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Entanglement in fermion systems

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We analyze the problem of quantifying entanglement in pure and mixed states of fermionic systems with a fixed number parity yet not necessarily a fixed particle number. The mode entanglement between one single-particle level and its orthogonal complement is first considered, and an entanglement entropy for such a partition of a particular basis of the single-particle Hilbert space $\mathcal{H}$ is defined. The sum over all single-particle modes of this entropy is introduced as a measure of the total entanglement of the system with respect to the chosen basis and it is shown that its minimum over all bases of $\mathcal{H}$ is a function of the one-body density matrix. Furthermore, we show that if minimization is extended to all bases related through a Bogoliubov transformation, then the entanglement entropy is a function of the generalized one-body density matrix. These results are then used to quantify entanglement in fermion systems with four single-particle levels. For general pure states of such a system a closed expression for the fermionic concurrence is derived, which generalizes the Slater correlation measure defined by J. Schliemann *et al.* [Phys. Rev. A **64**, 022303 (2001)], implying that particle entanglement may be seen as minimum mode entanglement. It is also shown that the entanglement entropy defined before is related to this concurrence by an expression analogous to that in the two-qubit case. For mixed states of this system the convex roof extension of the previous concurrence and entanglement entropy is evaluated analytically, extending the results in previous reference to general states.

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I. INTRODUCTION

Quantum entanglement is not only one of the key features of quantum mechanics but also an essential resource in quantum information processing [1]. It plays a central role in quantum teleportation [2] and quantum computation [3]. Consequently, the understanding and quantification of this resource have become a fundamental problem in quantum information theory [4]. They have also provided deep insights into the structure of correlations and quantum phase transitions in many-body systems [5–7].

If $|\Psi_{AB}\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$ is a pure state of a composite quantum system, its entanglement is quantified by the entanglement entropy $S(\rho_A) = S(\mathrm{Tr}_B|\Psi_{AB}\rangle\langle\Psi_{AB}|) = S(\rho_B)$, where $S(\rho) = -\mathrm{Tr}\rho\log_2\rho$ is the von Neumann entropy. It is then seen that the notion of entanglement in such systems relies on the tensor product structure of its state space [8]. In fermionic systems, however, the situation is less clear since the state space no longer has this structure due to indistinguishability.

When generalizing the notion of entanglement to systems of indistinguishable particles [9–18] mainly two approaches have been taken: *mode entanglement* [12–14,19,20] and *quantum correlations-particle entanglement* [9–11,15–18,21–23]. In the first case the parties share different modes of a given basis of the single-particle (SP) Hilbert space. Therefore, mode entanglement of a system does not remain invariant with respect to unitary transformations in the SP space. The second approach looks for correlations between particles and beyond antisymmetrization. In [9] and [11] a fermionic analog of the Schmidt decomposition and Schmidt number was introduced to quantify entanglement in two-fermion systems, and also a fermionic *concurrence* was defined. While these measures of entanglement remain invariant under unitary transformations in the SP space, they are restricted to states with a fixed particle number, which is not the general case in fermionic systems. The same problem arises in [15], where in order to share particles between parties it is necessary to project the original state onto subspaces with a definite particle number.

In this paper we first consider pure states of fermionic systems within a grand-canonical context, so the particle number is not necessarily fixed. Fermionic states with no fixed number of fermions arise, for instance, when considering the vacuum of quasiparticles defined through a Bogoliubov transformation [20,21,24], as well as by simply applying particle-hole transformations, such that the state is viewed as a vacuum of certain fermion operators plus particle-hole excitations. The fermion number parity of these states is nonetheless fixed, in agreement with fermionic superselection rules [25]. The entanglement between a single fermionic mode and the remaining SP orthogonal space in such states is first considered, and an entanglement entropy is defined in order to quantify these correlations. We then propose the sum over SP modes of this entropy as a measure of the total mode entanglement associated with the chosen SP basis and show that its minimum over all SP bases depends only on the eigenvalues of the one-body density matrix $\rho^{\mathrm{SP}}_{ij} = \langle c^\dagger_j c_i\rangle$, therefore being invariant under SP transformations. Furthermore, it is shown that if the minimization is extended to all quasiparticle bases, i.e., bases related through Bogoliubov transformations, the minimum entanglement entropy is just the von Neumann entropy of the generalized one-body density matrix ρ^{qsp}, which contains, in addition, the pair creation and annihilation contractions $\langle c^\dagger_j c^\dagger_i\rangle$ and $\langle c_j c_i\rangle$. Its convex roof extension for mixed states is also introduced. This quantity allows us to rigorously identify mixed states which cannot be written as convex mixtures of Slater determinants or quasiparticle vacua (or, in general, fermionic Gaussian states [21,22]), like thermal states of interacting fermion systems

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at sufficiently low temperatures, quantifying their quantum correlations.

We then focus on fermionic systems with SP space dimension 4. For general states it is shown that the minimum over all quasiparticle bases of the entanglement entropy can be written in terms of a fermionic analog of the concurrence [22,23,26], which reduces to the Slater correlation measure defined in [9] and [11] for two-fermion states. Its convex roof extension for mixed states is also evaluated analytically, extending explicitly the results in [9] to arbitrary mixed states with a fixed number parity. This allows us to evaluate in closed form the convex roof extension of the previous entanglement entropy. A simple illustrative example is provided.

II. FORMALISM

A. Single-level entanglement entropy

We start by considering a pure state $|\Psi\rangle$ of a fermion system with an n-dimensional SP Hilbert space $\mathcal{H}$. The system is described by a set of fermion annihilation and creation operators $\{c_j,c_j^\dagger\}$ satisfying

$$c_ic_j+c_jc_i=0,\quad c_ic_j^\dagger+c_j^\dagger c_i=\delta_{ij}, \tag{1}$$

such that $\{c_j^\dagger|0\rangle, j=1,\dots,n\}$ is an orthonormal basis of SP states ($|0\rangle$ denotes the vacuum of the operators c_j). We work within a general grand-canonical context, in which $|\Psi\rangle$ is not necessarily a state with a definite value of the fermion number $N=\sum_j c_j^\dagger c_j$. It may be, for instance, a vacuum of quasiparticle operators a_ν, related to the c_j's through a Bogoliubov transformation [24]. In this case, it is a sum of pure states with different fermion numbers (see Appendix), yet all having the same number parity,

$$P=\exp\left[i\pi\sum_j c_j^\dagger c_j\right], \tag{2}$$

such that $P|\Psi\rangle=\pm|\Psi\rangle$. Let us also recall that the elementary particle-hole Bogoliubov transformation

$$c_j\to c_j^\dagger,\quad c_j^\dagger\to c_j \tag{3}$$

leaves the anticommutation relations unchanged, so that, formally, it is a matter of choice whether one considers the particles or the holes as the "true" fermions. We take this basic symmetry into account in all the following correlation measures, such that they all remain invariant under the previous transformation. We just assume that all pure states involved have a definite number parity [25], which implies that $\langle c_j\rangle=0$ and also $\langle O\rangle=0$ for any operator O which is a product of an odd number of fermion operators c_j, $c_j^\dagger$.

We now consider a partition (A,B) of $\mathcal{H}$, where A denotes the single mode or "level" j, and B the remaining orthogonal SP space. Equation (1) implies that the operators,

$$\Pi_j=c_j^\dagger c_j,\quad \Pi_{\bar{j}}=c_jc_j^\dagger,\quad \Pi_j+\Pi_{\bar{j}}=1, \tag{4}$$

constitute a basic set of orthogonal projectors, defining a standard projective measurement on level j. Accordingly, we may decompose any state $|\Psi\rangle$ as

$$|\Psi\rangle=c_j^\dagger c_j|\Psi\rangle+c_jc_j^\dagger|\Psi\rangle \tag{5}$$
$$=\sqrt{p_j}\,|\Psi_j\rangle+\sqrt{p_{\bar{j}}}\,|\Psi_{\bar{j}}\rangle, \tag{6}$$

where the first (second) term in (5) selects the component of $|\Psi\rangle$ where state j is occupied (empty) and $|\Psi_j\rangle=\frac{1}{\sqrt{p_j}}c_j^\dagger c_j|\Psi\rangle$ and $|\Psi_{\bar{j}}\rangle=\frac{1}{\sqrt{p_{\bar{j}}}}c_jc_j^\dagger|\Psi\rangle$ are the corresponding normalized states. Here p_j ($p_{\bar{j}}$) is the probability of finding level j occupied (empty) in $|\Psi\rangle$:

$$p_j=\langle\Psi|c_j^\dagger c_j|\Psi\rangle,\quad p_{\bar{j}}=\langle\Psi|c_jc_j^\dagger|\Psi\rangle=1-p_j. \tag{7}$$

For an operator O_A depending just on c_j and $c_j^\dagger$, and O_B depending just on the complementary set $\{c_k,c_k^\dagger,k\neq j\}$, we then obtain, assuming $P|\Psi\rangle=\pm|\Psi\rangle$,

$$\langle\Psi|O_{A(B)}|\Psi\rangle=p_j\langle\Psi_j|O_{A(B)}|\Psi_j\rangle+p_{\bar{j}}\langle\Psi_{\bar{j}}|O_{A(B)}|\Psi_{\bar{j}}\rangle$$
$$=\mathrm{tr}_{A(B)}\rho_{A(B)}O_{A(B)}, \tag{8}$$

where $\rho_A=p_jc_j^\dagger|0\rangle\langle 0|c_j+p_{\bar{j}}|0\rangle\langle 0|$ and $\rho_B=p_jc_j|\Psi_j\rangle\langle\Psi_j|c_j^\dagger+p_{\bar{j}}|\Psi_{\bar{j}}\rangle\langle\Psi_{\bar{j}}|$ represent reduced density operators for systems A and B, respectively.

The entanglement between A and B can then be quantified by the entropy of the elementary distribution $\{p_j,p_{\bar{j}}=1-p_j\}$,

$$S(\rho_A)=S(\rho_B)=-p_j\log_2 p_j-(1-p_j)\log_2(1-p_j) \tag{9}$$
$$=h(p_j), \tag{10}$$

where $S(\rho)=-\mathrm{Tr}\rho\log_2\rho$ is the von Neumann entropy and $h(p)=-p\log_2 p-(1-p)\log_2(p)$ $[0\leqslant h(p)\leqslant 1]$. This entropy remains obviously invariant after a particle-hole transformation, (3). For a pure state $|\Psi\rangle$, Eq. (9) vanishes *if and only if* (iff) $|\Psi\rangle$ is separable with respect to this level, i.e., iff the level j is either occupied ($p_j=1$) or empty ($p_j=0$) in $|\Psi\rangle$, such that $|\Psi\rangle=c_j^\dagger c_j|\Psi\rangle$ or $|\Psi\rangle=c_jc_j^\dagger|\Psi\rangle$, respectively. Its maximum value 1 is attained for $p_j=1/2$.

B. One-body entanglement entropy

The sum

$$S_{\boldsymbol{c}}=\sum_j h(p_j) \tag{11}$$

is a measure of the entanglement associated with the SP basis determined by the operators $c_j^\dagger$. Equation (11) vanishes iff each level j of this basis is disentangled from its complementary SP space, i.e., iff each level is either occupied or empty in $|\Psi\rangle$, such that $|\Psi\rangle$ is a Slater determinant in this basis, $|\Psi\rangle=c_{j_1}^\dagger\dots c_{j_m}^\dagger|0\rangle$, for some subset of levels $\{j_1,\dots,j_m\}$.

Equation (11) depends on the choice of SP basis, i.e., on the choice of fermion operators $\boldsymbol{c}=(c_1\dots,c_n)^T$. We now consider the minimum of (11) over all SP bases of $\mathcal{H}$, i.e.,

$$S^{\rm SP}=\mathop{\rm Min}_{\boldsymbol{c}'}S_{\boldsymbol{c}'}, \tag{12}$$

where $S_{\boldsymbol{c}'}=\sum_j h(p'_j)$, with $p'_j=\langle\Psi|c'^\dagger_jc'_j|\Psi\rangle$ and $\boldsymbol{c}'=(c'_1,\dots,c'_n)^T$ an arbitrary set of fermion operators related to the c_j's through a unitary transformation,

$$\boldsymbol{c}' = U^\dagger \boldsymbol{c}\,, \tag{13}$$

with U an $n\times n$ unitary matrix [such that the fermionic relations (1) are preserved]. Equation (12) vanishes *iff* $|\Psi\rangle$ *is a Slater determinant*, i.e., $|\Psi\rangle = c'^\dagger_{k_1}\dots c'^\dagger_{k_m}|0\rangle$ for some operators c'_k of the form (13). Hence, $S^{\rm SP}=0$ iff there is an SP basis where every level is disentangled from its complementary SP space.

Defining the SP density matrix $\rho^{\rm SP} = 1-\langle \boldsymbol{c}\boldsymbol{c}^\dagger\rangle$ (with $\langle O\rangle \equiv \langle\Psi|O|\Psi\rangle$), of elements

$$\rho^{\rm SP}_{ij} = \langle c^\dagger_j c_i\rangle, \tag{14}$$

it is seen that the minimum, (12), is reached for those operators $\boldsymbol{c}'$ which *diagonalize* $\rho^{\rm SP}$, i.e., satisfying

$$\langle c'^\dagger_k c'_l\rangle = (U^\dagger\rho^{\rm SP}U)_{lk} = p'_k\delta_{kl}, \tag{15}$$

with p'_k the eigenvalues of $\rho^{\rm SP}$.

Proof. Equations (13)–(15) imply that $p_j = \rho^{\rm SP}_{jj} = \sum_k |U^2_{jk}|p'_k$. Hence, concavity of the function $h(p)$ entails $\sum_j h(p_j) \geqslant \sum_{j,k}|U^2_{jk}|h(p'_k) = \sum_k h(p'_k)$, with equality reached iff the p_j's are already the eigenvalues of $\rho^{\rm SP}$. ■

The minimum value (12) can then be expressed as

$$S^{\rm SP} = \sum_k h(p'_k) = {\rm tr}\, h(\rho^{\rm SP})\,, \tag{16}$$

being now apparent that $S^{\rm SP}$ vanishes iff the eigenvalues p'_k are either 0 or 1, i.e., iff $(\rho^{\rm SP})^2 = \rho^{\rm SP}$, a condition ensuring that $|\Psi\rangle$ is a Slater determinant [24].

Equation (16) has, in addition, the obvious meaning of quantifying how mixed or "hot" is $|\Psi\rangle$ with respect to the set of all one-body operators of the form

$$O = \sum_{i,j} o_{ij} c^\dagger_i c_j, \tag{17}$$

since their averages are completely determined just by $\rho^{\rm SP}$: $\langle\Psi|O|\Psi\rangle = {\rm tr}\,\rho^{\rm SP} o$. Accordingly, $S^{\rm SP}$ remains invariant under one-body unitary transformations $|\Psi\rangle \to \exp(-iO)|\Psi\rangle$, with O any Hermitian one-body operator of the form (17), since they lead to a unitary transformation of $\rho^{\rm SP}$ ($\rho^{\rm SP}\to U\rho^{\rm SP}U^\dagger$, with $U = e^{-io}$) and hence do not affect its eigenvalues.

C. Generalized one-body entanglement entropy

A quasiparticle vacuum, for instance, a superfluid or superconducting state in the BCS approximation [24], will lead to $S^{\rm SP}>0$, since $\rho^{\rm SP}$ will be *mixed*, i.e., it will have eigenvalues distinct from 0 or 1 (see Appendix). If fermion quasiparticles are to be allowed, we can extend the minimization in (12) to *all single-quasiparticle bases*, i.e.,

$$S^{\rm qsp} = \underset{\boldsymbol{a}}{\rm Min}\, S_{\boldsymbol{a}}, \tag{18}$$

where $S_{\boldsymbol{a}} = \sum_\nu h(\langle a^\dagger_\nu a_\nu\rangle)$ and $\boldsymbol{a}$ denotes a set of fermion operators a_ν linearly related to the original operators c_j, $c^\dagger_j$ through a general *Bogoliubov transformation* [24]:

$$a_\nu = \sum_j \bar U_{j\nu} c_j + V_{j\nu} c^\dagger_j\,. \tag{19}$$

Equation (19) can be written as

$$\begin{pmatrix}\boldsymbol{a}\\ \boldsymbol{a}^\dagger\end{pmatrix} = \mathcal{W}^\dagger\begin{pmatrix}\boldsymbol{c}\\ \boldsymbol{c}^\dagger\end{pmatrix},\quad \mathcal{W} = \begin{pmatrix}U & V\\ \bar V & \bar U\end{pmatrix}, \tag{20}$$

where the $2n\times 2n$ matrix $\mathcal{W}$ should be unitary (i.e., $UU^\dagger + VV^\dagger = 1$, $UV^T + VU^T = 0$) in order for the operators a_ν, $a^\dagger_\mu$ to fulfill the fermionic anticommutation relations, (1).

One should then consider the *extended* $2n\times 2n$ density matrix

$$\rho^{\rm qsp} = 1 - \left\langle \begin{pmatrix}\boldsymbol{c}\\ \boldsymbol{c}^\dagger\end{pmatrix}\begin{pmatrix}\boldsymbol{c}^\dagger & \boldsymbol{c}\end{pmatrix}\right\rangle = \begin{pmatrix}\rho^{\rm SP} & \kappa\\ -\bar\kappa & 1-\bar\rho^{\rm SP}\end{pmatrix}, \tag{21}$$

where κ is an $n\times n$ antisymmetric matrix containing the pair annihilation averages

$$\kappa_{ij} = \langle c_j c_i\rangle, \tag{22}$$

with $-\bar\kappa_{ij} = \langle c^\dagger_j c^\dagger_i\rangle$ and $(1-\bar\rho^{\rm SP})_{ij} = \langle c_j c^\dagger_i\rangle$. Equation (21) is a Hermitic matrix which can always be diagonalized by a suitable transformation, (20), such that

$$1 - \left\langle \begin{pmatrix}\boldsymbol{a}\\ \boldsymbol{a}^\dagger\end{pmatrix}\begin{pmatrix}\boldsymbol{a} & \boldsymbol{a}^\dagger\end{pmatrix}\right\rangle = \mathcal{W}^\dagger\rho^{\rm qsp}\mathcal{W} = \begin{pmatrix}f & 0\\ 0 & 1-f\end{pmatrix}, \tag{23}$$

with $f_{\mu\nu} = f_\nu\delta_{\mu\nu}$ and f_ν, $1-f_\nu$ the eigenvalues of $\rho^{\rm qsp}$ (which always come in pairs $(f_\nu, 1-f_\nu)$, with $f_\nu\in[0,1]$), entailing

$$\langle a^\dagger_\nu a_\mu\rangle = \delta_{\mu\nu} f_\nu,\quad \langle a_\mu a_\nu\rangle = 0. \tag{24}$$

It can then be easily shown that the minimum, (18), is

$$S^{\rm qsp} = -\sum_\nu f_\nu\log_2 f_\nu + (1-f_\nu)\log_2(1-f_\nu) \tag{25}$$

$$= -{\rm tr}'\,\rho^{\rm qsp}\log_2\rho^{\rm qsp}, \tag{26}$$

where ${\rm tr}'$ denotes the trace in the extended SP space.

Proof. Since both $p_j = \langle c^\dagger_j c_j\rangle$ and $1-p_j$ are the diagonal elements of $\rho^{\rm qsp}$, denoting by q_j and λ_ν the full set of diagonal elements and eigenvalues of $\rho^{\rm qsp}$, we obtain $q_j = \sum_\nu |\mathcal{W}^2_{j\nu}|\lambda_\nu$, and hence, due to the concavity of $f(p) = -p\log_2 p$, $S_{\boldsymbol{c}} = \sum_j f(q_j) \geqslant \sum_{j,\nu}|\mathcal{W}^2_{j\nu}|f(\lambda_\nu) = \sum_\nu f(\lambda_\nu) = S^{\rm qsp}$. ■

Equation (26) vanishes iff f_ν is either 0 or 1 for all ν, i.e., *iff* $|\Psi\rangle$ *is a particle or quasiparticle Slater determinant*. By an elementary particle-hole transformation we can always change such a state to a quasiparticle vacuum, so that we can say $S^{\rm qsp}=0$ iff $|\Psi\rangle$ is a quasiparticle vacuum. In other words, $S^{\rm qsp}=0$ iff there is a single-quasiparticle basis where *every* level is disentangled from the rest.

Equation (18) also measures the mixedness of $|\Psi\rangle$ with respect to the set of all *generalized one-body operators*, of the form

$$O = \sum_{i,j} o^{11}_{ij} c^\dagger_i c_j + \frac{1}{2}\left(o^{20}_{ij} c_i c_j + o^{02}_{ij} c^\dagger_i c^\dagger_j\right) - \frac{1}{2}{\rm tr}\, o^{11} \tag{27}$$

$$= \frac{1}{2}(\boldsymbol{c}^\dagger\, \boldsymbol{c})\mathcal{O}\begin{pmatrix}\boldsymbol{c}\\ \boldsymbol{c}^\dagger\end{pmatrix},\quad \mathcal{O} = \begin{pmatrix}o^{11} & o^{02}\\ o^{20} & -(o^{11})^T\end{pmatrix}, \tag{28}$$

i.e., general quadratic functions of $\boldsymbol{c}$, $\boldsymbol{c}^\dagger$ [the constant term in (27) is just added for convenience], since their averages are completely determined by $\rho^{\rm qsp}$:

$$\langle\Psi|O|\Psi\rangle = {\rm tr}\big[\rho^{\rm SP}o^{11} - \tfrac{1}{2}o^{11} + \tfrac{1}{2}(\kappa o^{20} - \bar{\kappa}o^{02})\big] = \tfrac{1}{2}{\rm tr}'\,\rho^{\rm qsp}\mathcal{O}. \quad (29)$$

The present scheme allows us then to properly treat states which do not have a definite fermion number and lead to nonzero contractions $\langle c_i c_j\rangle$. The whole formalism then becomes strictly invariant under arbitrary particle-hole transformations, (3), applied to some subset of levels, which will move elements from $\rho^{\rm SP}$ to κ, and vice versa, but which will not alter the spectrum of $\rho^{\rm qsp}$. The latter remains actually invariant under *arbitrary quasiparticle unitary transformations* $|\Psi\rangle \to \exp[-iO]|\Psi\rangle$, where O is a Hermitian generalized one-body operator of the form (27), since they just lead to a unitary transformation of $\rho^{\rm qsp}$, i.e., $\rho^{\rm qsp} \to \mathcal{W}\rho^{\rm qsp}\mathcal{W}^\dagger$, with $\mathcal{W} = e^{-i\mathcal{O}}$.

We note that a transformation $a_\nu \leftrightarrow a_\nu^\dagger$ obviously changes $f_\nu \leftrightarrow 1 - f_\nu$, so that there is no unique way to select which of the eigenvalues of $\rho^{\rm qsp}$ will be the f_ν's or the $1 - f'_\nu s$. One can choose the f_ν's as the lowest eigenvalues (such that $|\Psi\rangle$ becomes a quasiparticle vacuum when $S^{\rm qsp} = 0$), but it is also possible to set ${\rm Det}[U] \neq 0$, which ensures that the vacuum of the a_ν has the same number parity as $|0\rangle$ [Eq. (A1)]. These choices do not affect the entropy $S^{\rm qsp}$. We also remark that the maximally entangled state, i.e., that with the maximum $S^{\rm qsp}$, corresponds to the exceptional case $f_\nu = 1/2\ \forall\ \nu$, where $S^{\rm qsp} = n$ and $\rho^{\rm qsp} = I_{2n}/2$ becomes proportional to the identity matrix, then remaining invariant under *any* Bogoliubov transformation.

D. Generalized entropic inequalities and quadratic entropy

From their definitions, it follows that the entropies (11), (16), and (26) satisfy the inequality chain

$$S_c \geqslant S^{\rm SP} \geqslant S^{\rm qsp}. \quad (30)$$

Equation (30) actually holds for more general entropic forms. If $\tilde{\rho}^{\rm SP} = \begin{pmatrix}\rho^{\rm SP} & 0\\ 0 & 1-\rho^{\rm SP}\end{pmatrix}$ is the extended $\rho^{\rm SP}$ and $\tilde{\rho}^{\rm SP}_d$ the diagonal of $\tilde{\rho}^{\rm SP}$, we obtain, with the same previous arguments,

$$S_f\big(\tilde{\rho}^{\rm SP}_d\big) \geqslant S_f(\tilde{\rho}^{\rm SP}) \geqslant S_f(\rho^{\rm qsp}), \quad (31)$$

where

$$S_f(\rho) = {\rm tr}\, f(\rho), \quad (32)$$

with $f : [0,1] \to \mathbb{R}$ a strictly concave function satisfying $f(0) = f(1) = 0$, represents a generalized entropic form [27,28]. Moreover, these matrices fulfill the majorization relation [29]

$$\tilde{\rho}^{\rm SP}_d \prec \tilde{\rho}^{\rm SP} \prec \rho^{\rm qsp}, \quad (33)$$

where $\rho \prec \rho'$ means here $\sum_{i=1}^j \lambda_i \leqslant \sum_{i=1}^j \lambda'_i$ for $j = 1,\ldots,2n-1$, with λ_i and λ'_i the eigenvalues of ρ and ρ' sorted in decreasing order, since the sorted set of diagonal elements in an orthonormal basis of a Hermitian operator is always majorized by the sorted set of its eigenvalues [29]. Equation (33) allows us to extend (31) to any Schur-concave function [29] of the extended density matrices.

A particularly useful example, which plays an important role in the next section, is the quadratic entropy $S_2(\rho)$ (also denoted the linear entropy), obtained for $f(p) = 2p(1-p)$,

$$S_2(\rho^{\rm qsp}) = 2\,{\rm tr}'\,[\rho^{\rm qsp}(1-\rho^{\rm qsp})] = 4\,{\rm tr}[\rho^{\rm SP}(1-\rho^{\rm SP}) - \kappa^\dagger\kappa] \quad (34)$$

$$= 4\sum_\nu f_\nu(1-f_\nu), \quad (35)$$

where the factor 2 has been chosen such that its maximum value for a single level is 1. Unlike the von Neumman entropy, (26), $S_2(\rho^{\rm qsp})$ can be evaluated just by taking the trace in (34), without explicit knowledge of the eigenvalues f_ν of $\rho^{\rm qsp}$. Yet, like $S^{\rm qsp}$, it is non-negative and vanishes iff $|\Psi\rangle$ is a quasiparticle vacuum or Slater determinant. Equation (31) implies, in particular, that $\sum_j p_j(1-p_j) \geqslant \sum_k p'_k(1-p'_k) \geqslant \sum_\nu f_\nu(1-f_\nu)$.

E. Mixed states

Let us now consider mixed fermion states, assumed to be convex mixtures of pure states with definite number parity, i.e.,

$$\rho = \sum_i q_i|\Psi_i\rangle\langle\Psi_i|, \quad (36)$$

where $q_i \geqslant 0$, $\sum_i q_i = 1$, and $P|\Psi_i\rangle = \pm|\Psi_i\rangle$, such that $[\rho,P] = 0$. We can define an entanglement measure for these mixed states in a way similar to the entanglement of formation [30,31], through the convex roof extension of $S^{\rm qsp}$,

$$E^{\rm qsp}(\rho) = \underset{\{q'_i,|\Psi'_i\rangle\}}{\rm Min}\sum_i q'_i S^{\rm qsp}(|\Psi'_i\rangle), \quad (37)$$

where $\rho = \sum_i q'_i|\Psi'_i\rangle\langle\Psi'_i|$, $q'_i \geqslant 0$, and the minimization is over all decompositions of ρ as convex mixtures of pure states, assumed, again, to be of definite number parity. Equation (37) vanishes *iff ρ is a convex mixture of particle or quasiparticle Slater determinants*, i.e., of suitable quasiparticle vacua, and reduces to $S^{\rm qsp}$ for pure states. This quantity is evaluated exactly in the particular system in the next section.

As a general application of $E^{\rm qsp}$, let us consider an interacting fermion system at finite temperature T. For attractive two-body couplings, the static path approximation (SPA) [32,33] will lead to a classically correlated density operator $\rho_{\rm SPA}$, which is a convex mixture of (noncommuting) thermal states diagonal in a basis of particle or quasiparticle Slater determinants, associated with different values of the running effective order parameters. Hence, $E^{\rm qsp}(\rho_{\rm SPA}) = 0$, in agreement with the fact that $\rho_{\rm SPA}$ contains just static fluctuations around the mean field. This correlated but still unentangled approximation can be derived from the auxiliary field path integral representation [34] and becomes exact at sufficiently high T [33]. Its breakdown at low T reflects the onset of entanglement, i.e., of a finite value of $E^{\rm qsp}(\rho)$. Equation (37) defines a limit temperature T_L above which $E^{\rm qsp} = 0$. Mixtures of fermionic Gaussian states are also important in noisy fermionic quantum computation models [22,35].

III. THE CASE OF FOUR SINGLE-PARTICLE LEVELS

We now examine in detail the special case of a fermion system with SP space dimension $n = 4$. This is the lowest dimension at which nontrivial fermionic entanglement arises, i.e., at which $S^{\rm qsp}$ can be nonzero, as will be verified. We extend the results in [9], which considered just pure or mixed states with a definite fermion number, to general states which do not necessarily have a definite fermion number, yet still have a definite number parity P. This SP space can accommodate eight linearly independent pure states of the same number parity, so that the Hilbert-space dimension for fixed P is 8.

A. Pure states

1. Odd-parity states

We first consider pure states $|\Psi\rangle$ of this system with odd number parity: $P|\Psi\rangle = -|\Psi\rangle$. These states are then linear combinations of single-fermion states and three-fermion states, so a general odd state can be written as (Fig. 1, top)

$$|\Psi\rangle = \sum_{i=1}^{4}(\alpha_i c_i^\dagger|0\rangle + \bar{\beta}_i c_i|\bar{0}\rangle), \tag{38}$$

where $|\bar{0}\rangle = c_1^\dagger c_2^\dagger c_3^\dagger c_4^\dagger|0\rangle$ is the completely occupied state and $|\boldsymbol{\alpha}|^2 + |\boldsymbol{\beta}|^2 = 1$, with $\boldsymbol{\alpha}$, $\boldsymbol{\beta}$ four-dimensional complex vectors. It is easily seen that the single-hole states $c_i|\bar{0}\rangle$ are

$$c_i|\bar{0}\rangle = \frac{1}{3!}\sum_{j,k,l}\epsilon_{ijkl}c_j^\dagger c_k^\dagger c_l^\dagger|0\rangle, \tag{39}$$

where ϵ_{ijkl} denotes the completely antisymmetric Levi-Civita tensor in dimension 4. The elements of the generalized one-body density matrix, (21), are then given by

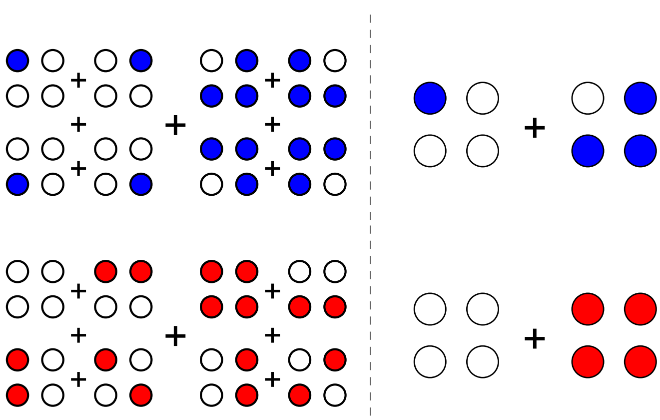

FIG. 1. (Color online) Schematic representation of pure fermion states with odd (top) or even (bottom) number parity. A general state with a definite number parity is a superposition of the eight states indicated to the left of the dashed vertical line, where a filled circle indicates an occupied level. In the normal form ($\rho^{\rm qsp}$ diagonal), obtained after a suitable Bogoliubov transformation, it can be reduced to the superposition of two states like those indicated on the right. The state is entangled (in the sense of not being a quasiparticle vacuum or Slater determinant) iff the product C [Eq. (43)] of the coefficients of the left and right groups of four states is nonzero, implying nonzero weight for both states of the normal representation.

$$\rho_{ij}^{\rm SP} = \langle c_j^\dagger c_i\rangle = \alpha_i\bar{\alpha}_j - \beta_i\bar{\beta}_j + |\boldsymbol{\beta}|^2\delta_{ij}, \tag{40}$$

$$\kappa_{ij} = \langle c_j c_i\rangle = \sum_{k,l}\epsilon_{ijkl}\bar{\alpha}_l\bar{\beta}_k, \tag{41}$$

i.e., $\rho^{\rm SP} = \boldsymbol{\alpha}\boldsymbol{\alpha}^\dagger - \boldsymbol{\beta}\boldsymbol{\beta}^\dagger + |\boldsymbol{\beta}|^2 I_4$. We now show that the ensuing eigenvalues f_ν of the 8×8 matrix $\rho^{\rm qsp}$ are *fourfold degenerate* and given by

$$f_\pm = \frac{1\pm\sqrt{1-C^2(|\Psi\rangle)}}{2}, \tag{42}$$

where $C(|\Psi\rangle)$ is fully determined by the S_2 entropy, (34),

$$C(|\Psi\rangle) = \sqrt{S_2(\rho^{\rm qsp})/4} = \sqrt{{\rm tr}\,[\rho^{\rm SP}(I_4-\rho^{\rm SP})-\kappa^\dagger\kappa]}$$
$$= 2|\boldsymbol{\beta}^\dagger\boldsymbol{\alpha}| = 2|\sum_{i=1}^{4}\bar{\beta}_i\alpha_i|, \tag{43}$$

and plays the role of a pure-state fermionic concurrence. It satisfies $0 \leqslant C \leqslant 1$, and as shown in the next subsection, it is the generalization of the Slater correlation measure defined in [9] and [11] for two fermion states. It also coincides with the quadratic invariant derived in [23] using a spinor classification-based approach. The entanglement entropy, (25), becomes

$$S^{\rm qsp} = 4h(f_+) = -4(f_+\log_2 f_+ + f_-\log_2 f_-). \tag{44}$$

Proof. We first consider a unitary transformation $\boldsymbol{c}\to U\boldsymbol{c}$ of the operators c_j, such that

$$\boldsymbol{\alpha}\to U^\dagger\boldsymbol{\alpha},\quad \boldsymbol{\beta}\to {\rm Det}[U^\dagger]U^\dagger\boldsymbol{\beta} \tag{45}$$

in (38), which does not affect the value of $C(|\Psi\rangle)$ [Eq. (43)]. By choosing an orthonormal basis of $\mathbb{C}^4$ such that the original vectors $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ are generated by the first two elements [for instance, $\boldsymbol{e}_1\propto\boldsymbol{\alpha}$ and $\boldsymbol{e}_2\propto\boldsymbol{\beta}-(\boldsymbol{\alpha}^\dagger\boldsymbol{\beta})\boldsymbol{\alpha}/|\boldsymbol{\alpha}|^2$], we can use this first transformation to set $\alpha_3=\alpha_4=0$, $\beta_3=\beta_4=0$ in the new basis. In this case, Eqs. (40) and (41) lead to

$$\rho^{\rm SP} = \begin{pmatrix}|\alpha_1|^2+|\beta_2|^2 & \alpha_1\bar{\alpha}_2-\beta_1\bar{\beta}_2 & 0 & 0\\ \alpha_2\bar{\alpha}_1-\beta_2\bar{\beta}_1 & |\alpha_2|^2+|\beta_1|^2 & 0 & 0\\ 0 & 0 & |\boldsymbol{\beta}|^2 & 0\\ 0 & 0 & 0 & |\boldsymbol{\beta}|^2\end{pmatrix},$$

$$\kappa = \begin{pmatrix}0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0\\ 0 & 0 & 0 & \bar{\alpha}_2\bar{\beta}_1-\bar{\alpha}_1\bar{\beta}_2\\ 0 & 0 & \bar{\alpha}_1\bar{\beta}_2-\bar{\alpha}_2\bar{\beta}_1 & 0\end{pmatrix}. \tag{46}$$

It is then seen that the diagonalization of $\rho^{\rm qsp}$ is achieved through (i) a unitary transformation of the operators c_1, c_2,

$$c_1 = ua_1 + va_2,\quad c_2 = -\bar{v}a_1 + ua_2, \tag{47}$$

with ${}^{\;u}_{|v|} = \sqrt{\frac{f_+-f_-\pm 2\epsilon}{2(f_+-f_-)}}$ and $\epsilon = |\alpha_1^2|+|\beta_2^2|-\frac{1}{2}$, which diagonalizes the first 2×2 block of $\rho^{\rm SP}$ and $1-\bar{\rho}^{\rm SP}$; plus (ii) a Bogoliubov transformation of the operators c_3, c_4,

$$c_3 = u'a_3 + v'a_4^\dagger,\quad c_4^\dagger = -\bar{v}'a_3 + u'a_4^\dagger, \tag{48}$$

with ${}^{\;u'}_{|v'|} = \sqrt{\frac{f_+-f_-\pm 2\epsilon'}{2(f_+-f_-)}}$ and $\epsilon' = |\boldsymbol{\beta}^2|-\frac{1}{2}$, which diagonalizes the rest of $\rho^{\rm qsp}$, comprising, again, two 2×2 blocks $\left(\begin{smallmatrix}|\boldsymbol{\beta}|^2 & \pm\kappa_{34}\\ \pm\bar{\kappa}_{34} & |\boldsymbol{\alpha}|^2\end{smallmatrix}\right)$.

These four 2×2 blocks all have trace 1 and determinant $C^2(|\Psi\rangle)/4$, leading then to the *same* eigenvalues $f_\pm$ of Eq. (42) (a 2×2 matrix with trace t and determinant d has eigenvalues $\frac{t\pm\sqrt{t^2-4d}}{2}$). ■

Note from (46) that if $\rho^{\rm qsp}$ is diagonal ($\rho^{\rm SP}$ diagonal and $\kappa=0$) and $C(|\Psi\rangle)<1$, then necessarily $\alpha_2=\beta_2=0$ or $\alpha_1=\beta_1=0$ in (46). This implies that after the previous transformations, $|\Psi\rangle$ can be written in the normal form (top-right scheme in Fig. 1),

$$|\Psi\rangle=\alpha' a_1^\dagger|0_{\boldsymbol a}\rangle+\bar\beta' a_1|\bar 0_{\boldsymbol a}\rangle, \tag{49}$$

i.e., $\boldsymbol\beta'\propto\boldsymbol\alpha'$, with $|0_{\boldsymbol a}\rangle$ the vacuum of the $\boldsymbol a$ operators, $|\bar 0_{\boldsymbol a}\rangle=a_1^\dagger a_2^\dagger a_3^\dagger a_4^\dagger|0_{\boldsymbol a}\rangle$, and $|\alpha'|^2=f_+$, $|\beta'|^2=f_-$ if $|\alpha'|\geqslant|\beta'|$, such that $C(|\Psi\rangle)=2|\alpha'\bar\beta'|$. This state leads to

$$\rho_a^{\rm qsp}=1-\left\langle\begin{pmatrix}\boldsymbol a\\ \boldsymbol a^\dagger\end{pmatrix}(\boldsymbol a^\dagger\quad \boldsymbol a)\right\rangle =\begin{pmatrix}|\alpha'|^2&0&0&0\\0&|\beta'|^2I_3&0&0\\0&0&|\beta'|^2&0\\ &0&0&|\alpha'|^2I_3\end{pmatrix}.$$

On the other hand, in the maximally entangled case $C(|\Psi\rangle)=1$, $f_\pm=1/2$ and $\rho^{\rm qsp}=I_8/2$ in *any* basis, i.e., after *any* Bogoliubov transformation. In this case $\boldsymbol\beta=e^{i\phi}\boldsymbol\alpha$, with $|\boldsymbol\alpha|=|\boldsymbol\beta|=1/\sqrt2$, and the form (49) is obtained just by choosing $\boldsymbol e_1$ in the direction of $\boldsymbol\alpha$.

It is apparent that if $\boldsymbol\beta=\boldsymbol 0$ in (38), $|\Psi\rangle$ can be written as a single-fermion state $a_1^\dagger|0\rangle$, where $a_1^\dagger=\sum_i\alpha_i c_i^\dagger$. Similarly, if $\boldsymbol\alpha=\boldsymbol 0$, $|\Psi\rangle$ can be written as a single-hole state $a_1|\bar 0\rangle$, with $a_1=\sum_i\bar\beta_i c_i$. Accordingly, $C(|\Psi\rangle)=0$ in these cases. The vanishing of $C(|\Psi\rangle)$ for nonzero but *orthogonal* $\boldsymbol\alpha$ and $\boldsymbol\beta$ [Eq. (43)] generalizes the previous result, showing that in this case $|\Psi\rangle$ can still be written as a single quasiparticle ($\beta'=0$) or quasihole ($\alpha'=0$) after a suitable Bogoliubov transformation of the original operators. This includes the three-level case, where, for instance, the fourth level is empty, which implies $\alpha_4=0$ and $\beta_i=0$ for $i=1,2,3$, leading necessarily to $\boldsymbol\beta^\dagger\boldsymbol\alpha=0$.

We also mention that the four eigenvalues of $\rho^{\rm SP}$ in Eq. (46) are $f_\pm$ and $|\boldsymbol\beta|^2$, the latter twofold degenerate. Since $C(|\Psi\rangle)\leqslant 2|\boldsymbol\alpha||\boldsymbol\beta|$,

$$f_+\geqslant\frac{1+\sqrt{1-4|\boldsymbol\alpha|^2|\boldsymbol\beta|^2}}{2}={\rm Max}[|\boldsymbol\alpha|^2,|\boldsymbol\beta|^2],$$

thus verifying that the eigenvalues of $\rho^{\rm SP}$ are majorized by those of $\rho^{\rm qsp}$ and, hence, that $S^{\rm SP}\geqslant S^{\rm qsp}$, $S_2^{\rm SP}\geqslant S_2^{\rm qsp}=4C^2(|\Psi\rangle)$.

Dualization. Equations (38) and (43) indicate that state $c_i|\bar 0\rangle$ plays the role of the partner or dual of state $c_i^\dagger|0\rangle$. We may obtain the partner state with the Hermitian operator

$$T=-\frac{1}{3!}\sum_{i,j,k,l}\varepsilon_{ijkl}[c_i^\dagger c_j^\dagger c_k^\dagger c_l+c_i^\dagger c_j c_k c_l], \tag{50}$$

such that for $i=1,\ldots,4$, $Tc_i^\dagger|0\rangle=c_i|\bar 0\rangle$, $Tc_i|\bar 0\rangle=c_i^\dagger|0\rangle$. We can then express Eq. (43) as

$$C(|\Psi\rangle)=|\langle\tilde\Psi|\Psi\rangle|,\quad |\tilde\Psi\rangle=T|\Psi\rangle^*, \tag{51}$$

where $|\Psi\rangle^*=\sum_j\bar\alpha_i c_i^\dagger|0\rangle+\beta_i c_i|\bar 0\rangle$ denotes the conjugated state in this basis. Note that the 8×8 matrix that represents T in the basis $(c_1^\dagger|0\rangle,\ldots,c_4^\dagger|0\rangle,c_1|\bar 0\rangle,\ldots,c_4|\bar 0\rangle)$ is just

$$T=\begin{pmatrix}0&I_4\\I_4&0\end{pmatrix}. \tag{52}$$

A generalization of (50) for higher dimensions is considered in [23].

2. Even-parity states

We now consider pure states of even number parity, $P|\Psi\rangle=|\Psi\rangle$. They can be obtained, for instance, by changing a particle for a hole in the odd-parity states. An even state is then a linear combination of the eight states shown in the bottom plots in Fig. 1, comprising the vacuum $|0\rangle$, six two-fermion states, and the completely full state $|\bar 0\rangle=c_1^\dagger c_2^\dagger c_3^\dagger c_4^\dagger|0\rangle$. We can write this state as

$$|\Psi\rangle=\alpha_1|0\rangle-\bar\beta_1|\bar 0\rangle+\sum_{j=2}^{4}\alpha_j c_j^\dagger c_1^\dagger|0\rangle+\bar\beta_j c_1 c_j|\bar 0\rangle, \tag{53}$$

which is just Eq. (38) with the replacements $c_1^\dagger\leftrightarrow c_1$ and $|0\rangle\leftrightarrow c_1^\dagger|0\rangle$, implying $|\bar 0\rangle\leftrightarrow -c_1|\bar 0\rangle$. Note that

$$c_1c_j|\bar 0\rangle=\frac{1}{2!}\sum_{k,l}\epsilon_{j1kl}c_k^\dagger c_l^\dagger|0\rangle. \tag{54}$$

In this notation, the eigenvalues of $\rho^{\rm qsp}$ are then given by Eq. (42) with the same expression, (43), for $C(|\Psi\rangle)$. The entanglement entropy $S^{\rm qsp}$ is given, again, by Eq. (44). Note, however, the minus sign in the term associated with $\bar\beta_1$. Expression (43) reduces to that in [9] for the case of two-fermion states ($\alpha_1=\beta_1=0$).

The state, (53), is then a Slater determinant or quasiparticle vacuum iff $C(|\Psi\rangle)=0$. As a check, the quasiparticle vacuum, (A1), corresponds in the present case to

$$\begin{aligned}&\boldsymbol\alpha\propto(1,T_{21},T_{31},T_{41}),\\ &\bar{\boldsymbol\beta}\propto(-T_{21}T_{43}-T_{31}T_{24}-T_{41}T_{32},T_{43},T_{24},T_{32}),\end{aligned} \tag{55}$$

therefore verifying that $\sum_{i=1}^4\bar\beta_i\alpha_i=0$. It is also shown that in the three-level case (i.e., level 4 empty, implying $\alpha_4=0$ and $\beta_j=0$ for $j=1,2,3$), $C(|\Psi\rangle)$ is always 0.

The normal form, (49), becomes here

$$|\Psi\rangle=\alpha'|0_{\boldsymbol a}\rangle-\bar\beta'|\bar 0_{\boldsymbol a}\rangle, \tag{56}$$

i.e., *a superposition of the vacuum and the maximally occupied state* (bottom-right scheme in Fig. 1) for the diagonalizing quasiparticle operators. Of course, after a trivial particle-hole transformation $a_j\leftrightarrow a_j^\dagger$ for $j=1,2$, we may always rewrite (56) as a sum of two two-fermion states, i.e.,

$$|\Psi\rangle=\alpha' a_2^\dagger a_1^\dagger|0_{\boldsymbol a}\rangle+\bar\beta' a_4^\dagger a_3^\dagger|0_{\boldsymbol a}\rangle, \tag{57}$$

which extends the results in [9] valid for two-fermion states to arbitrary definite-parity states.

The dualization operator, (50), here takes the form

$$T=-c_1^\dagger c_2^\dagger c_3^\dagger c_4^\dagger-c_4c_2c_3c_1-\frac14\sum_{i,j,k,l}\epsilon_{ijkl}c_i^\dagger c_j^\dagger c_k c_l, \tag{58}$$

which satisfies

$$T|0\rangle = -|\bar{0}\rangle, \quad T|\bar{0}\rangle = -|0\rangle,$$
$$Tc_i^\dagger c_j^\dagger|0\rangle = \frac{1}{2}\sum_{k,l}\epsilon_{ijkl}c_k^\dagger c_l^\dagger|0\rangle,$$

i.e., $Tc_i^\dagger c_1^\dagger|0\rangle = c_1 c_i|\bar{0}\rangle$, $Tc_1 c_i|\bar{0}\rangle = c_i^\dagger c_1^\dagger|0\rangle$. It is represented in the special basis $\{|0\rangle, c_2^\dagger c_1^\dagger|0\rangle, c_3^\dagger c_1^\dagger|0\rangle, c_4^\dagger c_1^\dagger|0\rangle, -|\bar{0}\rangle, c_4^\dagger c_3^\dagger|0\rangle, c_2^\dagger c_4^\dagger|0\rangle, c_3^\dagger c_2^\dagger|0\rangle\}$ by *the same matrix*, (52). We can then write, again, $C(|\Psi\rangle)$ in the form (51). If $\alpha_1 = \beta_1 = 0$, the ensuing expression reduces to that in [9].

The two-fermion states considered in [9] and [11] are only a particular case of the more general even states, (53). For two-fermion states the contractions $\langle c_i c_j\rangle$ obviously vanish ($\kappa = 0$), and the eigenvalues f_ν of the generalized one-body density matrix $\rho^{\rm qsp}$ reduce to those of the one-body density matrix $\rho^{\rm SP}$, implying that $S^{\rm SP} = S^{\rm qsp}$.

B. Mixed states and analytic evaluation of the concurrence

The fermionic concurrence for mixed states can be defined by the convex roof extension of Eq. (43). For two-fermion states an explicit expression was derived in [9]. We here generalize this expression to the present general states. Let

$$\rho = \sum_k \lambda_k |\Psi_k\rangle\langle\Psi_k| \tag{59}$$

be a mixed state with eigenvectors $|\Psi_k\rangle$ and eigenvalues λ_k, with $\lambda_k > 0$ for $k = 1\ldots,r$ and $r \leqslant 8$ the rank of ρ. We assume that all $|\Psi_k\rangle$'s have the same number parity, such that they are of the form (38) or (53), i.e., $|\Psi_k\rangle = \sum_{i=1}^4 \alpha_{ki}c_i^\dagger|0\rangle + \bar{\beta}_{ki}c_i|\bar{0}\rangle$ in the odd case. Every convex decomposition $\rho = \sum_{j=1}^{r'} p_j|\Phi_j\rangle\langle\Phi_j|$ can be obtained from these eigenvectors through an $r'\times r$ matrix U with orthonormal columns ($U^\dagger U = I_r$) such that $\sqrt{p_j}|\Phi_j\rangle = \sum_{k=1}^r U_{jk}\sqrt{\lambda_k}|\Psi_k\rangle$. Note that the states $|\Phi_j\rangle$ are normalized, so that $p_j = \sum_{k=1}^r \lambda_k|U_{jk}|^2$.

The average fermionic concurrence (generalized Slater measure) of this decomposition is

$$\langle C(\{p_j,|\Phi_j\rangle\})\rangle = \sum_j p_j C(|\Phi_j\rangle) = \sum_j p_j|\langle\tilde{\Phi}_j|\Phi_j\rangle| = \sum_j\left|\sum_{k,l}U_{jk}U_{jl}\sqrt{\lambda_k\lambda_l}\langle\tilde{\Psi}_k|\Psi_l\rangle\right|. \tag{60}$$

The matrix C of elements,

$$C_{kl} = \sqrt{\lambda_k\lambda_l}\langle\tilde{\Psi}_k|\Psi_l\rangle = \sqrt{\lambda_k\lambda_l}(\boldsymbol{\beta}_l^\dagger\boldsymbol{\alpha}_k + \boldsymbol{\beta}_k^\dagger\boldsymbol{\alpha}_l), \tag{61}$$

is complex symmetric. Therefore, it admits a decomposition of the form [9] $C = VDV^T$, where V is a unitary matrix and D is a real diagonal matrix whose diagonal elements $d_k \geqslant 0$ are the square root of the eigenvalues of $CC^\dagger = C\bar{C}$, sorted in *descending* order. Defining $S = UV$, Eq. (60) then reads

$$\langle C(\{p_j,|\Phi_j\rangle\})\rangle = \sum_j\left|\sum_k S_{jk}^2 d_k\right|. \tag{62}$$

Since $\sum_j|\sum_k S_{jk}^2 d_k| \geqslant \sum_j(d_1|S_{j1}^2| - \sum_{k\geqslant 2}|S_{jk}^2|d_k) = d_1 - \sum_{k\geqslant 2} d_k$, a necessary condition for the separability of ρ, i.e., for ρ to be a convex mixture of Slater determinants with the same number parity, is

$$d_1 \leqslant \sum_{k\geqslant 2} d_k. \tag{63}$$

As in the case of two-fermion states, we now show, following the scheme in [9], that this is also a sufficient condition for separability. Indeed, from (62) it is seen that ρ is separable if there is a matrix S with orthonormal columns such that for every j,

$$\left|\sum_{k=1}^r d_k S_{jk}^2\right| = 0. \tag{64}$$

Now, provided condition (63) is fulfilled, there are always phases $\theta_k, k = 2,\ldots,r$ such that $d_1 = |\sum_{k=2}^r d_k e^{i\theta_k}|$. Then a matrix with elements $S_{jk} = \frac{e^{i(\theta_k+\mu_{jk}\pi)}}{\sqrt{r'}}$, where $\mu_{jk} = 0,1$ and $\theta_1 = 0$, will give the desired decomposition if the signs $e^{i\mu_{jk}\pi}$ can be arranged such that the condition $S^\dagger S = I_r$ is satisfied. This can be ensured by taking $r' = 2$ if $r = 2$, $r' = 4$ if $r = 3,4$ [9], and $r' = 8$ if $5 \leqslant r \leqslant 8$, where we can set $\mu_{j1} = 0\ \forall\ j$ and $(\mu_{1k},\ldots,\mu_{8k})$ as $(0,0,0,0,1,1,1,1)$, $(0,0,1,1,0,0,1,1)$, $(0,0,1,1,1,1,0,0)$, $(0,1,0,1,0,1,0,1)$, $(0,1,0,1,1,0,1,0)$, $(0,1,1,0,0,1,1,0)$, $(0,1,1,0,1,0,0,1)$ for $k = 2,\ldots,8$. This completes the proof.

On the other hand, if condition (63) does not hold, the average, (62), is not smaller than $d_1 - \sum_{k=2}^r d_k$. This lower bound may be achieved with the same construction used above, choosing $\theta_k = \pi/2$ for $k \geqslant 2$. Then the minimizing decomposition is that where all the components have the same concurrence, which is the concurrence of state ρ,

$$C(\rho) = \text{Min}_{\{p_j,|\Phi_j\rangle\}}\sum_j p_j C(|\Phi_j\rangle) = \text{Max}\left[d_1 - \sum_{k=2}^r d_k, 0\right]. \tag{65}$$

Using the dualization matrix, (52), we may also obtain the eigenvalues d_k as those of

$$R = \sqrt{\rho^{1/2}T\rho^* T\rho^{1/2}}, \tag{66}$$

where ρ^* means conjugation in the basis where T takes the form (52).

Once C is obtained, we can evaluate the convex roof extension, (37), of $S^{\rm qsp}$ as

$$E^{\rm qsp}(\rho) = 4h\left(\frac{1+\sqrt{1-C^2(\rho)}}{2}\right), \tag{67}$$

in the same way as in the two-qubit case [26], since for pure states we have, similarly, $S^{\rm qsp} = 4h(\frac{1+\sqrt{1-C^2(|\Psi\rangle)}}{2})$ [Eq. (44)], which is a *convex* increasing function of $C(|\Psi\rangle)$. The quantity $\frac{1+\sqrt{1-C^2(\rho)}}{2}$ is also the maximum fidelity between ρ and a convex mixture of Gaussian states, as shown in [22] with a different treatment based on group representation theory.

A general mixed state ρ satisfying $[\rho,P] = 0$ will be a convex mixture of pure states with even and odd number parity. It can be written as a convex mixture of even and odd parts, i.e.,

$$\rho = p_+\rho_+ + p_-\rho_-, \tag{68}$$

where $\rho_{\pm} = \frac{1}{2p_{\pm}}(1 \pm P)\rho$ are the even and odd components of ρ, and $p_{\pm} = \text{Tr}\,\rho(1 \pm P)/2$ the corresponding probabilities. Since we just consider pure states with a definite number parity, for the general mixed states, (68), we may just take $E^{\text{qsp}}(\rho) = p_+E^{\text{qsp}}(\rho_+) + p_-E^{\text{qsp}}(\rho_-)$, with $E^{\text{qsp}}(\rho_{\pm})$ evaluated with Eqs. (65) and (67).

As an illustration, we consider a definite-parity mixture of a maximally entangled state $|\Psi\rangle$ ($C(|\Psi\rangle) = 1$) with the fully mixed state,

$$\rho = p|\Psi\rangle\langle\Psi| + (1-p)I_8/8, \tag{69}$$

where $0 \leqslant p \leqslant 1$. In the odd-parity case, $|\Psi\rangle$ can be written in the form

$$|\Psi\rangle = \tfrac{1}{\sqrt{2}}(c_1^\dagger|0\rangle + c_1|\bar{0}\rangle) = \tfrac{1}{\sqrt{2}}(c_1^\dagger + c_2^\dagger c_3^\dagger c_4^\dagger)|0\rangle, \tag{70}$$

whereas in the even-parity case we can take $|\Psi\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |\bar{0}\rangle)$ or $\frac{1}{\sqrt{2}}(c_1^\dagger c_2^\dagger + c_3^\dagger c_4^\dagger)|0\rangle$. A direct calculation using (65) leads to

$$C(\rho) = \text{Max}\left[\frac{7p-3}{4}, 0\right], \tag{71}$$

indicating entanglement for $p > 3/7$, i.e., $q > 1/2$, where $q = \langle\Psi|\rho|\Psi\rangle = p + (1-p)/8$ is the total weight of $|\Psi\rangle$. A similar calculation but considering just two-fermion states, $\rho_2 = p|\Psi\rangle\langle\Psi| + (1-p)I_6/6$, leads instead to $C(\rho_2) = \text{Max}[\frac{5p-2}{3}, 0]$, implying entanglement above a slightly smaller value of p [$p > 2/5$, entailing, again, $q = p + (1-p)/6 > 1/2$], with $C(\rho_2) > C(\rho)$ for $p \in (2/5, 1)$. As in the two-qubit case, the existence of a finite threshold probability p for nonzero C, and hence E^{qsp}, implies a finite limit temperature for entanglement T_L if ρ represents a thermal state [$\frac{q}{(1-p)/8} \propto e^{-\beta(E_0-E_1)}$, with E_0 the energy of $|\Psi\rangle$ and $E_1 > E_0$ that of the remaining seven levels], which is larger in the second canonical case.

IV. CONCLUSIONS

We have presented a general consistent formalism for describing entanglement-like correlations in general fermion states with no definite fermion number yet a fixed number parity. We have first defined a single-level entanglement entropy that quantifies the entanglement between an SP mode and its orthogonal complement, through the definition of suitable reduced states for such a partition of a given basis of the SP space. The sum over all SP modes of this entropy, S_c, can be taken as a measure of the total entanglement of the system with respect to this basis, and its minimum over all SP bases, S^{SP}, is shown to be a function of the one-body density matrix, then being invariant with respect to unitary transformations in the SP space. Moreover, if minimization is extended over all quasiparticle bases, the resulting entanglement entropy, S^{qsp}, is a function of the generalized one-body density matrix, therefore remaining invariant under general Bogoliubov transformations. This entropy vanishes iff there is an SP or quasiparticle basis in which every level is separable from its orthogonal complement, i.e., iff each of these levels is either empty or occupied. These entanglement entropies satisfy the inequality chain $S_c \geqslant S^{\text{SP}} \geqslant S^{\text{qsp}}$. The convex roof extension of S^{qsp} was also introduced, its vanishing rigorously identifying classically correlated mixed fermion states which can be expressed as convex mixtures of pure states or quasiparticle vacua, like those emerging at sufficiently high temperatures in interacting many-fermion systems through approaches like the SPA.

In the case of fermion systems with four SP levels, a fermionic analog of the two-qubit pure-state concurrence was defined in terms of ρ^{qsp}, which reduces to the Slater correlation measure defined in [9] and [11] for two-fermion states. The eigenvalues of the generalized one-body density matrix, which are fourfold degenerate, can be written as functions of this concurrence, and consequently, the entanglement entropy S^{qsp} is related to the fermionic concurrence by an expression analogous to that in the two-qubit case. This result suggests that particle entanglement may be seen as a minimum mode entanglement. For mixed states with fixed number parity in this system, an explicit expression for the fermionic concurrence, defined as the convex roof extension of the pure-state concurrence, was derived, in complete analogy with the two-qubit case, which generalizes the result in [9] and [11] and provides a closed analytic expression for the convex roof extension of S^{qsp}.

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APPENDIX: QUASIPARTICLE VACUUM

According to the Thouless theorem [36] the vacuum $|0_{\boldsymbol{a}}\rangle$ of the quasiparticle fermion operators, (19), is given, if $\text{Det}\,U \neq 0$, by [24]

$$\begin{aligned} |0_{\boldsymbol{a}}\rangle &= \gamma \exp\left[\frac{1}{2}\sum_{i,j} T_{ij}c_i^\dagger c_j^\dagger\right]|0\rangle \\ &= \gamma\left[1 + \frac{1}{2}\sum_{i,j} T_{ij}c_i^\dagger c_j^\dagger + \dots\right]|0\rangle, \end{aligned} \tag{A1}$$

where $\gamma = \sqrt{|\text{Det}\,U|}$ and $T = -U^{-1}V$ is an antisymmetric matrix, with $|0\rangle$ the vacuum of the c_j operators. Equation (A1) can be verified by directly applying a_ν to (A1) [if $\text{Det}\,U = 0$, $|0_a\rangle$ can be obtained by applying additional creation operators $c_j^\dagger$ to Eq. (A1)].

If $|\Psi\rangle = |0_{\boldsymbol{a}}\rangle$, then $f_\nu = \langle 0_{\boldsymbol{a}}|a_\nu^\dagger a_\nu|0_{\boldsymbol{a}}\rangle = 0\ \forall\ \nu$, implying that $S^{\text{qsp}} = 0$. However, it is easy to see that

$$\rho^{\text{SP}} = 1 - \langle 0_{\boldsymbol{a}}|\boldsymbol{c}\boldsymbol{c}^\dagger|0_{\boldsymbol{a}}\rangle = VV^\dagger, \tag{A2}$$

implying that $S^{\text{SP}} > 0$ if $V \neq 0$. The eigenvalues p_k of ρ^{SP} are then just the square of the singular values of V. The state $|\Psi\rangle$ appears, therefore, mixed at the SP level, reflecting that it cannot be written as a Slater determinant in operators of the form (13).

[1] M. A. Nielsen and I. L. Chuang, *Quantum Computation and Quantum Information* (Cambridge University Press, Cambridge, UK, 2000).
[2] C. H. Bennett, G. Brassard, C. Crepeau, R. Jozsa, A. Peres, and W. K. Wootters, Phys. Rev. Lett. **70**, 1895 (1993).
[3] R. Josza and N. Linden, Proc. R. Soc. London Sec. A **459**, 2011 (2003); G. Vidal, Phys. Rev. Lett. **91**, 147902 (2003).
[4] R. Horodecki, P. Horodecki, M. Horodecki, and K. Horodecki, Rev. Mod. Phys. **81**, 865 (2009).
[5] G. Vidal, J. I. Latorre, E. Rico, and A. Kitaev, Phys. Rev. Lett. **90**, 227902 (2003).
[6] L. Amico, R. Fazio, A. Osterloh, and V. Vedral, Rev. Mod. Phys. **80**, 517 (2008).
[7] J. Eisert, M. Cramer, and M. B. Plenio, Rev. Mod. Phys. **82**, 277 (2010).
[8] A. Peres, *Quantum Theory, Concepts and Methods* (Kluwer Academic, Dordrecht, The Netherlands, 1995).
[9] J. Schliemann, J. I. Cirac, M. Kus, M. Lewenstein, and D. Loss, Phys. Rev. A **64**, 022303 (2001).
[10] J. Schliemann, D. Loss, and A. H. MacDonald, Phys. Rev. B **63**, 085311 (2001).
[11] K. Eckert, J. Schliemann, D. Bruß, and M. Lewenstein, Ann. Phys. **299**, 88 (2002).
[12] P. Zanardi, Phys. Rev. A **65**, 042101 (2002).
[13] Y. Shi, Phys. Rev. A **67**, 024301 (2003).
[14] N. Friis, A. R. Lee, and D. E. Bruschi, Phys. Rev. A **87**, 022338 (2013).
[15] H. M. Wiseman and J. A. Vaccaro, Phys. Rev. Lett. **91**, 097902 (2003).
[16] G. C. Ghirardi and L. Marinatto, Phys. Rev. A **70**, 012109 (2004).
[17] A. Plastino, D. Manzano, and J. Dehesa, Europhys. Lett. **86**, 20005 (2009).
[18] F. Iemini and R. O. Vianna, Phys. Rev. A **87**, 022327 (2013); F. Iemini, T. O. Maciel, and R. O. Vianna, Phys. Rev. B **92**, 075423 (2015).
[19] F. Benatti, R. Floreanini, and U. Marzolino, Phys. Rev. A **89**, 032326 (2014).
[20] X. M. Puspus, K. H. Villegas, and F. N. C. Paraan, Phys. Rev. B **90**, 155123 (2014).
[21] C. V. Kraus, M. M. Wolf, J. I. Cirac, and G. Giedke, Phys. Rev. A **79**, 012306 (2009).
[22] M. Oszmaniec, J. Gutt, and M. Kuś, Phys. Rev. A **90**, 020302(R) (2014); M. Oszmaniec and M. Kuś, *ibid.* **90**, 010302(R) (2014); **88**, 052328 (2013).
[23] G. Sárosi and P. Lévay, J. Phys. A **47**, 115304 (2014); Phys. Rev. A **90**, 052303 (2014); **89**, 042310 (2014).
[24] P. Ring and P. Schuck, *The Nuclear Many-Body Problem* (Springer, Berlin, 1980).
[25] N. Friis, arXiv:1502.04476.
[26] S. Hill and W. K. Wootters, Phys. Rev. Lett. **78**, 5022 (1997); W. K. Wootters, *ibid.* **80**, 2245 (1998).
[27] N. Canosa and R. Rossignoli, Phys. Rev. Lett. **88**, 170401 (2002).
[28] N. Gigena and R. Rossignoli, Phys. Rev. A **90**, 042318 (2014).
[29] R. Bhatia, *Matrix Analysis* (Springer, New York, 1997).
[30] R. F. Werner, Phys. Rev. A **40**, 4277 (1989).
[31] C. H. Bennett, D. P. DiVincenzo, J. A. Smolin, and W. K. Wootters, Phys. Rev. A **54**, 3824 (1996).
[32] B. Mühlschlegel, D. J. Scalapino, and R. Denton, Phys. Rev. B **6**, 1767 (1972).
[33] Y. Alhassid and J. Zingman, Phys. Rev. C **30**, 684 (1984); P. Arve, G. Bertsch, B. Laurizten and G. Puddu, Ann. Phys. (NY) **183**, 309 (1988); R. Rossignoli, A. Ansari, and P. Ring, Phys. Rev. Lett. **70**, 1061 (1993); R. Rossignoli, N. Canosa, and P. Ring, *ibid.* **80**, 1853 (1998).
[34] J. Hubbard, Phys. Rev. Lett. **3**, 77 (1959); R. L. Stratonovich, Dokl. Akad. Nauk. SSSR **115**, 1097 (1957) [Soviet Phys. Doklady **2**, 416 (1957)].
[35] F. de Melo, P. Ćwikliński, and B. M. Terhal, New J. Phys. **15**, 013015 (2013).
[36] D. J. Thouless, Nucl. Phys. **21**, 225 (1960).