Entanglement in fermionic systems

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The anticommuting properties of fermionic operators, together with the presence of parity conservation, affect the concept of entanglement in a composite fermionic system. Hence different points of view can give rise to different reasonable definitions of separable and entangled states. Here we analyze these possibilities and the relationship between the different classes of separable states. We illustrate the differences by providing a complete characterization of all the sets defined for systems of two fermionic modes. The results are applied to Gibbs states of infinite chains of fermions whose interaction corresponds to a XY-Hamiltonian with transverse magnetic field.

I. INTRODUCTION

The definition of entanglement in a composite quantum system \[ \mathbf{I} \] depends on a notion of locality which is typically assigned to a tensor product structure or to commuting sets of observables \([4, 5, 6]\). Various a priori different definitions can then be formulated depending on requirements concerning preparation, representation, observation and application. Fortunately, most of them usually coincide. \([3]\)

In the present article we investigate systems of fermions where several of these definitions differ due to indistinguishability, anti-commutation relations and the parity superselection rule. We will provide a systematic study of the different definitions of entanglement and determine the relations between them. To this end, we will consider fermionic systems in second quantization. That is, the entanglement will be between sets of modes or regions in space rather than between particles. The latter case was studied in first quantization in \([4, 5, 6]\) whereas entanglement between distinguishable modes of fermions has been calculated for various systems in \([3, 8, 9, 10, 11, 12]\).

That the presence of superselection rules affects the concept of entanglement has been pointed out and studied in detail in \([13, 14, 15, 16, 17]\). There, the existence of states was shown which are convex combinations of product states but not locally preparable, thus two reasonable definitions of entanglement already differ.

In the following the differences will mainly arise from an interplay between the parity superselection rule and the anti-commutation relation of fermionic operators. The different mathematical definitions will carry physically motivated meanings corresponding to different abilities to prepare, use or observe the entanglement, as well as to differences between the single copy case and the asymptotic regime.

In section \([11]\) we introduce the basic ideas and tools used in the rest of the paper. We start by defining the different sets of product states in section \([13]\). From them, several sets of separable states are constructed by convex combination in section \([14]\). It is shown that they all correspond to four different classes each of which contains the previous ones as proper subsets:

1. States which are preparable by means of local operations and classical communication (LOCC).
2. Convex combinations of product states in Fock space.
3. Convex combinations of states for which products of locally measurable observables factorize.
4. States for which all locally measurable correlations can as well arise from a state within class 3 above.

Section \([14]\) analyzes the asymptotic properties of the various sets of separable states. As an illustration of all these concepts, section \([17]\) shows the complete characterization of the different sets in the case of a \(1 \times 1\)-modes system, and their application to the thermal state of an infinite chain of fermions interacting with a particular Hamiltonian. In order to improve the readability of the paper, we have compiled the detailed proofs of all the relations in section \([17]\).

II. PRELIMINARIES

The basic objects for describing a fermionic system of \(m\) modes are the creation and annihilation operators, which satisfy canonical anticommutation relations. Alternatively, \(2m\) Majorana operators can be defined, \(c_{2k-1} := a_k + a_k^\dagger, c_{2k} := (-i)(a_k^\dagger - a_k)\), for \(k = 1, \ldots 2m\), which satisfy \(\{c_i, c_j\} = \delta_{ij}\). Each set generates the algebra \(\mathcal{C}\) of all observables. A bipartition of the system is defined by two subset of modes, \(A = 1, \ldots m_A\) and \(B = m_A + 1, \ldots m\). We will denote by \(\mathcal{A}\) (\(\mathcal{B}\)) the operator subalgebra spanned by the \(m_A\) \((m_B)\) modes in \(A\) (\(B\)).
If \( n_k \) is the occupation number of the \( k \)-th mode, i.e. the expectation value of the operator \( a_k^\dagger a_k \), the Fock basis can be defined by

\[
| n_1, \ldots, n_m \rangle = (a_1^\dagger)^{n_1} \cdots (a_m^\dagger)^{n_m} | 0 \rangle.
\]

The Jordan-Wigner transformation maps the fermionic algebra onto Pauli spin operators so that

\[
c_{2k-1} = \prod_{i=1}^{k-1} a_{2i}^\dagger \sigma_x^{(i)} \sigma_y^{(k)}, \quad c_{2k} = \prod_{i=1}^{k-1} a_{2i}^\dagger \sigma_x^{(i)} \sigma_x^{(k)}.
\]

The Hilbert space associated to \( m \) fermionic modes (Fock space) is isomorphic to the \( m \)-qubit space. Due to the anticommutation relations, however, the action of fermionic operators in Fock space is non-local.

For the fermionic systems under consideration, conservation of the parity of the fermion number, \( \tilde{P} = \sum 1 c_k \), implies that the accessible state space is the direct sum of positive (even) and negative (odd) parity eigenspaces. Any physical state or observable commutes with the operator \( \tilde{P} \), so that we can define the set of physical states

\[ \Pi := \{ \rho : [\rho, \tilde{P}] = 0 \} \]

Correspondingly, \( A_x \) and \( B_x \) will designate the sets of local observables, commuting with the local parity operators \( \tilde{P}_A \) and \( \tilde{P}_B \), respectively.

We will call an observable even if it commutes with the parity operator, whereas an odd observable will be that anticommuting with \( \tilde{P} \). Notice that with this nomenclature, odd observables are not the ones supported on the odd parity eigenspace. On the contrary, an observable with such support will be even in this notation, as it commutes with \( \tilde{P} \). It will be convenient to make use of the projectors onto the well-defined parity subspaces, \( \mathbb{P}_\pi \). Any state (or operator) commuting with parity has a block diagonal structure \( \rho = \mathbb{P}_\pi \rho \mathbb{P}_\pi + \mathbb{P}_\bar{\pi} \rho \mathbb{P}_\bar{\pi} \). In the local subspaces, a parity conserving operator can be written \( A_\pi = \mathbb{P}_\pi A \mathbb{P}_\pi + \mathbb{P}_{\bar{\pi}} A \mathbb{P}_{\bar{\pi}} \).

One subset of states of particular physical interest is that of Gaussian states. They describe the equilibrium and excited states of quadratic Hamiltonians. Moreover, important variational states (e.g. the BCS state) belong to this category. In various respects Gaussian states exhibit relevant extremality properties \[18, 19\]. Fermionic Gaussian states are those whose density matrix can be written as an exponential of a quadratic form in the fermionic operators \[20\],

\[
\rho = \exp \left( -\frac{i}{4} c^T M c \right),
\]

for some real antisymmetric matrix \( M \). The covariance matrix of any fermionic state is a real antisymmetric matrix defined by

\[
\Gamma_{kl} = \frac{i}{2} \text{tr} (\rho [c_k, c_l]),
\]

which necessarily satisfies \( i \Gamma \leq \mathbf{1} \). According to Wick’s theorem, the covariance matrix determines completely all the correlation functions of a Gaussian state. Pure fermionic Gaussian states satisfy \( \Gamma^2 = -\mathbf{1} \), and they can be written as a tensor product of pure states involving at most one mode of each partition \[21\].

### III. Product States

We start by defining product states of a bipartite fermionic system formed by \( m = m_A + m_B \) modes, where \( m_A (m_B) \) is the number of modes in partition \( A (B) \).

The entanglement of such system can be studied at the level of operator subalgebras or in the Fock space representation, thus the possibility to define different sets of product states. In Fock space, the isomorphism to a system of \( m_A + m_B \) qubits allows separability to be studied with respect to the tensor product \( \mathbb{C}^{2^{m_A}} \otimes \mathbb{C}^{2^{m_B}} \). At the level of the operator subalgebras, on the other hand, one should study the entanglement between \( A \) and \( B \) subalgebras. However the observables in them do not commute, in general, and have non-local action in Fock space. On the contrary, \( A_x \) and \( B_x \), i.e. the subalgebras of parity conserving operators, commute with each other, so that they can be considered local to both parties. It is then natural to study the entanglement between them.

#### A. General states

With these considerations, we may give the following definitions of a product state. They are summarized in Table IV.

- We may call a state product if there exists some state acting on the Fock space of the form \( \rho = \tilde{A} \otimes \tilde{B} \), and producing the same expectation values for all local observables. Formally, \[22\],

\[
\mathcal{P} 0 := \{ \rho : \exists \tilde{A}, \tilde{B}, [\tilde{A} \tilde{B}^\dagger], \tilde{P} \tilde{A} \tilde{B}^\dagger] = 0 \text{ s.t.} \\
\rho(\tilde{A}_x \tilde{B}_x) = \tilde{A}(\tilde{A}_x) \tilde{B}(\tilde{B}_x) \forall \tilde{A}_x \in A_x, \tilde{B}_x \in B_x \}.
\]

- Alternatively, product states may be defined as those for which the expectation value of products of local observables factorizes,

\[
\mathcal{P} 1 := \{ \rho : \rho(\tilde{A}_x \tilde{B}_x) = \tilde{A}(\tilde{A}_x) \tilde{B}(\tilde{B}_x) \forall \tilde{A}_x \in A_x, \tilde{B}_x \in B_x \}.
\]

- At the level of the Fock representation, a product state can be defined as that writable as a tensor
The two first definitions are equivalent, $\mathcal{P}0 \equiv \mathcal{P}1$. They correspond to states with a separable projection onto the diagonal blocks that preserve parity in each of the subsystems. This means that

$$\sum_{\alpha, \beta = e, o} P^A_\alpha \otimes P^B_\beta \rho^A_\alpha \otimes P^B_\beta,$$

is a product in the sense of $\mathcal{P}2$.

The three remaining sets are strictly different. In particular $\mathcal{P}2 \subset \mathcal{P}1$ and $\mathcal{P}3 \subset \mathcal{P}1$, but $\mathcal{P}3 \neq \mathcal{P}2$. The inclusion $\mathcal{P}2, \mathcal{P}3 \subset \mathcal{P}1$ is immediate from the definitions. The non equality of the sets can be seen by explicit examples as those shown in Table I. The difference between $\mathcal{P}3$ and $\mathcal{P}2$, however, is limited to non-physical states, i.e. those not commuting with parity $\hat{\pi}$.

### B. Physical states

Being parity a conserved quantity in the systems of interest, the only physical states will be those commuting with $\hat{\pi}$. It makes then sense to restrict the study of entanglement to such states. By applying each of the above definitions to the physical states, $\mathcal{P}$, we obtain the following sets of physical product states.

### IV. Separable states

For pure states, all $\mathcal{P}i_\pi$ reduce to the same set. If the state vector is written in a basis of well-defined parity in each subsystem, it is possible to show that the condition of $\mathcal{P}1_\pi$ requires that such expansion has a single non-vanishing coefficient, and thus the state can be written as a tensor product also with the definition of $\mathcal{P}2$.

### C. Pure states

For pure states, all $\mathcal{P}i_\pi$ reduce to the same set. If the state vector is written in a basis of well-defined parity in each subsystem, it is possible to show that the condition of $\mathcal{P}1_\pi$ requires that such expansion has a single non-vanishing coefficient, and thus the state can be written as a tensor product also with the definition of $\mathcal{P}2$.
VII B summarizes the definitions and mutual relations among product states. The strict character of the inclusion between product sets can be seen with an example, in particular in the subset \( S_3 \cap \Pi \). It can be shown that any parity preserving state in \( S_3 \) has a decomposition in terms of only parity preserving terms, and is thus in \( S_3 \).  

As shown in Fig. 1, we may take the physical states that satisfy the definitions for separability introduced in the previous subsection, and hence use \( S_i \cap \Pi \) as the definition of separable states. This yields the sets

- \( S_1 \cap \Pi \equiv S_{1,\pi} \),
- \( S_{2,\pi} := S_2 \cap \Pi \),
- \( S_2 \cap \Pi \equiv S_{2,\pi} \).

Only \( S_{2,\pi} \) is different from the separable sets defined above. Actually, given an \( S_1 \) state that commutes with \( \hat{P} \), it is possible to construct a decomposition according to \( S_{1,\pi} \) by taking the parity preserving part of each term in the original convex combination. Therefore \( S_1 \cap \Pi \subseteq S_{1,\pi} \), while the converse inclusion is evident. For \( S_3 \cap \Pi \), on the other hand, it was shown in [23] that any parity preserving state in \( S_3 \) has a decomposition in terms of only parity preserving terms, and is thus in \( S_{3,\pi} \).

All the considerations above leave us with three strictly different sets of separable physical states,

\[
S_{2,\pi} \subset S_{2,\pi}^' \subset S_{1,\pi}
\]  

From the definitions, it is immediate that \( S_{2,\pi} \subseteq S_{2,\pi}^' \). The inclusion is strict because not every state \( \rho \in S_{2,\pi}^' \) has a decomposition in terms of products of even states (see example \( \rho_{S_{2,\pi}^'} \) in Table I). The condition for \( S_{2,\pi} \) is then more restrictive.

From the relation between product sets, \( S_2 \subseteq S_1 \), and \( S_{2,\pi} \subseteq S_{1,\pi} \). The strict inclusion can be shown by constructing an explicit example of a \( P_{1,\pi} \) state without positive partial transpose (PPT) [24] in the 2×2-modes system.

The detailed proofs of the equivalences and inclusions above are shown in section VII B.

C. Equivalence classes

If one is only interested in the measurable correlations of the state, rather than in its properties after further evolution or processing, it makes sense to define an equivalence relation between states by

\[
\rho_1 \sim \rho_2 \text{ if } \rho_1(A_\pi B_\pi) = \rho_2(A_\pi B_\pi) \forall A_\pi \in A_\pi, B_\pi \in B_\pi,
\]

i.e., two states are equivalent if they produce the same expectation values for all physical local operators. Therefore, two states that are equivalent cannot be distinguished by means of local measurements.

With the restriction of parity conservation, the states that can be locally prepared are of the form \( S_{2,\pi} \), i.e.
\[ \rho = \sum \lambda_k \rho_k^{A} \otimes \rho_k^{B}, \ \text{where} \ [\rho_k^{A(B)}, \hat{P}_{A(B)}] = 0. \] 

Since the only locally accessible observables are local, parity preserving operators, i.e. quantities of the form \[ \rho(A_x B_y), \] 

it makes sense to say that a given state is separable if it is equivalent to a state that can be prepared locally. With this definition, the set of separable states is equal to the equivalence class of \( S^{2\pi} \) with respect to the equivalence relation above.

Generalizing this concept, we may construct the equivalence classes for each of the relevant separability sets,

\[ [S^{i}] := \{ \rho : \exists \tilde{\rho} \in S^{i} \pi, \ \rho \sim \tilde{\rho} \}, \ i = 1; 2'. \]

From the inclusion relation among the separability sets, \( [S^{2\pi}] \subseteq [S^{2'2\pi}] \subseteq [S^{1\pi}] \). And, obviously, \( S^{i} \pi \subseteq [S^{i}] \).

On the other hand, any state \( \rho \in [S^{1}] \) has also an equivalent state in \( S^{2\pi} \) (see section VII B), so that

\[ [S^{2\pi}] = [S^{2'2\pi}] = [S^{1\pi}] \].

This equivalence class includes then all the separability sets described in the previous subsection. However, it is strictly larger, as can be seen by the explicit example \( \rho \in S^{1\pi} \) in Table II.



**D. Characterization**

It is possible to give a characterization of the previously defined separability sets in terms of the usual mathematical concept of separability, i.e. with respect to the tensor product. This allows us to use standard separability criteria (see [23] for a recent review) in order to decide whether a given state is in each of these sets.

The definition \( S^{2\pi} \) corresponds to the separability in the sense of the tensor product, i.e. the standard notion \[ \bigotimes \], applied to parity preserving states.

As convex hull of \( P^{2} \cap \Pi \), the set \( S^{2\pi} \) consists of states with a decomposition in terms of tensor products, with the additional restriction that every factor commutes with the local version of the parity operator. Using the block diagonal structure \( P_a \rho P_B + P_B \rho P_a \) of any parity preserving state, each block must have independent decompositions in the sense of the tensor product. Then a state will be in \( S^{2\pi} \) iff both \( P_a \rho P_B \) and \( P_B \rho P_a \) are in \( S^{2'\pi} \).

A state \( \rho \) is in \( P^{0\pi} \) if its diagonal blocks are a tensor product,

\[ \sum_{\alpha, \beta = e, o} P_{\alpha}^{A} \otimes P_{\beta}^{B} \rho P_{\alpha}^{A} \otimes P_{\beta}^{B} = \tilde{\rho}^{A} \otimes \tilde{\rho}^{B} \in P^{2\pi}. \]  

The set \( S^{1\pi} \) is characterized as the convex hull of \( P^{1\pi} \equiv P^{0\pi} \), i.e. it is formed by convex combinations of states that can be written as the sum of a parity preserving tensor product plus some off–diagonal terms.

Finally, the equivalence class \( [S^{1\pi}] \equiv [S^{2\pi}] \) is completely defined in terms of the expectation values of observable products \( A_x B_y \). These have no contribution from off–diagonal blocks in \( \rho \), so the class can be characterized in terms of the diagonal blocks alone. Therefore a state is in \( [S^{1\pi}] \) iff

\[ \sum_{\alpha, \beta = e, o} P_{\alpha}^{A} \otimes P_{\beta}^{B} \rho P_{\alpha}^{A} \otimes P_{\beta}^{B} \in S^{2'\pi}. \]
Since the condition involves only the block diagonal part of the state, it is equivalent to the individual separability (with respect to the tensor product) of each of the blocks.

\section*{V. MULTIPLE COPIES}

The definitions introduced in the previous sections apply to a single copy of the fermionic state. It is nevertheless interesting to see the stability of the different criteria when several copies are considered, and, in particular, to understand their asymptotic behaviour when \( N \to \infty \).

The criteria \( S_2' \pi \) and \( S_2 \pi \) are stable when several copies of the state are considered.

\begin{itemize}
  \item \( \rho^{\otimes 2} \in S_2' \pi \iff \rho \in S_2' \pi \),
  \item \( \rho^{\otimes 2} \in S_2 \pi \iff \rho \in S_2 \pi \).
\end{itemize}

Moreover, it was shown in \cite{15} that the entanglement cost of \( S_2 \pi \) converges to that of \( S_2' \pi \), so that asymptotically both definitions are equivalent.

On the other hand, \( S_1 \pi \) and \( \pi \) do not show the same stability, although the corresponding individual separability is a necessary condition for the separability of the multiple copies state.

\begin{itemize}
  \item \( \rho^{\otimes 2} \in S_1 \pi \Rightarrow \rho \in S_1 \pi \),
  \item \( \rho^{\otimes 2} \in \pi \Rightarrow \rho \in \pi \).
\end{itemize}

It is also possible to prove (see section \textbf{VIIC}) that

\begin{itemize}
  \item \( \rho^{\otimes 2} \in S_1 \pi \Rightarrow \rho \) PPT.
\end{itemize}

Therefore, an NPPT state \( \rho \) is also non separable according to the broadest definition \( \pi \) when one takes several copies. This is true, in particular, for distillable states \cite{26,27}. This suggests that the differences between the various definitions of separability may vanish in the asymptotic regime. The strict equivalence of the classes in this limit, however, is proved only for the case of \( 1 \times 1 \) modes, as detailed in the following section.

\section*{VI. 1×1 MODES}

In the case of a small system of only two modes, it is possible to apply all the definitions above to the most general density matrix and find the complete characterization of each of the sets. Table \textbf{III} shows this characterization.

A generic state of a \( 1 \times 1 \)-mode system can be written in the Fock representation as

\[
\rho = \begin{pmatrix}
1 - x - y + z & p & q & r \\
p^* & x - z & s & t \\
q^* & s^* & y - z & w \\
r^* & t^* & w^* & z
\end{pmatrix},
\]

where \( x, y, z \) are real parameters, and with the additional restrictions that ensure \( \rho \geq 0 \), which include \( z \leq x, y \), and \( 1 + z \geq x + y \).

States in \( P_1 \) must satisfy a single relation between expectation values, namely \( \langle c_1 c_2 c_3 c_4 \rangle = \langle c_1 c_2 \rangle \langle c_3 c_4 \rangle \), which reads, in terms of the given parametrization, \( z = x y \). This condition is also necessary for states in \( P_2 \) or \( P_3 \).

If a state is in \( P_2 \), it can be written as the tensor product of two \( 1 \)-mode matrices, each of them determined by one real and one complex parameter. This imposes a number of restrictions on the general parameters above, that can be read in Table \textbf{III}. Since \( S_2 \) corresponds to separability in the isomorphic qubit system, a state will be in \( S_2 \) iff it has PPT \cite{28}.

According to \cite{23}, a state in \( P_3 \) has zero expectation value for all observable products \( A \pi B \pi \), and one of the restrictions of \( \rho \) to the subsystems is odd with respect to the parity transformation. There are then two generic forms of a product state \( P_3 \) in this system, as shown in the table.

If we restrict the study to physical states, i.e. those commuting with \( P \), the density matrix has a block diagonal structure, and the most general even \( 1 \times 1 \) state can be written

\[
\rho = \begin{pmatrix}
1 - x - y + z & 0 & 0 & r \\
0 & x - z & s & 0 \\
0 & s^* & y - z & 0 \\
r^* & 0 & 0 & z
\end{pmatrix},
\]

Particularizing the conditions for general product states to this form of the density matrix, where \( p = q = t = w = 0 \), gives the explicit characterization of the physical product states according to each definition.

In particular, the state \( \| 12 \rangle \) is in \( P_1 \) iff \( z = x y \). Convex combinations of this kind of states will produce density matrices that fulfill \( |s|^2 \leq z(1 - x - y + z) \) and \( |r|^2 \leq (x - z)(y - z) \), and thus have PPT. This shows that, for this small system, \( S_1 \pi \equiv S_2' \pi \).

The independent separability of both blocks of \( \rho \), that determines separability according to \( S_2' \pi \), requires that \( r = s = 0 \), i.e. that the density matrix is diagonal in this basis.

Finally, the characterization \( \| 10 \rangle \) of \( S_1 \pi \) applied to \( \| 11 \rangle \) yields the condition that the diagonal of \( \rho \) is sep-
arable according to the tensor product, so that all even states of $1 \times 1$-modes are in $[S_{1\pi}]$.

If we look at several copies of such a $1 \times 1$-modes system, it is possible to show that

$$\rho^{\otimes 2} \in [S_{1\pi}] \iff \rho \in S_{2\pi}'.$$

Therefore, in this case all the definitions of entanglement converge when we look at a large number of copies.

### A. Thermal states of fermionic chains

All the concepts above can be applied to a particular example. We consider a 1D chain of $N$ fermions subject to the Hamiltonian

$$H = \frac{1}{2} \sum_n (a_n^\dagger a_{n+1}^\dagger + \text{h.c.}) - \lambda \sum_n a_n^\dagger a_n$$

$$+ \gamma \sum_n (a_n^\dagger a_{n+1}^\dagger + \text{h.c.}).$$

This Hamiltonian can be obtained as the Jordan-Wigner transformation of an XY spin chain with transverse magnetic field [24, 30]. The Hamiltonian can be exactly diagonalized by means of Fourier and Bogoliubov transformations, yielding

$$H = \sum_{k=-N/2}^{N/2-1} \Lambda_k b_k^\dagger b_k,$$

with $\Lambda_k = \sqrt{\left[\cos \frac{2\pi k}{N} - \lambda\right]^2 + 4\gamma^2 \sin^2 \frac{2\pi k}{N}}$, $b_k = \cos \theta_k a_k + i \sin \theta_k a_k^\dagger$, $2\theta_k = \frac{\cos \frac{2\pi k}{N} - \lambda}{\Lambda_k}$ and $a_k = \frac{1}{\sqrt{N}} \sum_n e^{-i \frac{2\pi k n}{N}} a_n$.

We consider the thermal state $\rho = \frac{e^{-\beta H}}{Z(\beta)}$, with inverse temperature $\beta$, and calculate the reduced density matrix for two adjacent modes in the limit of an infinite chain, by numerical integration of the relevant expectation values as a function of the three parameters of this model, $\lambda$, $\gamma$ and $\beta$.

First we may study which values of the parameters make the two modes entangled according to each of the definitions. As mentioned above, for a 2-mode system there is no distinction between the sets $S_{1\pi}$ and $S_{2\pi}'$. Therefore we look for the limits of the separability regions $S_{2\pi}'$ and $S_{2\pi}$ for a fixed value of the parameter $\lambda$. The results are shown in Fig. 2. For every value of $\lambda$ we may see that the reduced density matrix is in $S_{2\pi}$ only if $\beta = 0$, i.e. for all finite values of the temperature two adjacent fermions will be entangled according to this criterion. The region $S_{2\pi}'$, on the contrary, changes with the parameters, as shown by the plots.

From a quantitative point of view, the entanglement with respect to $S_{2\pi}'$ can be measured by the entanglement of formation [31],

$$E_F(\rho) = \min_{\{\psi_i\}} \sum_i p_i E(\psi_i).$$

With respect to $S_{2\pi}$, it is natural to define the entanglement of formation conforming to parity conservation.

\[
\begin{array}{|c|c|}
\hline
&P1 & P2 & P3 & \Pi \\
\hline
\rho & 1 - x - y + z & p & q & r \\
\hline
z = x y & & & & \\
\rho^A \otimes \rho_B & & & & \\
\hline
S_{1\pi} & S_{1\pi} & r = s = 0 & All \rho \geq 0 \\
S_{2\pi} & |s|^2 \leq z(1 - x - y + z) & & & \\
S_{2\pi}' & |r|^2 \leq (x - z)(y - z) & & & \\
\hline
\end{array}
\]

**TABLE III:** Characterization of the sets for a $1 \times 1$-modes system.

\[
\begin{array}{|c|c|}
\hline
P & \text{characterization} \\
\hline
\rho & \left(\begin{array}{cccc}
p & q & r \\
p^* & x - z & s & t \\
q^* & s^* & y - z & w \\
r^* & t^* & w^* & z \\
\end{array}\right) \\
\hline
P1 & z = x y \\
\hline
P2 & \rho = \rho_A \otimes \rho_B \quad \text{i.e.} \\
& \left\{ \begin{array}{c}
z = x y \\
p = (1 - y)w \\
x q = (1 - x)t \\
x y r = t w \\
x y s = t w^* \\
\end{array} \right. \quad \left\{ \begin{array}{c}
q = t = 0 \\
(1 - y)w = -yp \\
(1 - x)t = x q \\
\end{array} \right. \\
\hline
P3 & r = s = 0 \\
\hline
\Pi & p = q = t = w = 0 \\
\hline
\end{array}
\]
as

\[ E^p_F(\rho) = \min_{\{i, \psi\}} \sum_i p_i E(\psi_i), \]

where the minimization is performed over ensembles all whose \( \psi_i \) have well-defined parity \([14]\). Both quantities can be calculated. The results as a function of the temperature \( \beta \), for fixed values of \( \lambda \) and \( \gamma \), are shown in Fig. 3. Consistently with the results in Fig. 2 there is always non-zero entanglement with respect to \( S^2_\pi \), for \( \beta \neq 0 \). The entanglement of formation with respect to \( S^2_\pi \) is, for any other value of the temperature, strictly smaller, and in fact the reduced density matrix starts to be entangled at a finite value of \( \beta \).

VII. DETAILED PROOFS

This section contains the detailed proofs of all the inclusions and equivalences that appear in the text. Table II summarizes all the definitions and the relations among sets.

A. Product states

A.1. \( \mathcal{P}0 \equiv \mathcal{P}1 \)

**Proof.** States in \( \mathcal{P}1 \) satisfy the restriction that

\[ \rho(A_\pi B_\pi) = \hat{\rho}_A(A_\pi)\hat{\rho}_B(B_\pi) \]

for some product state \( \hat{\rho} \) and all parity conserving operators \( A_\pi, B_\pi \). Since the only elements or \( \rho \) contributing to such expectation values are in the diagonal blocks \( \mathbb{P}^A_\alpha \otimes \mathbb{P}^B_\beta \rho \mathbb{P}^A_\alpha \otimes \mathbb{P}^B_\beta, (\alpha, \beta = e, o) \), the condition is equivalent to saying that the sum of these blocks is equal to the (parity commuting) product state \( \hat{\rho} = \hat{\rho}_A \otimes \hat{\rho}_B \).

The condition for \( \rho \in \mathcal{P}1 \) turns out to be equivalent to this. We may decompose the state as a sum

\[ \rho = \sum_{\alpha, \beta = e, o} \mathbb{P}^A_\alpha \otimes \mathbb{P}^B_\beta \rho \mathbb{P}^A_\alpha \otimes \mathbb{P}^B_\beta + R := \rho' + R, \]

where \( \rho' \) is a density matrix commuting with \( \hat{P}_A \) and \( \hat{P}_B \), and \( R \) contains only the terms that violate parity in some subspace. It is easy to check that \( R \) gives no contribution to expectation values of the form \( \rho(A_\pi B_\pi) \), so that \( \rho'(A_\pi B_\pi) = \rho'(A_\pi)\rho'(B_\pi) \).

A.2. \( \mathcal{P}2 \subset \mathcal{P}1 \)

**Proof.** The inclusion \( \mathcal{P}2 \subseteq \mathcal{P}1 \) is immediate from the fact that the products of even observables in the \( A_\pi B_\pi \) correspond, via a Jordan-Wigner transformation, to products of local even operators \( \hat{A}_\pi \hat{B}_\pi \) in the Fock representation, and thus they factorize for any state in \( \mathcal{P}2 \). The strict character of the inclusion is shown with an explicit example as \( \rho_{P1} \), in Table II.

A.3. \( \mathcal{P}3 \subset \mathcal{P}1 \)

**Proof.** The inclusion \( \mathcal{P}3 \subseteq \mathcal{P}1 \) in immediate from the definitions of both sets. The example \( \rho_{P1} \notin \mathcal{P}3 \) (Table II) shows it is strict.

A.4. \( \mathcal{P}2 \neq \mathcal{P}3 \)

**Proof.** The example

\[ \rho_{P2} = \frac{1}{4} \begin{pmatrix} 1 & 1 & -1 & -1 \\ 1 & 1 & -1 & -1 \\ -1 & -1 & 1 & 1 \\ -1 & -1 & 1 & 1 \end{pmatrix}, \]

fulfills \( \rho_{P2} \in \mathcal{P}2 \), but \( \rho_{P2} \notin \mathcal{P}3 \) because it has non vanishing expectation value for products of odd operators, f.i. \( \langle e_2 c_3 \rangle_{\rho_{P2}} = i \neq 0 \).

On the other hand, it is also possible to construct a state as

\[ \rho_{P3} = \frac{1}{6} \begin{pmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & -1 \end{pmatrix}, \]

satisfying \( \rho_{P3} \in \mathcal{P}3 \) (it is easy to check the explicit characterization for \( 1 \times 1 \) modes of Table III), but \( \rho_{P3} \notin \mathcal{P}2 \) because it is not possible to write it as a tensor product.

A.5. \( \mathcal{P}2_\pi \subset \mathcal{P}1_\pi \)

**Proof.** The non strict inclusion is immediate from the result for general states (A.2). Actually, the same example \( \rho_{P1} \) is parity preserving and then shows the non equivalence of both sets.

A.6. \( \mathcal{P}2_\pi \equiv \mathcal{P}3_\pi \)

**Proof.** For any physical state \( [\rho, \hat{P}] = 0 \), the expectation value of any odd operator is null. On the other hand, all \( \mathcal{P}3 \) states (in particular those in \( \mathcal{P}3_\pi \)) fulfill \( \rho(A_\pi B_\pi) = \rho'(A_\pi)\rho'(B_\pi) \).
Since a state in $\mathcal{P}_{2\pi}$ can be written as a product of two factors each of them commuting with the local parity operator, then the only non–vanishing expectation values in these sets of states correspond to products of parity conserving local observables. It is then enough to check that
\[\rho(A_{\pi}B_{\pi}) = \rho(A_{\pi})\rho(B_{\pi}) \iff \rho = \rho_A \otimes \rho_B.\]

Given the state $\rho$ we can look at the Fock representation and write it as an expansion in the Pauli operator basis, where coefficients correspond to expectation values of products $\sigma_{a_1}^{(1)} \otimes \ldots \otimes \sigma_{a_m}^{(m)}$.

Making use of the Jordan-Wigner transformation, any product of even observables in the Fock space is mapped to a product of even operators in the subalgebras $\mathcal{A}, \mathcal{B}$. So it is easy to see that the property of factorization is equivalent in both languages and thus
\[\rho \in \mathcal{P}_{2\pi} \iff \rho \in \mathcal{P}_{3\pi}.\]

This equivalence implies also that of the convex hulls, $S_{2\pi} \equiv S_{3\pi}$. \qed
**A.7.** For pure states $P1_\pi \iff P2_\pi$

Proof. A pure state $|\Psi\rangle\langle\Psi| \in \Pi$ is such that $\hat{P}\Psi = \pm \Psi$. We consider the even case (the same reasoning applies for the odd one). Since such a state vector is a direct sum of two components, one of them even with respect to both $P_A$, $P_B$ and the other one odd with respect to both local operations, and applying the Schmidt decomposition to each of those components, it is always possible to write the state as

$$|\Psi\rangle = \sum_i \alpha_i |e_i\rangle |\varepsilon_i\rangle + \sum_i \beta_i |\alpha_i\rangle |\theta_i\rangle,$$

where $\{|e_i\rangle\}$ ($\{|\varepsilon_i\rangle\}$) are mutually orthogonal states with $P_A|e_i\rangle = +|e_i\rangle$ ($P_B|\varepsilon_i\rangle = +|\varepsilon_i\rangle$) and $\{|\alpha_i\rangle\}$ ($\{|\theta_i\rangle\}$) are mutually orthogonal states with $P_A|\alpha_i\rangle = -|\alpha_i\rangle$ ($P_B|\theta_i\rangle = -|\theta_i\rangle$).

The condition of $P1_\pi$ imposes that $\langle\Psi|A_\pi B_\pi |\Psi\rangle = \langle\Psi|A_\pi|\Psi\rangle\langle\Psi|B_\pi |\Psi\rangle$ for all parity preserving observables. In particular, we may consider those of the form

$$A_\pi = \sum_k A^e_k |e_k\rangle \langle e_k| + A^{\varepsilon}_k |\varepsilon_k\rangle \langle \varepsilon_k|,$$

$$B_\pi = \sum_k B^e_k |e_k\rangle \langle e_k| + B^{\varepsilon}_k |\varepsilon_k\rangle \langle \varepsilon_k|.$$

On these observables the restriction reads

$$\left( \sum_i |\alpha_i|^2 A^e_i + \sum_i |\beta_i|^2 A^\varepsilon_i \right) \left( \sum_i |\alpha_i|^2 B^e_i + \sum_i |\beta_i|^2 B^{\varepsilon}_i \right) = \sum_i |\alpha_i|^2 A^e_i B^e_i + \sum_i |\beta_i|^2 A^{\varepsilon}_i B^{\varepsilon}_i.$$

Let us assume that the state $\Psi$ has more than one term in the even-even sector, i.e. $\alpha_1 \neq 0$ and $\alpha_2 \neq 0$ (we may reorder the sum, if necessary). Then we apply the condition to $A_\pi = A^e_1 |e_1\rangle \langle e_1|$, $B_\pi = B^{\varepsilon}_2 |\varepsilon_2\rangle \langle \varepsilon_2|$, and applying the equality we deduce $|\alpha_1|^2 A^e_1 |\alpha_1|^2 B^{\varepsilon}_2 = 0$, and thus $|\alpha_1| |\alpha_2| = 0$, so that there can only be a single term in the $|e_1\rangle |\varepsilon_2\rangle$ sum. An analogous argument shows that also the sum of $|\alpha_i\rangle |\theta_i\rangle$ must have at most one single contribution, for the state to be in $P1_\pi$.

By applying the equality to operators $A_\pi = A^e_0 |\alpha_0\rangle \langle \alpha_0|$ and $B_\pi = B^{\varepsilon}_1 |\varepsilon_1\rangle \langle \varepsilon_1|$ we also rule out the possibility that $\Psi$ has a contribution from each sector. Then, if $\Psi \in P1_\pi$, it has one single term in the Schmidt decomposition, and therefore it is a product in the sense of $P2_\pi$. \[\square\]

**B. Separable states**

**B.1.** $S2 \subset S1$ and $S2' \subset S1$

Proof. The first (non strict) inclusion is immediate from the relation between product states \[\square\] To see that both sets are not equal, we use again an explicit example. It is possible to construct a state in $P1_\pi \subset S1_\pi$ which has non-positive partial transpose and is thus not in $S2$. However, this has to be found in bigger systems than the previous counterexamples, as in a 2-mode system the conditions for $S1_\pi$ and $S2_\pi$ are identical, as shown in Table II.

By constructing random matrices $\rho_A \otimes \rho_B$ in the parity preserving sector, and adding off-diagonal terms $R$ which are also randomly chosen, we find a counterexample $\rho_{S1_\pi}$ in a $2 \times 2$-system such that $\rho_{S1_\pi} \in P1_\pi$ by construction, but its partial transposition with respect to the subsys-
tem B, \( \rho_{S_1^1} \) has a negative eigenvalue.

When taking intersection with the set of physical states, the inclusion still holds, and it is again strict, since the counterexample \( \rho_{S_1^1} \) is in particular in \( P_{1} \).

**B.2.** \( S_{1} \equiv S_1 \cap \Pi \)

**Proof.** Obviously, \( S_{1} \subseteq S_1 \cap \Pi \). To see the converse direction of the inclusion, we consider a state \( \rho \in S_1 \cap \Pi \). Then there is a decomposition \( \rho = \sum \lambda_i \rho \), with \( \rho_i \in P_{1} \), but not necessarily in \( \Pi \). We may split the sum into the even and odd terms under the parity operator,

\[
\rho = \rho_e + \rho_o := \sum \lambda_i \frac{1}{2} (\rho_i + \hat{P} \rho_i \hat{P}) + \sum \lambda_i \frac{1}{2} (\rho_i - \hat{P} \rho_i \hat{P}).
\]

The second term, \( \rho_o \), gives no contribution to operators that commute with \( \hat{P} \). Since \( \rho \) is physical, this term also gives zero contribution to odd observables, so that

\[
\rho = \sum \lambda_i \frac{1}{2} (\rho_i + \hat{P} \rho_i \hat{P}).
\]

It only remains to be shown that each \( \rho_i \) is a product state in \( P_{1} \). But since for parity commuting observables all the contributions come from the symmetric part of the density matrix, \( \rho_i (A_{l}B_{l}) = \rho_i (A_{l}B_{l}) \), and the condition for \( P_{1} \) holds for \( \rho_i \). Therefore we have found a convex decomposition of \( \rho \) in terms of product states all of them conforming to the symmetry.

The analogous relation for \( S_{2} \) was shown in [23].

**B.3.** \( S_{2} \subset S_{2}^{\prime} \)

**Proof.** Since \( P_{2} = P_{2} \cap \Pi \), taking convex hulls and intersecting again with \( \Pi \) implies that \( S_{2} \subset S_{2}^{\prime} \). However, not all separable states can be decomposed as a convex sum of product states all of them conforming to the parity symmetry. In particular, the state

\[
\rho_{S_{2}^{\prime}} \equiv \frac{1}{4} \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 1 & 0 \\
0 & 1 & 1 & 0 \\
0 & 0 & 0 & 1
\end{pmatrix},
\]

which has PPT and is thus in \( S_{2}^{\prime} \), is not in \( S_{2} \) (recall that for the 1 \( \times \) 1-system, only density matrices which are diagonal in the number basis are in \( S_{2} \)).

**B.4.** \( [S_{1}] = [S_{2}^{\prime}] = [S_{2}] \)

**Proof.** From the relations \( S_{2} \subset S_{2}^{\prime} \subset S_{1} \) and the definition of the equivalence classes it is evident that \( [S_{2}] \subseteq [S_{2}^{\prime}] \subseteq [S_{1}] \). To show the equivalence of all sets it is enough to prove that any state \( \rho \in [S_{1}] \) is also in \( [S_{2}] \), i.e. that there exists a state in \( S_{2} \) equivalent to \( \rho \).

For \( \rho \in [S_{1}] \), there is a \( \tilde{\rho} \in S_{1} \), i.e. \( \tilde{\rho} = \sum \lambda_i \tilde{\rho}_i \) with each \( \tilde{\rho}_i \in P_{1} \), producing identical expectation values for products of even operators \( A_{l}B_{l} \). If we define

\[
\rho_{\lambda} \equiv \sum_{\alpha,\beta=\epsilon,\sigma} P_{\alpha} A_{\alpha} \otimes P_{\beta} B_{\beta} \tilde{\rho}_{\alpha} A_{\alpha} \otimes P_{\beta} B_{\beta},
\]

it is evident that \( \rho' = \sum \lambda \tilde{\rho}_i \) produces the same expectation values as \( \tilde{\rho} \) for the relevant operators (see proof [A.1]). Therefore, \( \rho \sim \rho' \). Moreover, since \( \rho_{\lambda}(A_{\epsilon}B_{\epsilon}) = 0 \) for all odd-odd products, every \( \tilde{\rho}_i \in P_{2} \), and so \( \rho' \in S_{2} \).

**C.** Multiple copies

**C.1.** \( \rho^{\otimes 2} \in [S_{1}] \Rightarrow \rho \in [S_{1}] \)

**Proof.** An arbitrary state can be decomposed in two terms, \( \rho = \rho_{E} + \rho_{O} \), where

\[
\rho_{E} := \sum_{\alpha,\beta=\epsilon,\sigma} P_{\alpha} A_{\alpha} \otimes P_{\beta} B_{\beta} \tilde{\rho}_{\alpha} A_{\alpha} \otimes P_{\beta} B_{\beta},
\]

and

\[
\rho_{O} := \sum_{\alpha,\beta,\gamma,\delta = \epsilon,\sigma} \rho_{\alpha} \tilde{\rho}_{\beta} \otimes P_{\gamma} B_{\gamma} \otimes P_{\delta} B_{\delta}.
\]

For any state in \( S_{1} \), there exists a decomposition \( \rho_{E} = \sum \lambda \tilde{\rho}_i \), \( \rho_{O} = \sum \lambda \tilde{\rho}_i \), such that \( \rho_{E} + \rho_{O} \in P_{1} \). Let us consider two copies of a state such that \( \tilde{\rho} := \rho^{\otimes 2} \). Then, using the above decomposition of \( \tilde{\rho} \), and taking the partial trace with respect to the second system, we obtain a decomposition of the single copy, \( \rho = \rho_{E} + \rho_{O} = \sum \lambda \tilde{\rho}_i \), \( \tilde{\rho}_i \), where \( \sum \lambda \tilde{\rho}_i \in P_{2} \). If we consider \( \tilde{\rho} := \rho^{\otimes 2} = \rho_{E} + \rho_{O} \), the condition \([S_{1}]\) on the state of the two copies reads

\[
\rho_{E} = \rho_{E} \otimes \rho_{E} + \rho_{O} \otimes \rho_{O} \in S_{2}^{\prime},
\]

in terms of the components of the single copy state. Taking the trace with respect to one of the copies, then, and using the fact that \( \rho_{O} \) is traceless, \( \rho_{E} \in S_{2}^{\prime} \), so that \( \rho \in [S_{1}] \).

**C.3.** \( \rho \text{ NPPT} \Rightarrow \rho^{\otimes 2} \notin [S_{1}] \)
We may restrict the proof to states such that $C.2$. Written in a basis of well-defined local parities, any density matrix that commutes with the parity operator has a block structure (analogous to that of (12) for the $1 \times 1$ case).

$$\rho = \begin{pmatrix} \rho_{ee} & 0 & 0 & C \\ 0 & \rho_{eo} & D & 0 \\ 0 & D^\dagger & \rho_{oo} & 0 \\ C^\dagger & 0 & 0 & \rho_{oo} \end{pmatrix}. \quad (13)$$

The diagonal blocks correspond to the projections onto simultaneous eigenspaces of both parity operators, $\rho_{\alpha\beta} = P_\alpha \otimes P_\beta \rho P_\alpha \otimes P_\beta$, whereas $C = P_A \otimes P_B \rho P_A \otimes P_B^\dagger$ and $D = P_A^\dagger \otimes P_B^\dagger \rho P_A \otimes P_B$.

From the characterization of separability, the state is in $[S1_{1\pi}]$ iff all the diagonal blocks $\rho_{\alpha\beta}$ are in $S_{2\pi}'$. It is then enough to prove that the partial transpose of $\rho$ is positive iff $P_A^\dagger \otimes P_B^\dagger \rho \otimes \rho P_A \otimes P_B^\dagger$ has PPT. Non positivity of the partial transpose of $\rho$ implies then the non separability of $S_{2\pi}'$ of the one of the diagonal blocks of $\rho \otimes \rho$.

The partial transposition of the above matrix yields

$$\rho_{TB} = \begin{pmatrix} \rho_{ee} & 0 & 0 & D' \\ 0 & \rho_{eo} & C' & 0 \\ 0 & (C'^\dagger) & \rho_{oe} & 0 \\ (D')^\dagger & 0 & 0 & \rho_{oo} \end{pmatrix}, \quad (14)$$

where $X' := X_{TB}$, and the $T_B$ operation acts on each block transposing the last $m_B - 1$ indices.

If we take two copies of the state, we find for the corresponding uppermost diagonal block $\rho_{ee} := P_A^\dagger \otimes P_B^\dagger \rho \otimes \rho P_A^\dagger \otimes P_B$, $\rho_{ee} =$

$$\begin{pmatrix} \rho_{ee} & 0 & 0 & C \\ 0 & \rho_{eo} & D \otimes D & 0 \\ 0 & D^\dagger \otimes D^\dagger & \rho_{oe} \otimes \rho_{oo} & 0 \\ C^\dagger \otimes C^\dagger & 0 & 0 & \rho_{oo} \otimes \rho_{oo} \end{pmatrix}, \quad (15)$$

and for the partial transposition

$$\rho_{ee}^{TB} = \begin{pmatrix} \rho_{ee} & 0 & 0 & D' \otimes D' \\ 0 & \rho_{eo} \otimes \rho_{eo} & C' \otimes C' & 0 \\ 0 & C'^\dagger \otimes C'^\dagger & \rho_{oe} \otimes \rho_{oo} & 0 \\ D'^\dagger \otimes D'^\dagger & 0 & 0 & \rho_{oo} \otimes \rho_{oo} \end{pmatrix}. \quad (16)$$

The matrices (13) and (16) are the direct sum of two blocks. Thus they are positive definite iff each such block is positive definite. Let us consider one of the blocks of (16), namely

\[ \begin{pmatrix} \rho_{ee} & \rho_{ee}' \\ D \otimes D' & (D' \otimes D')^{\dagger} \end{pmatrix}. \quad (17) \]

Let us first assume that $\rho_{ee}'$ is non-singular. Applying a standard theorem in matrix analysis and making use of the fact that our $\rho \in [S1_{1\pi}]$, so that each diagonal block is PPT, we obtain that (17) is positive iff

$$\rho_{ee}' \otimes \rho_{ee} \geq (D' \otimes D')(\rho_{ee}^{-1} \otimes \rho_{ee}^{-1})(D'^\dagger \otimes D'^\dagger),$$

which holds iff

$$\rho_{ee}' \geq (D' \rho_{ee})^{-1} D'^\dagger. \quad (18)$$

The result holds also if the assumption of non-singularity of $\rho_{ee}$ ($\rho_{oe}$ for the second block) is not valid. In that case, we may take $\rho_{oo}$ diagonal and then, by positivity of $(\rho_{ee})_{TB}$ (or $\rho_{TB}$ for the reverse implication), find that $D'$ must have some null columns. This allows us to reduce both matrices to a similar block structure, where the reduced $\rho_{oo}$ ($\rho_{oe}$) is non-singular.

\section{C.4. For $1 \times 1$ systems, $\rho \otimes 2 \in [S1_{\pi}] \iff \rho \in S_{2\pi}'$}

Proof. One of the directions is immediate, and valid for an arbitrarily large system, since $\rho \in S_{2\pi}'$ implies $\rho \otimes 2 \in S_{2\pi}' \subset S_{1\pi} \subset [S1_{\pi}]$. On the other hand, if we take $\rho := \rho \otimes 2 \in [S1_{\pi}]$, then the diagonal blocks of this state are separable, in particular $P_A^\dagger \otimes P_B^\dagger \rho P_A \otimes P_B^\dagger \in S_{2\pi}'$, which was calculated in (15). For the case of $1 \times 1$ modes, with $\rho$ given by (12), this block reads

$$\begin{pmatrix} 1 - x - y + z \quad 0 \quad 0 \quad r^2 \\ 0 \quad (x - z)^2 \quad s^2 \quad 0 \\ 0 \quad (s^*)^2 \quad (y - z)^2 \quad 0 \\ (r^*)^2 \quad 0 \quad 0 \quad z^2 \end{pmatrix}. $$

This is in $S_{2\pi}'$ iff it has PPT, and this happens if and only if $\rho$ has PPT, i.e. $\rho \in S_{2\pi}'$.

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