldsymbol{c} \\ \boldsymbol{c}^{\dagger} \end{pmatrix}, \quad \mathcal{W} = \begin{pmatrix} U & V \\ \bar{V} & \bar{U} \end{pmatrix}, \quad (12)$$

where the $2n \times 2n$ matrix \mathcal{W} should be unitary $(UU^{\dagger} + VV^{\dagger} = 1, UV^{T} + VU^{T} = 0)$ in order that $a_{\nu}, a_{\nu}^{\dagger}$ fulfill the fermionic anticommutation relations (1). It can be shown [31] that the minimum is reached for those operators $\{a_{\mu}, a_{\mu}^{\dagger}\}$ that diagonalize the *extended* $2n \times 2n$ density matrix,

$$\rho^{\rm qsp} = 1 - \left\langle \begin{pmatrix} \boldsymbol{c} \\ \boldsymbol{c}^{\dagger} \end{pmatrix} (\boldsymbol{c}^{\dagger} \quad \boldsymbol{c}) \right\rangle = \begin{pmatrix} \rho^{\rm sp} & \kappa \\ -\bar{\kappa} & 1 - \bar{\rho}^{\rm sp} \end{pmatrix}, \quad (13)$$

where $\kappa_{ij} = \langle c_j c_i \rangle$, $-\bar{\kappa}_{ij} = \langle c_j^{\dagger} c_i^{\dagger} \rangle$, and $(1 - \bar{\rho}^{sp})_{ij} = \langle c_j c_i^{\dagger} \rangle$. Equation (13) is an hermitic matrix which can always be diagonalized by a suitable transformation (12), such that

$$1 - \left\langle \begin{pmatrix} \boldsymbol{a} \\ \boldsymbol{a}^{\dagger} \end{pmatrix} (\boldsymbol{a} \quad \boldsymbol{a}^{\dagger}) \right\rangle = \mathcal{W}^{\dagger} \rho^{\operatorname{qsp}} \mathcal{W} = \begin{pmatrix} f & 0 \\ 0 & 1 - f \end{pmatrix},$$

with $f_{kl} = f_k \delta_{kl}$ and f_k , $1 - f_k$ the eigenvalues of ρ^{qsp} [which come in pairs $(f_k, 1 - f_k)$, with $f_k \in [0,1]$], entailing $\langle a_k^{\dagger} a_k \rangle = \delta_{kl} f_k$, $\langle a_k a_l \rangle = 0$. The generalized one-body entanglement entropy is therefore

$$S^{qsp}(|\psi\rangle) = -\sum_{k} f_k \log_2 f_k + (1 - f_k) \log_2(1 - f_k)$$

= $-\text{tr}' \rho^{qsp} \log_2 \rho^{qsp},$ (14)

with tr' the trace in the extended single-particle space. Hence, $S^{qsp}(|\psi\rangle) = 0$ iff all eigenvalues f_k are 0 or 1, i.e., $(\rho^{qsp})^2 = \rho^{qsp}$, which implies that ρ is a vacuum or in general a quasiparticle Slater determinant.

B. Information loss due to a single-mode measurement

Let us now consider a single-mode measurement on a general mixed state ρ of a fermion system (assumed to satisfy $[\rho, P] = 0$). The state after finding that sp state $|k\rangle$ is

occupied or empty is $\rho'_k = \prod_k \rho \prod_k / p_k$, or $\rho'_{\bar{k}} = \prod_{\bar{k}} \rho \prod_{\bar{k}} / p_{\bar{k}}$, respectively, with $p_k = \langle c_k^{\dagger} c_k \rangle = \text{Tr } \rho c_k^{\dagger} c_k$ and $p_{\bar{k}} = 1 - p_k$. Therefore, after an unread measurement of that level the state of the system is

$$\rho'(k) = p_k \,\rho'_k + p_{\bar{k}} \,\rho'_{\bar{k}} = \Pi_k \,\rho \,\Pi_k + \Pi_{\bar{k}} \,\rho \,\Pi_{\bar{k}}. \tag{15}$$

For instance, if ρ is a pure state $|\psi\rangle\langle\psi|$ [Eq. (4)],

$$\rho'(k) = p_k |\psi_k\rangle \langle \psi_k| + p_{\bar{k}} |\psi_{\bar{k}}\rangle \langle \psi_{\bar{k}}|.$$
(16)

The ensuing reduced state of A is given by (6) while $\rho_B = p_k c_k \rho'_k c^{\dagger}_k + p_{\bar{k}} \rho'_{\bar{k}}$. Since $\rho = \rho'(k) + \Pi_k \rho \Pi_{\bar{k}} + \Pi_{\bar{k}} \rho \Pi_k$, the last two terms are lost after such measurement.

The entropy $S(\rho'(k)) = -\text{Tr } \rho'(k) \log_2 \rho'(k)$ of the postmeasurement state (15) then cannot be lower than the entropy $S(\rho)$ of the original state, due to the information contained in the lost elements. In fact, the eigenvalues of $\rho'(k)$ are just the diagonal elements of ρ in a basis different from that of its eigenvectors, and it is well known that any such diagonal is always majorized by the eigenvalues of ρ [38]. We have then

$$S(\rho'(k)) \ge S(\rho), \tag{17}$$

with equality if and only if $\rho'(k) = \rho$. This last condition is obviously equivalent to

$$[\rho, c_k^{\dagger} c_k] = 0, \qquad (18)$$

since if $\rho = \rho'(k)$, Eq. (18) holds, while if (18) is valid, there is common basis of eigenvectors of ρ and $c_k^{\dagger}c_k$ and hence $\rho = \rho'(k)$. The difference,

$$I^{c_k}(\rho) = S(\rho'(k)) - S(\rho),$$
(19)

quantifies then this loss of information. It clearly satisfies $I^{c_k}(\rho) \ge 0$, with $I^{c_k}(\rho) = 0$ iff (18) applies. It is a fermionic version of the information deficit $\Delta^{\rightarrow}(\rho) = S(\rho') - S(\rho)$ [12], defined for systems of distinguishable constituents (there is here no minimization involved because the occupation of mode $|k\rangle$ is a classical variable). Furthermore, it is worth noting from (15) that

$$S(\rho'(k)) = S(k) + S(\rho|k),$$
 (20)

where

$$S(k) = -p_k \log_2 p_k - p_{\bar{k}} \log_2 p_{\bar{k}} = h(p_k)$$
(21)

is the entropy of mode k and

$$S(\rho|k) = p_k S(\rho'_k) + p_{\bar{k}} S(\rho'_{\bar{k}})$$
(22)

is the conditional entropy of the set of remaining modes, given that the state of mode k (occupied or empty) is known. Therefore, the deficit (19) can be written as

$$S(\rho'(k)) - S(\rho) = S(\rho|k) - (S(\rho) - S(k)), \quad (23)$$

which is a difference of classical-like and quantum conditional entropies with respect to mode k and represents the quantum discord [8] with respect to this mode. Hence, for single-mode measurements the extension of quantum deficit coincides with that of the quantum discord. For a pure state $\rho = |\psi\rangle\langle\psi|$, ρ'_k and ρ'_k are both pure [Eq. (16)], implying that I^{c_k} becomes coincident with the entanglement entropy (8) of mode k:

$$I^{c_k}(|\psi\rangle) = S(k) = E_k(|\psi\rangle).$$
⁽²⁴⁾

The conditional entropy (22) can be interpreted, following the general results of [39], as an entanglement of formation between the set of remaining modes $k' \neq k$ and a complementary system (which can also be a set of new fermionic modes) which purifies the whole system [see appendix, Eq. (A9)]. Besides, the arguments of [13,16] imply that the information deficit (19) is an indicator of the entanglement generated between the measurement device and the system after a measurement of mode k. In fact, by adding a qubit ancilla C in an initial state $|0\rangle$ to the fermionic system and performing the unitary transformation $U = e^{-i\frac{\pi}{2}(c_k c_k^{\dagger}) \otimes \sigma_y}$, we obtain

$$U(|\psi\rangle|0\rangle) = \sqrt{p_k} |\psi_k\rangle|0\rangle + \sqrt{p_k} |\psi_k\rangle|1\rangle.$$
(25)

Hence, for a general mixed fermion state ρ ,

$$\operatorname{Tr}_{C}[U(\rho \otimes |0\rangle\langle 0|)U^{\dagger}] = \rho'(k).$$
(26)

Therefore $I^{c_k}(\rho)$ is the difference between the entropy of the fermionic subsystem $\rho_F = \text{Tr}_C \rho_{FC} = \rho'(k)$ in $\rho_{FC} = U(\rho \otimes |0\rangle \langle 0|) U^{\dagger}$ and that of the whole system, $S(\rho_{FC}) = S(\rho)$. Such difference [the negative of the conditional entropy $S(\rho_{FC}) - S(\rho_F)$] can be positive only if ρ_{FC} is entangled, according to the entropic separability criterion [40–42], and is a lower bound to the one-way distillable entanglement [13,16,43]. On the other hand, if $\rho'(k) = \rho$, such that $p_k = 0$ or 1 for any eigenstate of ρ , then ρ_{FC} is clearly separable and no entanglement is created.

C. One-body information loss

We now take the sum, over all the states of a given basis of S, of I^{c_k} in (19),

$$I^{c}(\rho) = \sum_{k} I^{c_{k}}(\rho) = \sum_{k} S(\rho'(k)) - S(\rho), \qquad (27)$$

as a measure of the loss of information due to an unread measurement in this basis. The minimum over all sp bases of this difference,

$$I^{\mathrm{sp}}(\rho) = \underset{c}{\mathrm{Min}} \ I^{c}(\rho) = \underset{\{c_k\}}{\mathrm{Min}} \sum_{k} I^{c_k}(\rho), \qquad (28)$$

measures then the minimum loss of information due to such type of measurement. This *one-body information loss* clearly satisfies $I^{sp}(\rho) \ge 0$, since it is a sum of non-negative terms, with $I^{sp}(\rho) = 0$ iff fermion operators c_k exist such that $\rho'(k) = \rho \forall k$, i.e., iff

$$[\rho, c_k^{\dagger} c_k] = 0, \quad k = 1, \dots, n,$$
(29)

which occurs iff ρ is diagonal in a set of Slater determinants $\{\prod_k (c_k^{\dagger})^{n_k} | 0\rangle\}$ in the same sp basis (the common eigenvectors of all $c_k^{\dagger} c_k$). Such states include the typical uncorrelated thermal-like states $\rho \propto \exp[-\beta H]$, with $H = \sum_k \varepsilon_k c_k^{\dagger} c_k$, but also any convex combination of Slater determinants in the same basis. These combinations play here the role of "classically" correlated states.

Note that if (29) holds, for $k \neq l$ we have $\langle c_k^{\dagger} c_l \rangle = \langle [c_k^{\dagger} c_k, c_k^{\dagger} c_l] \rangle = 0$, so that the operators c_k diagonalize the sp density matrix: $\langle c_k^{\dagger} c_l \rangle = \lambda_k \delta_{kl}$. Therefore, even though the operators minimizing $I^c(\rho)$ may not diagonalize $\rho^{\rm sp}$ in

general, they will if $I^{sp}(\rho) = 0$. Thus, $I^{c}(\rho) > 0$ in all sp bases diagonalizing ρ^{sp} imply $I^{sp}(\rho) > 0$.

For a pure state $\rho = |\psi\rangle\langle\psi|$ Eq. (24) implies

$$I^{c}(|\psi\rangle) = \sum_{k} S(k) = \sum_{k} h(p_{k}), \qquad (30)$$

which is just a concave function of the diagonal elements of ρ^{sp} . Therefore, in this case its minimum over all bases is obtained when p_k are its eigenvalues, i.e., when the c_k 's are the fermion operators diagonalizing ρ^{sp} :

$$I^{\rm sp}(|\psi\rangle) = \operatorname{tr} h(\rho^{\rm sp}) = S^{\rm sp}(|\psi\rangle). \tag{31}$$

This result coincides with the entanglement entropy defined in the previous section, in analogy with the information loss for the distinguishable case [14], which also coincides with the entanglement entropy for pure states.

On the other hand, it is seen from (20) that for a general mixed state ρ , $S(\rho'(k)) \ge S(k) = h(p_k)$ and hence,

$$\operatorname{Min}_{\{c_k\}} \sum_{k} S(\rho'(k)) \ge \operatorname{tr} h(\rho^{\operatorname{sp}}).$$
(32)

As in the case of the one-body entanglement entropy, if quasiparticle mode measurements are to be allowed then the minimization extends to all quasiparticle bases, i.e., sets of operators $\{a_k, a_k^{\dagger}\}$ related to the original fermion operators $\{c_i, c_i^{\dagger}\}$ through a Bogoliubov transformation (12). It can be seen by repeating the argument used above that this information loss,

$$I^{qsp}(\rho) = \min_{\{a_k\}} \sum_k [S(\rho'(k)) - S(\rho)],$$
 (33)

satisfies $I^{\text{qsp}}(\rho) \ge 0$, with equality iff quasiparticle operators a_k exist such that

$$[\rho, a_k^{\dagger} a_k] = 0, \quad k = 1, \dots, n, \tag{34}$$

i.e., iff ρ is diagonal in a set of *quasiparticle* Slater determinants in the same basis (common eigenvectors of all $a_k^{\dagger}a_k$). Moreover, as this extended minimization includes the previous one as a particular case, we have

$$I^{\rm qsp}(\rho) \leqslant I^{\rm sp}(\rho). \tag{35}$$

For pure states, the minimum I^{qsp} is obtained for those a_k^{\dagger} diagonalizing the extended density matrix (13), which in analogy with (31) yields

$$I^{qsp}(|\psi\rangle) = -\text{tr}'\rho^{qsp}\log_2\rho^{qsp} = S^{qsp}(|\psi\rangle), \qquad (36)$$

where S^{qsp} is the generalized entanglement entropy (14). As in the previous case, if (34) holds, the operators a_k diagonalize ρ^{qsp} , implying that even though such operators may not minimize $I^a(\rho)$ in general, they will if $I^{qsp}(\rho) = 0$.

Let us also remark that $I^{sp}(\rho)$ remains invariant under standard unitary one-body transformations,

$$\rho \to U\rho U^{\dagger}, \quad U = \exp\left[-it\sum_{i,j}h_{ij}c_i^{\dagger}c_j\right], \quad (37)$$

with $h_{ij} = h_{ji}^*$, since they just imply a unitary transformation of the fermion operators $\boldsymbol{c} = (c_1, \dots, c_n)^T$:

$$\boldsymbol{c} \to U \boldsymbol{c} U^{\dagger} = \exp[ith]\boldsymbol{c},$$
 (38)

with $\rho^{sp} \rightarrow \exp[ith]\rho^{sp} \exp[-ith]$. These transformations map Slater determinants onto Slater determinants. Similarly, $I^{qsp}(\rho)$ remains invariant under general one-body transformations,

$$\rho \to W \rho W^{\dagger}, \quad W = \exp[-itH],$$

$$H = \sum_{i,j} h_{ij} c_i^{\dagger} c_j + \frac{1}{2} \Delta_{ij} (c_i^{\dagger} c_j^{\dagger} + c_j c_i) \qquad (39)$$

$$= \frac{1}{2} (\boldsymbol{c}^{\dagger} \ \boldsymbol{c}) \mathcal{H} \begin{pmatrix} \boldsymbol{c} \\ \boldsymbol{c}^{\dagger} \end{pmatrix}, \quad \mathcal{H} = \begin{pmatrix} h & \Delta \\ -\Delta^* & -h^* \end{pmatrix}, \quad (40)$$

where $\Delta^T = -\Delta$, since they just imply a Bogoliubov transformation of the fermion operators:

$$\begin{pmatrix} \boldsymbol{c} \\ \boldsymbol{c}^{\dagger} \end{pmatrix} \rightarrow \exp[it\mathcal{H}] \begin{pmatrix} \boldsymbol{c} \\ \boldsymbol{c}^{\dagger} \end{pmatrix},$$

with $\rho^{qsp} \rightarrow \exp[it\mathcal{H}]\rho^{qsp} \exp[-it\mathcal{H}]$. Therefore, evolution under Hamiltonians H of the previous form will not alter the value of $I^{qsp}(\rho)$.

Finally, it is worth remarking that

$$I^{\rm qsp}(\rho) = 0, \tag{41}$$

for any state ρ with support in a *two-dimensional* sp space (n = 2) which commutes with the parity *P*.

Proof. Let

$$\rho = \sum_{\nu=1,2} q_{\nu}^{-} |\psi_{-}^{\nu}\rangle \langle \psi_{-}^{\nu}| + q_{\nu}^{+} |\psi_{+}^{\nu}\rangle \langle \psi_{+}^{\nu}|$$
(42)

be the spectral decomposition of such ρ , with

$$\psi_{-}^{\nu}\rangle = \left(\alpha_{1}^{\nu}c_{1}^{\dagger} + \alpha_{2}^{\nu}c_{2}^{\dagger}\right)|0\rangle, \quad |\psi_{+}^{\nu}\rangle = \left(\beta_{1}^{\nu} + \beta_{2}^{\nu}c_{2}^{\dagger}c_{1}^{\dagger}\right)|0\rangle,$$

its odd and even parity orthogonal eigenstates $[\alpha_j^2 = (-)^j \bar{\alpha}_{3-j}^1, \beta_j^2 = (-)^j \bar{\beta}_{3-j}^1]$. It is easily seen that these states can be all written as zero-, one- or two-quasiparticle states in a common basis. In fact, $\langle c_2^{\dagger} c_1 \rangle = (q_1^- - q_2^-) \bar{\alpha}_2^{\dagger} \alpha_1^1, \langle c_2^{\dagger} c_1^{\dagger} \rangle = (q_1^+ - q_2^+) \bar{\beta}_2^1 \beta_1^1$. Hence, in terms of the quasiparticle operators a_k that diagonalize ρ^{qsp} ($\langle a_2^{\dagger} a_1 \rangle = (q_1^- - q_2^-) \bar{\alpha}_2^{\dagger} \alpha_1^{\prime 1} = 0, \langle a_2^{\dagger} a_1^{\dagger} \rangle = (q_1^+ - q_2^+) \bar{\beta}_2^{\dagger} \beta_1^{\prime 1} = 0)$, necessarily $|\psi_{-}^{\perp} \rangle \propto a_2^{\dagger} |0' \rangle, |\psi_{+}^{\perp} \rangle \propto |0' \rangle$ and $|\psi_{+}^2 \rangle \propto a_2^{\dagger} a_1^{\dagger} |0' \rangle$ if $q_1^{\pm} \neq q_2^{\pm}$, with $|0' \rangle$ the vacuum of these quasiparticles (of the same parity as $|0\rangle$). And in case of degeneracy we may always choose the eigenstates $|\psi_{\pm}^{\psi} \rangle$ of the previous forms. Hence ρ is always diagonal in a quasiparticle Slater determinant basis, implying $I^{qsp}(\rho) = 0$.

Note, however, that $I^{\text{sp}}(\rho) > 0$ unless $[\rho, N] = 0$, i.e., $\langle c_2^{\dagger} c_1^{\dagger} \rangle = 0$, and that ρ is not necessarily of the uncorrelated form $\propto \exp[-\sum_{\nu=1,2} \varepsilon_{\nu} a_{\nu}^{\dagger} a_{\nu}]$ unless $\langle a_1^{\dagger} a_1 a_2^{\dagger} a_2 \rangle = \langle a_1^{\dagger} a_1 \rangle \langle a_2^{\dagger} a_2 \rangle$, i.e., $q_2^+ = (q_1^- + q_2^+)(q_2^- + q_2^+)$.

On the other hand, if the support is a three-dimensional sp space (n = 3), then $I^{qsp}(\rho) = 0$ for any ρ of *definite* parity (but not for any ρ commuting with P).

Proof. Let $\rho = \sum_{\nu=1}^{4} q_{\nu} |\psi^{\nu}\rangle \langle \psi^{\nu}|$ be the spectral decomposition of ρ . If its eigenstates have all odd parity, i.e.,

$$|\psi^{\nu}\rangle = \left(\sum_{j=1}^{3} \alpha_{j}^{\nu} c_{j}^{\dagger} + \alpha_{4}^{\nu} c_{3}^{\dagger} c_{2}^{\dagger} c_{1}^{\dagger}\right)|0\rangle, \quad \nu = 1, \dots, 4,$$

then $\langle c_j^{\dagger} c_k \rangle = \sum_{\nu} q_{\nu} (\bar{\alpha}_j^{\nu} \alpha_k^{\nu} + \delta_{jk} | \alpha_4^{\nu} |^2), \quad \langle c_j^{\dagger} c_k^{\dagger} \rangle = -\sum_{\nu,l} q_{\nu} \epsilon_{jkl} \bar{\alpha}_4^{\nu} \alpha_l^{\nu}, \text{ with } \epsilon_{jkl} \text{ the fully antisymmetric tensor.}$ Hence, if expressed in terms of the quasiparticle operators a_k that diagonalize $\rho^{qsp} (c_j^{\dagger} \rightarrow a_j^{\dagger}, |0\rangle \rightarrow |0'\rangle, \alpha_j^{\nu} \rightarrow \alpha'_j^{\nu},$ with $\langle a_j^{\dagger} a_k \rangle = f_j \delta_{jk}, \quad \langle a_j^{\dagger} a_k^{\dagger} \rangle = 0$, the previous relations together with $\langle \psi^{\nu} | \psi^{\nu'} \rangle = \sum_{\mu=1}^{4} \bar{\alpha}_{\mu}^{\nu} \alpha'_{\mu}^{\nu} = \delta^{\nu\nu'}$ imply, for distinct $q^{\nu}s, \quad \alpha'_{\mu}^{\nu} \propto \delta_{\mu}^{\nu}, \text{ i.e., } |\psi^{\nu}\rangle \propto a_{\nu}^{\dagger}|0'\rangle, \quad \nu = 1,2,3, \text{ and}$ $|\psi^4\rangle \propto a_3^{\dagger} a_2^{\dagger} a_1^{\dagger}|0'\rangle.$ Hence ρ is diagonal in a quasiparticle Slater determinant basis and $I^{qsp}(\rho) = 0$ [but $I^{sp}(\rho) \neq 0$ if $[\rho, N] \neq 0$]. The same procedure can be applied for an even parity ρ (which can be recast in the previous odd-parity form after a particle-hole transformation $c_i^{\dagger} \rightarrow c_i$ of one of the operators).

Note, however, that if ρ contains eigenstates of different parity, $I^{\text{qsp}}(\rho)$ can be positive since the fermion quasiparticle operators of the normal form for each parity will not coincide in general.

D. General stationary condition

Let us now derive the general stationary equations that must be satisfied by the set of operators $\{a_k\}$ minimizing the generalized one-body information loss (33). After a measurement of the occupancy of a corresponding level k, the ensuing state $\rho'(k)$, Eq. (15) has eigenstates $|\phi_{k(\bar{k})}^{\mu}\rangle$ with eigenvalues,

$$q_{k(\bar{k})}^{\mu} = \left\langle \phi_{k(\bar{k})}^{\mu} \middle| \rho(k) \middle| \phi_{k(\bar{k})}^{\mu} \right\rangle = \left\langle \phi_{k(\bar{k})}^{\mu} \middle| \rho \middle| \phi_{k(\bar{k})}^{\mu} \right\rangle.$$

Consider now a small variation of the measurement basis determined by a general one-body transformation,

$$W = \exp[-i\epsilon H] \approx 1 - i\epsilon H,$$

with *H* of the general form (39) and (40). We then have $\delta q_{k(\bar{k})}^{\mu} = -i\epsilon \langle \phi_{k(\bar{k})}^{\mu} | [\rho, H] | \phi_{k(\bar{k})}^{\mu} \rangle$ up to lowest order in ϵ , which implies, for the information loss (33),

$$\delta I^{\rm qsp}(\rho) = \sum_{k,\mu} f'(q_k^{\mu}) \delta q_k^{\mu} + f'(q_{\bar{k}}^{\mu}) \delta q_{\bar{k}}^{\mu}$$
$$= -i\epsilon \operatorname{Tr}\left(\left[\sum_k f'(\rho'(k)), \rho\right] H\right), \qquad (43)$$

where $f'(\rho) = -\log_2 \rho$. The condition $\delta I^{qsp}(\rho) = 0$ for *arbitrary* H then leads to the stationary equations $\operatorname{Tr} [\sum_k f'(\rho'(k)), \rho] c_i^{\dagger} c_j = 0$, $\operatorname{Tr} [\sum_k f'(\rho'(k)), \rho] c_i^{\dagger} c_j^{\dagger} = 0 \forall i, j$, which reduce to

Tr
$$\rho \left[f'(\rho'(k)) + f'(\rho'(l)), a_k^{\dagger} a_l \right] = 0,$$
 (44)

Tr
$$\rho \left[f'(\rho'(k)) + f'(\rho'(l)), a_k^{\dagger} a_l^{\dagger} \right] = 0,$$
 (45)

 $\forall k \neq l$ when expressed in terms of the quasiparticle operators determining the measurement basis $([\rho'(k), a_k^{\dagger}a_k] = 0 \forall k)$, since Tr $[f'(\rho(k)), \rho]a_j^{\dagger}a_l = 0$ if $j \neq k \neq l$, and also if j = l = k. In the case of $I^{\text{sp}}(\rho)$, just Eq. (44) is to be considered $(\Delta = 0 \text{ in } H)$.

For a pure state $\rho = |\psi\rangle\langle\psi|$, Eqs. (44) and (45) become

$$[g(p_k) - g(p_{\bar{k}}) - g(p_l) + g(p_{\bar{l}})]\langle \psi | a_k^{\dagger} a_l | \psi \rangle = 0, \quad (46)$$

$$[g(p_k) - g(p_{\bar{k}}) + g(p_l) - g(p_{\bar{l}})]\langle \psi | a_k^{\dagger} a_l^{\dagger} | \psi \rangle = 0, \quad (47)$$

for $k \neq l$, where g(p) = f'(p) and $p_{k(\bar{k})}$ are the probabilities of finding state *k* occupied (empty) in $|\psi\rangle$. It is then verified that they are fulfilled by those a_k diagonalizing the extended density matrix (13) ($\langle a_k^{\dagger} a_l \rangle = \langle a_k^{\dagger} a_l^{\dagger} \rangle = 0$).

E. Generalized one-body information loss

We may directly extend all previous considerations to more general entropic forms. We first consider the generalized trace form entropies [42,44],

$$S_f(\rho) = \operatorname{Tr} f(\rho), \tag{48}$$

where $f : [0,1] \to \mathbb{R}$ is a smooth strictly concave real function satisfying f(0) = f(1) = 0. For $f(\rho) = -\rho \log_2 \rho$, $S_f(\rho)$ becomes the von Neumann entropy $S(\rho)$, whereas for $f(\rho) = 2\rho(1-\rho)$, it becomes the quadratic entropy $S_2(\rho)$, which is just a decreasing function of the purity Tr ρ^2 and corresponds to the linear approximation $-\rho \ln \rho \approx \rho(1-\rho)$. It does not require the explicit knowledge of the eigenvalues of ρ , being then easier to determine than $S(\rho)$ [45,46]. Moreover, the associated generalization of the one-body entanglement entropy (14), $S_f^{\text{qsp}}(|\psi\rangle) = \text{tr}' f(\rho'^{\text{qsp}})$ [31], becomes

$$S_2^{\text{qsp}}(|\psi\rangle) = 2 \operatorname{tr}' \rho^{\text{qsp}}(1 - \rho^{\text{qsp}}) = 4 \sum_k f_k (1 - f_k), \quad (49)$$

which is just the sum of the *fluctuations* of the occupancies of all single quasiparticle levels. More generally, these entropies include the family of Tsallis entropies [47], obtained for $f(\rho) = (\rho - \rho^q)/(1 - 2^{1-q})$ with q > 0, $q \neq 1$, which become proportional to the von Neumann and quadratic entropies for $q \rightarrow 1$ and q = 2, respectively. We use here the normalization $\operatorname{Tr} f(\rho) = 1$ for a maximally mixed single qubit state ρ .

A function f defined with the properties stated above ensures that all entropies $S_f(\rho)$ satisfy [42,44] (i) $S_f(\rho) \ge 0 \forall \rho$, with $S_f(\rho) = 0$ iff $\rho^2 = \rho$, (ii) $S_f(\sum_i q_i \rho_i) \ge \sum_i q_i S_f(\rho_i)$ for $q_i \ge 0$, $\sum_i q_i = 1$ (concavity), and (iii)

$$\rho' \prec \rho \Rightarrow S_f(\rho') \ge S_f(\rho), \tag{50}$$

where $\rho' \prec \rho$ indicates that the sorted set $\{q'_i\}$ of eigenvalues of $\rho' (q'_i > q'_j \text{ if } i < j)$ is *majorized* [14,38,42] by the sorted set $\{q_i\}$ of eigenvalues of ρ :

$$\rho' \prec \rho \Leftrightarrow \sum_{i=1}^k q'_i \leqslant \sum_{i=1}^k q_i, \quad k = 1, \dots, d,$$

with $\sum_{i=1}^{d} q'_i = \sum_{i=1}^{d} q_i$. Therefore, $S_f(\rho)$ increases with increasing mixedness of ρ .

This last property allows the straightforward extension of the results of the previous section to the present more general entropic forms. Indeed, $\rho'(k)$ in (15) is majorized by the original state ρ , $\rho'(k) \prec \rho$, implying $S_f(\rho'(k)) \ge S_f(\rho)$ and hence

$$I_f^{c_k}(\rho) \equiv S_f(\rho'(k)) - S_f(\rho) \ge 0, \tag{51}$$

with $I_f^{c_k}(\rho) = 0$ iff $\rho'(k) = \rho$. Equation (51) is a measure of the information loss due to the unread measurement of the occupation of the sp state k, and is also an indicator of the entanglement generated between the system and measurement device, according to the generalized entropic separability criterion [42]. By summing over all states in a basis and minimizing over all possible bases of S we obtain

$$I_{f}^{\rm sp}(\rho) = \min_{\{c_{k}\}} \sum_{k} I_{f}^{c_{k}} = \min_{\{c_{k}\}} \sum_{k} S_{f}(\rho'(k)) - S_{f}(\rho), \quad (52)$$

which satisfies $I_f^{\text{sp}}(\rho) \ge 0$, with $I_f^{\text{sp}}(\rho) = 0$ iff ρ is diagonal in a set of Slater determinants in the same sp basis ($[\rho, c_k^{\dagger} c_k] = 0 \forall k$). The minimization may again be extended to all quasiparticle bases through a Bogoliubov transformation, leading to the quantity,

$$I_{f}^{qsp}(\rho) = \min_{\{a_{k}\}} \sum_{k} S_{f}(\rho'(k)) - S_{f}(\rho),$$
(53)

which satisfies $0 \leq I_f^{qsp}(\rho) \leq I_f^{sp}(\rho)$, with $I_f^{qsp}(\rho) = 0$ iff ρ is diagonal in a basis of quasiparticle Slater determinants $([\rho, a_k^{\dagger} a_k] = 0 \forall k)$. For pure states $\rho^2 = \rho$, $I_f^{qsp}(\rho) = S_f(\rho^{qsp})$ becomes the generalized entropy of the extended one-body density matrix. Let us remark that the general stationary conditions (44)–(47) remain valid for the present generalization, with f' denoting now the derivative of the entropic function f.

Equation (50) remains also valid for Schur-concave functions of ρ [38], which include, in particular, increasing functions of the previous entropies $S_f(\rho)$. An example is provided by the quantum version of the Renyi entropies [48],

$$S_q^R(\rho) = \frac{\log_2(\operatorname{Tr} \rho^q)}{1-q} = \frac{\log_2[1 - (1 - 2^{1-q})S_q(\rho)]}{1-q}, \quad (54)$$

where q > 0, $q \neq 1$, which are just increasing functions of the Tsallis entropies $S_q(\rho)$ and approach the von Neumann entropy for $q \rightarrow 1$. The definition of information loss straightforwardly extends to these entropies. The logarithm in (54) implies additivity, i.e., $S_q^R(\rho \otimes \sigma) = S_q^R(\rho) + S_q^R(\sigma)$, which ensures that the addition of an uncorrelated ancilla to the system $(\rho \rightarrow \rho \otimes \sigma)$ has no effect on the associated information deficit [49] $I_{R_q}(\rho) = \sum_k S_q^R(\rho'(k)) - S_q^R(\rho)$. Nonetheless, the optimization problem for $I_{R_q}(\rho)$ is the same as that for $I_q(\rho) = \sum_k S_q(\rho'(k)) - S_q(\rho)$.

We finally mention that for fermions we may consider yet another way of adding an ancilla to our system *S*, by expanding its sp Hilbert space $S \to S \oplus A$. A noncorrelated state of the system S + A will then have the form $\rho_S \rho_A$, where ρ_A and ρ_B involve creation and annihilation operators of singleparticle states in *S* and *A*, respectively (see appendix). We have Tr $\rho_S \rho_A = \text{Tr } \rho_S \text{Tr} \rho_A$ if traces are taken in a grand canonical ensemble (as we are here assuming), and hence $S_q^R(\rho_S \rho_A) =$ $S_q^R(\rho_S) + S_q^R(\rho_A)$.

III. APPLICATION

A. Mixture of pure state plus maximally mixed state

Let us now consider the mixture,

$$\rho = w|\psi\rangle\langle\psi| + \frac{1-w}{d}I_d, \tag{55}$$

with $0 \le w \le 1$ and *d* the dimension of the state space. After an unread measurement of mode $|k\rangle$ the state reads

$$\rho'(k) = w(p_k|\psi_k\rangle\langle\psi_k| + p_{\bar{k}}|\psi_{\bar{k}}\rangle\langle\psi_{\bar{k}}|) + \frac{1-w}{d}I_d, \quad (56)$$

with $p_{k(\bar{k})} = \langle c_k^{\dagger} c_k \rangle$ ($\langle c_k c_k^{\dagger} \rangle$) the probability of finding mode *k* occupied (empty) in $|\psi\rangle$. Its eigenvalues are $q_{k(\bar{k})} = w p_{k(\bar{k})} + \frac{1-w}{d}$ and $\frac{1-w}{d}$, so that

$$S_{f}(\rho'(k)) = f(q_{k}) + f(q_{\bar{k}}) + (d-2)f\left(\frac{1-w}{d}\right), \quad (57)$$

$$I_{f}^{e}(\rho) = \sum_{k} [S(\rho'(k)) - S(\rho)]$$

$$= \sum_{k} \left[f(q_{k}) + f(q_{\bar{k}}) - f\left(w + \frac{1-w}{d}\right) - f\left(\frac{1-w}{d}\right) \right]. \quad (58)$$

We now show that the minimum of $I_f^c(\rho)$ over all sp basis of S is reached for the operators $\{c'_k\}$ that diagonalize the onebody density matrix $\rho_{ij}^{\text{sp}} = \langle c_j^{\dagger} c_i \rangle$, while the minimum over all quasiparticle basis is attained for those $\{a_k\}$ diagonalizing the corresponding extended one-body density matrix ρ^{qsp} .

Proof. Denoting with $\{\lambda_k = \langle c_k^{\dagger} c_k^{\prime} \rangle\}$ the set of eigenvalues of the one-body density matrix ρ^{sp} , such that $\langle c_k^{\dagger} c_j^{\prime} \rangle = \lambda_k \delta_{kj}$, this distribution majorizes any other diagonal of the matrix, implying $\{p_k = \langle c_k^{\dagger} c_k \rangle\} \prec \{\lambda_k\}$ for the sorted sets. Hence, $\{q_k\} \prec \{q_k^{\prime}\}$ if $q_k^{\prime} = w\lambda_k + \frac{1-w}{d}$ and $0 \le w \le 1$, and also $\{q_{\bar{k}}\} \prec \{q_k^{\prime}\}$ if $q_k^{\prime} = w\lambda_{\bar{k}} + \frac{1-w}{d}$, since $\{p_k\} \prec \{\lambda_k\}$ implies $\{p_{\bar{k}} = 1 - p_k\} \prec \{\lambda_{\bar{k}} = 1 - \lambda_k\}$. Therefore, Eq. (50) leads to

$$\sum_{k} f(q_{k}) + f(q_{\bar{k}}) \ge \sum_{k} f(q'_{k}) + f(q'_{\bar{k}}), \qquad (59)$$

implying $I_f^{sp}(\rho) = \operatorname{Min}_{\boldsymbol{c}} I_f^{\boldsymbol{c}}(\rho) = I_f^{\boldsymbol{c}'}(\rho)$. This result also follows directly from the concavity of f and the relation $q_{k(\bar{k})} = \sum_{k'} |U_{kk'}|^2 q'_{k'(\bar{k}')}$, with U the unitary matrix diagonalizing ρ^{sp} .

When quasiparticles are also considered, we note that both p_k and $p_{\bar{k}} = 1 - p_k$ are diagonal elements of ρ^{qsp} , so that the enlarged sorted set $\{p_k, p_{\bar{k}}\}$ is majorized by the whole sorted set $\{f_k = \langle a_k^{\dagger} a_k \rangle, f_{\bar{k}} = 1 - f_k\}$ of eigenvalues of $\rho^{qsp} (\langle a_k^{\dagger} a_l \rangle = \delta_{kl} f_k, \langle a_k^{\dagger} a_l^{\dagger} \rangle = 0)$. Therefore, $\{q_k, q_{\bar{k}}\} \prec \{q'_k, q'_{\bar{k}}\}$ for $q'_{k(\bar{k})} = wf_{k(\bar{k})} + \frac{1-w}{d}$, implying Eq. (59) and hence $I_f^{qsp}(\rho) = I_f^a(\rho)$. This result also follows from the relation $q_k = \sum_{k'} |W_{kk'}|^2 q'_{k'}$ between the elements of the enlarged sets, with W the matrix diagonalizing ρ^{qsp} .

These results are valid for the von Neumann entropy as well as for the generalized entropic forms S_f , and are evidently in agreement with the stationary conditions (44) and (45), since for the state (55) they become proportional to Eqs. (46) and (47). They also hold if ρ has a definite parity P, i.e., if I_d stands for the projector onto the same parity as that of $|\psi\rangle$, in which case $d \to d/2$ in (55)–(59). And if $|\psi\rangle$ has definite fermion number N, they are also valid in a canonical ensemble, with $d \to {n \choose N}$.

The previous arguments also imply that if $|\psi'\rangle$ is a state whose one-body density matrix is majorized by that of $|\psi\rangle$, $\rho'^{qsp} \prec \rho^{qsp}$, and $\rho' = w |\psi'\rangle \langle \psi'| + (1 - w)I_d/d$, then

$$I_f^{\rm qsp}(\rho') \ge I_f^{\rm qsp}(\rho), \tag{60}$$

 $\forall w \in [0,1]$, and $\forall S_f$. This general inequality reflects the rigorously stronger entanglement of $|\psi'\rangle$, in the sense that $S_f^{qsp}(|\psi'\rangle) = S_f(\rho'^{qsp}) \ge S_f(\rho^{qsp})$ for all entropies S_f if $\rho'^{qsp} \prec \rho^{qsp}$, and indicates that the value of I_f^{qsp} in the mixture (55) is indeed driven by the entanglement of the pure state. The same relation holds for I_f^{sp} if $\rho'^{sp} \prec \rho^{sp}$.

Let us point out that $I_f^{qsp}(\rho)$ is a strictly increasing function of w for any concave f, with $I_f^{qsp}(\rho) > 0$ for any w > 0. From Eq. (58) it is seen that it exhibits for small w a *universal* initial quadratic increase, given by

$$I_f^{\rm qsp}(\rho) \approx w^2 |f''(d^{-1})| \sum_k f_k (1 - f_k), \tag{61}$$

with f_k the eigenvalues of the ρ^{qsp} determined by $|\psi\rangle$, which is just proportional to the quadratic entanglement of $|\psi\rangle$, Eq. (49). For $I_f^{sp}(\rho)$ we should just replace f_k by the eigenvalues λ_k of ρ^{sp} . In the case of the quadratic entropy S_2 , Eq. (61) is of course *exact* $\forall w \in [0,1]$ and independent of $d(|f''(d^{-1})| = 4)$.

Previous results are then similar to those obtained for distinguishable bipartite quantum systems [14], where the role played here by the basis diagonalizing ρ^{qsp} corresponds there to the local part of the Schmidt basis of the pertinent pure state.

B. The case of four single-particle levels

We now focus on the special case of a fermion system with $n = \dim(S) = 4$, where the entanglement of formation for general states can be analytically evaluated [23,31]. For simplicity we will consider mixed states with definite parity, which will be chosen as odd. A general pure state will be then a linear combination of single fermion states and three fermion states. Therefore, it can be written as

$$|\psi\rangle = \sum_{i}^{4} (\alpha_{i} c_{i}^{\dagger} |0\rangle + \bar{\beta}_{i} c_{i} |\bar{0}\rangle), \qquad (62)$$

where $|\bar{0}\rangle = c_1^{\dagger} c_2^{\dagger} c_3^{\dagger} c_4^{\dagger} |0\rangle$ is the fully occupied state and $\boldsymbol{\alpha}, \boldsymbol{\beta}$ are four-dimensional complex vectors satisfying $|\boldsymbol{\alpha}|^2 + |\boldsymbol{\beta}|^2 = 1$. It can be shown [31] that the eigenvalues of the generalized one-body density matrix ρ^{qsp} of such state are fourfold degenerate and given by

$$f_{\pm} = \frac{1 \pm \sqrt{1 - C^2(|\psi\rangle)}}{2},\tag{63}$$

where $C(|\psi\rangle) = 2|\beta^{\dagger}\alpha|$ is the *generalized Slater correlation measure*, satisfying $0 \le C \le 1$. This result implies that there is always a quasiparticle basis in which the state (62) takes the normal form,

$$|\psi\rangle = (\sqrt{f_+} a_1^{\dagger} + \sqrt{1 - f_+} a_2^{\dagger} a_3^{\dagger} a_4^{\dagger})|0\rangle,$$
 (64)



FIG. 1. Quadratic (dashed line) and von Neumann (solid line) information loss $I^{qsp}(\rho)$ and entanglement of formation $S^{qsp}(\rho)$ (normalized to their maximum values), as a function of w for the mixture (55) with n = 4 and definite odd parity, for a maximally entangled state $|\psi\rangle$.

with $|0\rangle$ denoting now the vacuum of the operators a_i . In terms of *C* the entanglement entropy (14) becomes then

$$S^{\text{qsp}}(|\psi\rangle) = 4h\left(\frac{1+\sqrt{1-C^2(|\psi\rangle)}}{2}\right),$$
 (65)

so $C(|\psi\rangle)$ plays the role of a fermionic concurrence. As in the two-qubit case, for a mixed state ρ the convex roof extension of S^{qsp} can be similarly evaluated as

$$S^{qsp}(\rho) = 4h\left(\frac{1+\sqrt{1-C^2(\rho)}}{2}\right),$$
 (66)

where $C(\rho)$ is the convex roof extension of the pure state concurrence defined above [31]. This quantity vanishes iff ρ can be written as a convex combination of particle or quasiparticle Slater determinants.

Let us now consider the state (55) with a maximally entangled state $|\psi\rangle = \frac{1}{\sqrt{2}}(a_1^{\dagger} + a_2^{\dagger}a_3^{\dagger}a_4^{\dagger})|0\rangle$, which leads to $f_{\pm} = 1/2$. The fermionic concurrence is then $C(\rho) = \text{Max}[(7w - 3)/4, 0]$ [46] and therefore, Eq. (66) leads to

$$S^{\text{qsp}}(\rho) = \begin{cases} 0 & w \leq 3/7 \\ 4h\left(\frac{4+\sqrt{7[1+w(6-7w)]}}{8}\right) & w > 3/7 \end{cases}$$
(67)

The information loss $I_f^{qsp}(\rho)$ can be easily evaluated from Eq. (58), since all single-particle levels have probability 1/2 of being occupied:

$$I_f^{\rm qsp}(\rho) = 4 \left[2f\left(\frac{3w+1}{8}\right) - f\left(\frac{7w+1}{8}\right) - f\left(\frac{1-w}{8}\right) \right].$$
(68)

Figure 1 depicts this information loss in the von Neumann case $(f(p) = -p \log_2 p)$ and in the quadratic case (f(p) = 2p(1-p)), together with the corresponding entanglement of formations $S^{qsp}(\rho)$ and $S^{qsp}_2(\rho) = 4C^2(\rho)$, as a function of w. While there is a threshold value, w = 3/7, below which the state remains separable, $I_f^{qsp}(\rho) > 0$ as soon as ρ departs from the maximally mixed state, as given by Eq. (61), implying

that the information loss detects "nonclassical" correlations beyond entanglement. In addition, it is worth noting that while $I_2^{qsp}(\rho)$ is an upper bound to $S_2^{qsp}(\rho)$ for the present states $\forall w \in (0,1)$, this is not strictly the case for the von Neumann–based quantities, as $I^{qsp}(\rho) < S^{qsp}(\rho)$ for w below but very close to 1.

C. Two fermion states

We now assume $|\psi\rangle$ in (55) is a two-fermion state. These states are of the form,

$$|\psi\rangle = \frac{1}{2} \sum_{i,j} M_{ij} c_i^{\dagger} c_j^{\dagger} |0\rangle, \qquad (69)$$

where *M* is a $n \times n$ complex antisymmetric matrix satisfying $\frac{1}{2}$ Tr $MM^{\dagger} = 1$. As shown by Zumino in [50], for any such matrix there is a unitary matrix *U* such that $U^{\dagger}M\bar{U} = D$, where *D* is a block diagonal matrix with 2 × 2 blocks of the form,

$$D_k = \sqrt{\lambda_k} \begin{pmatrix} 0 & 1\\ -1 & 0 \end{pmatrix},\tag{70}$$

with λ_k a real number. With the corresponding unitary transformation c = Ua of the fermion operators, we can then split the sp space as $S = S_A \oplus S_B$ and rewrite the state (69) in the normal form,

$$|\psi\rangle = \sum_{k} \sqrt{\lambda_k} a_{k(A)}^{\dagger} a_{k(B)}^{\dagger} |0\rangle \,. \tag{71}$$

Equation (71) is the *Slater decomposition* [23] of $|\psi\rangle$, a fermionic analog (for two-fermion states) of the Schmidt decomposition for distinguishable bipartite systems. The associated one-body density matrix is

$$\rho^{\rm sp} = M M^{\dagger} = U D D^T U^{\dagger}, \tag{72}$$

which entails that the numbers λ_k are its *eigenvalues* (twofold degenerate), as is also evident from Eq. (71). The Slater basis then diagonalizes ρ^{sp} (and hence ρ^{qsp} , as there are here no pairing contractions). We then obtain $S^{\text{qsp}}(|\psi\rangle) = S^{\text{sp}}(|\psi\rangle) = 2\sum_k h(\lambda_k)$, which is the sum of the entanglement entropies of all sp modes of the Slater basis. We also have $S_f^{\text{sp}}(|\psi\rangle) = 2\sum_k f(\lambda_k) + f(1 - \lambda_k)$.

Let us now consider the one-body information loss $I_f^{\text{sp}}(\rho)$ for the ensuing mixture (55). Since the operators $a_{k(A)}$, $a_{k(B)}$ are the fermion operators where the one-body density matrix is diagonal, the measurement minimizing $I_f^{\text{sp}}(\rho)$ [which coincides here with $I^{\text{qsp}}(\rho)$] is that on the Slater basis of $|\psi\rangle$ and is then a function of the eigenvalues λ_k :

$$I_{f}^{\rm sp}(\rho) = 2\sum_{k} \left[f\left(w\lambda_{k} + \frac{1-w}{d}\right) + f\left(w(1-\lambda_{k}) + \frac{1-w}{d}\right) - f\left(w + \frac{1-w}{d}\right) - f\left(w + \frac{1-w}{d}\right) - f\left(\frac{1-w}{d}\right) \right], \quad (73)$$

with $d = 2^n$ in a grand canonical ensemble, $d = 2^{n-1}$ in an even parity ensemble, and $d = \frac{n(n-1)}{2}$ in a canonical ensemble. Present results are then formally similar to those obtained for

similar mixtures in bipartite distinguishable systems [14], with the Slater basis replacing the local Schmidt basis.

IV. CONCLUSIONS

We have discussed the problem of quantifying one-body discordlike correlations in general pure and mixed states of fermion systems, which may not have a fixed particle number (but which commute with the number parity). First, the correlation between a single-particle mode and its orthogonal complement in the single-particle state space S is considered. The measurement of the occupancy of a single-particle mode is properly defined and an entropic measure of the loss of information due to this projective measurement is introduced. The sum over all modes in a given basis of S of this quantity, minimized over all such bases, is defined as the one-body information loss, a measure of the minimum loss of information due to an unread measurement. It is a non-negative quantity, invariant under arbitrary unitary transformations in S, which vanishes if and only if the state of the system can be written as a convex combination of Slater determinants in a common basis of \mathcal{S} , i.e., if it remains invariant after the unread measurement of the occupancy of *any* sp level of this basis. For pure states it reduces to the fermionic entanglement entropy defined in [31]. These properties still hold if quasiparticle level occupancy measurements are allowed, in which case minimization is to be extended to all bases related through a Bogoliubov transformation. The defined quantities are then extended to more general entropic forms, including trace form entropies and quantum Renyi entropies. The general stationary condition to be satisfied by the minimizing measurement was also derived.

As application, we considered the mixture of a general pure state with the maximally mixed state for arbitrary space dimension. The minimum information loss was shown to be always reached for a measurement on the basis diagonalizing the generalized one-body density matrix, and to exhibit a universal quadratic initial increase with the mixing parameter, proportional to the quadratic entanglement entropy of the pure state. This fact implies that it can measure nonclassical correlations beyond entanglement, as explicitly verified for dim(S) = 4 (first nontrivial dimension for definite parity).

The approach can be applied in both canonical and grand-canonical ensembles, and for general states such as mixtures of independent quasiparticle states or vacua, being then suitable for studying correlations in strongly interacting fermion systems and requiring just an sp basis optimization. Its extension to more general partitions of the sp space may yield further insight into the structure of the state and is currently under investigation.

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APPENDIX: ENTANGLEMENT OF PARTITIONS OF THE FERMIONIC SINGLE-PARTICLE SPACE

We discuss here the entanglement associated with a general partition of a single-particle (sp) space S of a fermionic system.

Let us assume S is of dimension n, and consider a partition of S in two orthogonal subspaces S_A and S_B , generated, respectively, by m and n - m orthogonal sp states of a given basis of S, such that $S = S_A \oplus S_B$. Any Slater determinant in this basis can then be written, except for a global phase, as

$$|\psi_{sd}\rangle = \prod_{i \in S_A} (c_i^{\dagger})^{n_i} \prod_{j \in S_B} (c_j^{\dagger})^{n_j} |0\rangle \equiv |\mu\nu\rangle,$$

where $n_{i(j)} = 0, 1$ is the occupation number of level *i* (*j*) and $\mu = \{n_i, i \in S_A\}, \nu = \{n_j, j \in S_B\}$ indicate the collection of these numbers. The full set of states $|\mu\nu\rangle$, with $\mu = 1, \dots, 2^m$. $\nu = 1 \dots 2^{n-m}$, form an orthonormal basis of the full (grand canonical) space of many fermion states in S, of dimension $d = 2^n$. Any pure fermion state $|\psi\rangle$ with definite number parity can then be written as

$$|\psi\rangle = \sum_{\mu,\nu} C_{\mu\nu} |\mu\nu\rangle, \qquad (A1)$$

where the sum is restricted to states $|\mu\nu\rangle$ of the same number parity as $|\psi\rangle$ (i.e., $|++\rangle$ or $|--\rangle$ states for $|\psi\rangle$ of even parity). This implies that the matrix C of elements $C_{\mu\nu}$ is blocked in two submatrices (C^+ and C^-). After a singular value decomposition $C = UDV^{\dagger}$, with D a "diagonal" $2^m \times$ 2^{n-m} matrix of non-negative elements $D_{kl} = \sigma_k \delta_{kl}$, and U, Vunitary matrices, we may rewrite this state as

$$|\psi\rangle = \sum_{k} \sigma_{k} |k_{A}k_{B}\rangle, \tag{A2}$$

with $|k_A k_B\rangle = \sum_{\mu,\nu} U_{\mu k} V_{\nu k}^* |\mu \nu\rangle$ orthonormal states. This is the Schmidt decomposition associated with this partition. Of course, U and V are also blocked, so that all states $|k_A k_B\rangle$ have the same number parity as $|\psi\rangle$.

The entanglement entropy associated with the previous partition is then

$$E_{AB} = S(\rho_A) = S(\rho_B) = -\sum_k p_k \log_2 p_k,$$
 (A3)

with $p_k = \sigma_k^2$ the eigenvalues of CC^{\dagger} (or $C^{\dagger}C$) and

$$\rho_A = \sum_{\mu,\mu'} (CC^{\dagger})_{\mu\mu'} |\mu\rangle \langle \mu'| = \sum_k p_k |k_A\rangle \langle k_B|, \quad (A4)$$

$$\rho_B = \sum_{\nu,\nu'} (C^{\dagger}C)_{\nu\nu'} |\nu\rangle \langle\nu'| = \sum_k p_k |k_B\rangle \langle k_B|, \quad (A5)$$

the reduced states associated with subspaces S_A and S_B , such that any observable $O_{A(B)}$ containing operators c_i^{\dagger} , c_i with $i \in \mathcal{S}_{A(B)}$ can be obtained as

$$\langle O_{A(B)} \rangle = \text{Tr} \rho_{A(B)} O_{A(B)}.$$

A Slater determinant in a given sp basis is then completely separable, in the sense that $E_{AB} = 0$ for any bipartition (m,n-m) of S in this basis. On the other hand, if a state is not a Slater determinant there is no sp basis in which it is completely separable. Note that $\rho_{A(B)}$ commutes with number parity but will contain in general eigenstates of both parities.

In particular, if S_A contains just a single state (say k), Eq. (A1) becomes

$$\begin{aligned} |\psi\rangle &= \sum_{\nu} C_{0\nu} |0\nu\rangle + \sum_{\nu'} C_{1\nu'} |1\nu'\rangle \\ &= \sqrt{p_0} |0\psi_0\rangle + \sqrt{p_1} |1\psi_1\rangle, \end{aligned} \tag{A6}$$

where $p_i = \sum_{\nu} |C_{i\nu}|^2$ and $|i\psi_i\rangle = \sum_{\nu} C_{i\nu} |i\nu\rangle / \sqrt{p_i}$ for i =0,1. Equation (A6), equivalent to (4), is the Schmidt decomposition of $|\psi\rangle$ since the states $|\psi_0\rangle$ and $|\psi_1\rangle$ have opposite parity and are therefore orthogonal. The ensuing entanglement (A3) is then given by Eq. (8).

Let us now consider the entanglement of mixed states. If a partition of S_B in two subspaces S_{B_1} and S_{B_2} is made, we may define the associated entanglement of formation of ρ_B , $E_{B_1B_2}(\rho_B)$, as the minimum of the average entanglement entropies,

$$\sum_{\alpha} p_{\alpha} E_{B_1 B_2}(|\alpha\rangle \langle \alpha|) = \sum_{\alpha} p_{\alpha} S(\rho_{B_1}^{\alpha}), \qquad (A7)$$

over all decompositions $\rho_B = \sum_{\alpha} p_{\alpha} |\alpha\rangle \langle \alpha|$, with $p_{\alpha} \ge 0$, $\sum_{\alpha} p_{\alpha} = 1, \rho_{B_1}^{\alpha}$ the reduced state of B_1 in the state $|\alpha\rangle$ and $|\alpha\rangle$ normalized many-fermion states in S_B , with the restriction (since $[\rho_B, P_B] = 0$) that all states $|\alpha\rangle$ have definite number parity. This implies that $E_{B_1B_2}$ will be the average of the entanglement of formations for each parity, i.e., $E_{B_1B_2}(\rho_B) =$ $p_+E_{B_1B_2}(\rho_B^+) + p_-E_{B_1B_2}(\rho_B^-)$ if $\rho_B = p_+\rho_B^+ + p_-\rho_B^-$.

In particular, if S_A is a single state, Eq. (A6) leads to

$$\rho_B = p_0 |\psi_0\rangle \langle \psi_0| + p_1 |\psi_1\rangle \langle \psi_1|, \qquad (A8)$$

with $|\psi_0\rangle$ and $|\psi_1\rangle$ of opposite parity. Therefore, in this case the decomposition is unique and the entanglement of formation reads

$$E_{B_1B_2} = p_0 S(\rho_{B_1}^0) + p_1 S(\rho_{B_2}^1) = S(B_1|A), \quad (A9)$$

where $S(B_1|A)$, equivalent to Eq. (22), denotes the *conditional* entropy of subsystem B_1 after a measurement of the single level of A in the mixed state ρ_{AB_1} , in agreement with the general result of [39].

It is worth remarking that a general fermionic mixed state ρ_A defined over a given sp space S_A (and commuting with P) can be purified in many ways, but in particular (and efficiently) by the addition of a complementary fermionic sp space S_B , as is evident from the previous discussion. In a grand canonical context, if ρ_A is, say, of rank 2^n , with $2^n/2$ eigenstates of each parity, it is sufficient to add n orthogonal sp states generating an orthogonal sp space S_B , and then form a pure state like (A2) or (A1), which should have a definite number parity if physically realizable. If all eigenstates of ρ_A are of the same parity then n + 1 sp states should be added and just many-fermion states of definite parity should be considered.

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