Entanglement in fermionic systems

Mari-Carmen Bañuls,* J. Ignacio Cirac, and Michael M. Wolf
Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Strasse 1, 85748 Garching, Germany
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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. The behavior of the various classes when taking multiple copies of a state is also studied, showing that some of the differences vanish in the asymptotic regime. In particular, in the case of only two fermionic modes all the classes become equivalent in this limit. We illustrate the differences and relations 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.

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I. INTRODUCTION

The definition of entanglement in a composite quantum system [1] depends on a notion of locality, which is typically assigned to a tensor product structure or to commuting sets of observables [2]. Various *a priori* different definitions can then be formulated depending on requirements concerning preparation, representation, observation, and application. Fortunately, most of them usually coincide [32].

In the present paper we investigate systems of fermions where several of these definitions differ due to indistinguishability, anticommutation 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, we study the entanglement between sets of modes or regions in space rather than between particles. The latter case was studied in first quantization in [3–5] whereas entanglement between distinguishable modes of fermions has been calculated for various systems in [6–12].

The presence of superselection rules affects the concept of entanglement, as it has been pointed out and studied in detail in [13–17]. There, the existence of states was shown, which are convex combinations of product states but not locally preparable, since the superselection rule restricts local operations to those commuting with the conserved quantity. 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 anticommutation 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 Sec. II we introduce the basic ideas and tools used in the rest of the paper. First we define the different sets of product states in Sec. III. From them, several sets of separable states are constructed by convex combination in Sec. IV. It is shown that they all correspond to four different classes, each of them containing the previous ones as proper subsets:

(1) States which are preparable by means of local operations and classical communication (LOCC_S) [33].

(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 V analyzes the asymptotic properties of the various sets of separable states. Our results suggest that the various definitions become equivalent in the asymptotic regime. This equivalence is strictly proven in the case of a system with only two fermionic modes. As an illustration of all these concepts, Sec. VI shows the complete characterization of the different sets in the case of a 1×1-mode system, and their application to the thermal state of an infinite chain of fermions interacting with a particular Hamiltonian. Section VII summarizes all the results to provide a global view of this work. In order to improve the readability of the paper, we have compiled the detailed proofs of all the relations in the Appendix.

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, $c_{2k-1}:=a_k^\dagger+a_k$, $c_{2k}:=(-i)(a_k^\dagger-a_k)$, for $k=1,\ldots m$, which satisfy $\{c_i,c_j\}=\delta_{ij}$. Either set generates the algebra $\mathcal{C}$ of all observables. A bipartition of the system is defined by two subsets 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 kth mode, i.e., the expectation value of the operator $a_k^\dagger a_k$, the Fock basis can be defined by

*banu1sm@mpq.mpg.de

$$|n_1, \ldots, n_m\rangle = (a_1^\dagger)^{n_1} \cdots (a_m^\dagger)^{n_m}|0\rangle. \tag{1}$$

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

$$c_{2k-1} = \prod_{i=1}^{k-1} \sigma_z^{(i)}\sigma_x^{(k)}, \quad c_{2k} = \prod_{i=1}^{k-1} \sigma_z^{(i)}\sigma_y^{(k)}. \tag{2}$$

Thus, 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 nonlocal. In the same sense, not all the operators in $\mathcal{A}$ ($\mathcal{B}$) can be considered local to one of the partitions.

For the fermionic systems under consideration, conservation of the parity of the fermion number,

$$\hat{P} = i^m \prod_k c_k = \prod_k (1 - 2a_k^\dagger a_k),$$

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 $\hat{P}$, so that we can define the set of physical states

$$\Pi \coloneqq \{\rho : [\rho, \hat{P}] = 0\}.$$

Correspondingly, $\mathcal{A}_\pi$ and $\mathcal{B}_\pi$ will designate the sets of local physical observables, commuting with the local parity operators $\hat{P}_A$ and $\hat{P}_B$, respectively.

In the following, we use the expression "even observable" for those observables that commute with the parity operator, i.e., that can be written as a sum of products of an even number of fermionic operators c_k (equivalently a_k, $a_k^\dagger$). Correspondingly, an "odd" observable will be one that anticommutes with $\hat{P}$, and is thus decomposable as a sum of odd products of fermionic operators. Notice that even and odd observables do not correspond to the even and odd eigenspaces of $\hat{P}$, for instance an observable with support on the subspace of odd parity will be "even" in the former nomenclature, since it commutes with $\hat{P}$.

It will be convenient to make use of the projectors onto the well-defined parity subspaces $\mathbb{P}_{e(o)}$. Any state (or operator) commuting with parity has a block diagonal structure $\rho = \mathbb{P}_e \rho \mathbb{P}_e + \mathbb{P}_o \rho \mathbb{P}_o$. In the local subspaces, correspondingly, a parity conserving operator can be written $A_\pi = \mathbb{P}_e^A A_\pi \mathbb{P}_e^A + \mathbb{P}_o^A A_\pi \mathbb{P}_o^A$.

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]. In the case of fermionic systems, 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

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

which necessarily satisfies $i\Gamma \leq \mathbb{1}$. According to Wick's theorem, the covariance matrix determines completely all the correlation functions of a Gaussian state. Pure fermionic Gaussian states satisfy $\Gamma^2 = -\mathbb{1}$, 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 a 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 $\mathbb{C}^{2m_A} \otimes \mathbb{C}^{2m_B}$. At the level of the operator subalgebras, on the other hand, one could study the entanglement between $\mathcal{A}$ and $\mathcal{B}$ subalgebras. However, the observables in them do not commute, in general, and have nonlocal action in Fock space. On the contrary, $\mathcal{A}_\pi$ and $\mathcal{B}_\pi$, i.e., the subalgebras of parity conserving operators, commute with each other, and they can be considered local to both parties in a physical sense, as discussed in the previous section. 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 I.

(1) We may call a state ρ a product if there exists some state, acting on the Fock space, of the form $\tilde{\rho} = \tilde{\rho}_A \otimes \tilde{\rho}_B$, such that it yields the same expectation values as ρ for all local observables. Formally,

$$\mathcal{P}0 \coloneqq \{\rho : \exists\, \tilde{\rho}_A, \tilde{\rho}_B, [\tilde{\rho}_{A(B)}, \hat{P}_{A(B)}] = 0 \quad \text{such that} \quad \rho(A_\pi B_\pi) = \tilde{\rho}_A(A_\pi)\tilde{\rho}_B(B_\pi)\ \forall\ A_\pi \in \mathcal{A}_\pi, B_\pi \in \mathcal{B}_\pi\}. \tag{3}$$

Notice that in the expression above, as in the following, we use for the expectation values the notation $\rho(X) \coloneqq \mathrm{tr}(\rho X)$.

(2) Alternatively, product states may be defined as those for which all the expectation values of products of local observables factorize,

$$\mathcal{P}1 \coloneqq \{\rho : \rho(A_\pi B_\pi) = \rho(A_\pi)\rho(B_\pi)\ \forall\ A_\pi \in \mathcal{A}_\pi, B_\pi \in \mathcal{B}_\pi\}. \tag{4}$$

(3) At the level of the Fock representation, a product state can be defined as that writable as a tensor product,

TABLE I. Relations among sets of product states.

Set	Definition	Relation	Example in 1×1
$\mathcal{P}0$	$\rho(A_\pi B_\pi)=\tilde{\rho}(A_\pi B_\pi)$, $\tilde{\rho}\in\mathcal{P}2$	$\mathcal{P}0=\mathcal{P}1$	$\rho_{\mathcal{P}1}=\frac{1}{16}\begin{pmatrix}9 & 0 & 0 & -i\\ 0 & 3 & -i & 0\\ 0 & i & 3 & 0\\ i & 0 & 0 & 1\end{pmatrix}\in\mathcal{P}1_\pi\backslash\mathcal{P}2_\pi$
$\mathcal{P}1$	$\rho(A_\pi B_\pi)=\rho(A_\pi)\rho(B_\pi)$	$\mathcal{P}2\subset\mathcal{P}1$	
$\mathcal{P}2$	$\rho=\rho_A\otimes\rho_B$	$\mathcal{P}3\subset\mathcal{P}1$	$\rho\mathcal{P}2=\frac{1}{4}\begin{pmatrix}1 & 1 & -1 & -1\\ 1 & 1 & -1 & -1\\ -1 & -1 & 1 & 1\\ -1 & -1 & 1 & 1\end{pmatrix}\in\mathcal{P}2\backslash\mathcal{P}3$
$\mathcal{P}3$	$\rho(AB)=\rho(A)\rho(B)$	$\mathcal{P}2\neq\mathcal{P}3$	$\rho_{\mathcal{P}3}=\frac{1}{6}\begin{pmatrix}2 & 2 & 0 & 0\\ 2 & 2 & 0 & 0\\ 0 & 0 & 1 & -1\\ 0 & 0 & -1 & 1\end{pmatrix}\in\mathcal{P}3\backslash\mathcal{P}2$

$$\mathcal{P}2 \coloneqq \{\rho : \rho = \rho_A \otimes \rho_B\}. \tag{5}$$

(4) From the point of view of the entanglement between the subalgebras of observables for both partitions, one may ignore the commutation with the parity operator and require factorization of any product of observables [22]. This yields another set of product states,

$$\mathcal{P}3 \coloneqq \{\rho : \rho(AB) = \rho(A)\rho(B) \quad \forall\ A \in \mathcal{A}, B \in \mathcal{B}\}. \tag{6}$$

The two first definitions are equivalent, $\mathcal{P}0 \equiv \mathcal{P}1$. They correspond to states whose projection onto the diagonal blocks, i.e., those that preserve parity in each of the subsystems, is separable. This means that

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

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 $\mathcal{P}2, \mathcal{P}3 \subseteq \mathcal{P}1$ is immediate from the definitions. The nonequality of the sets can be seen by explicit examples as those shown in Table I (each example is discussed in detail in Appendix A 1). The difference between $\mathcal{P}3$ and $\mathcal{P}2$, however, is limited to nonphysical states, i.e., those not commuting with parity [22].

B. Physical states

Physical states must commute with $\hat{P}$, since parity is a conserved quantity in the systems under analysis. It makes sense then to restrict the study of entanglement to such states. By applying each of the above definitions to the physical states Π we obtain the following sets of physical product states:

$$\mathcal{P}1_\pi \coloneqq \mathcal{P}1 \cap \Pi = \mathcal{P}0 \cap \Pi.$$

$$\mathcal{P}2_\pi \coloneqq \mathcal{P}2 \cap \Pi.$$

$$\mathcal{P}3_\pi \coloneqq \mathcal{P}3 \cap \Pi.$$

We notice that $\rho \in \mathcal{P}2_\pi$ is equivalent to $\rho = \rho_A \otimes \rho_B$ where both factors are also parity conserving.

With the parity restriction, the three sets are related by

$$\mathcal{P}3_\pi = \mathcal{P}2_\pi \subset \mathcal{P}1_\pi. \tag{7}$$

The proofs of all the relations above are shown in Appendix A 1.

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 an expansion has a single nonvanishing coefficient, and thus the state can be written as a tensor product also with the definition of $\mathcal{P}2$.

IV. SEPARABLE STATES

Generally speaking, separable states are those that can be written as convex combinations of product states. The convex hulls of the different sets of product states introduced in the previous section define then various separability sets. Figure 1 outlines the procedure to obtain each of these sets. Table II summarizes the different definitions and the relations between them.

A. General states

Taking the convex hull of the general product states, we define the sets

$$\mathcal{S}1 \coloneqq \mathrm{co}(\mathcal{P}1),$$

$$\mathcal{S}2 \coloneqq \mathrm{co}(\mathcal{P}2),$$

$$\mathcal{S}3 \coloneqq \mathrm{co}(\mathcal{P}3).$$

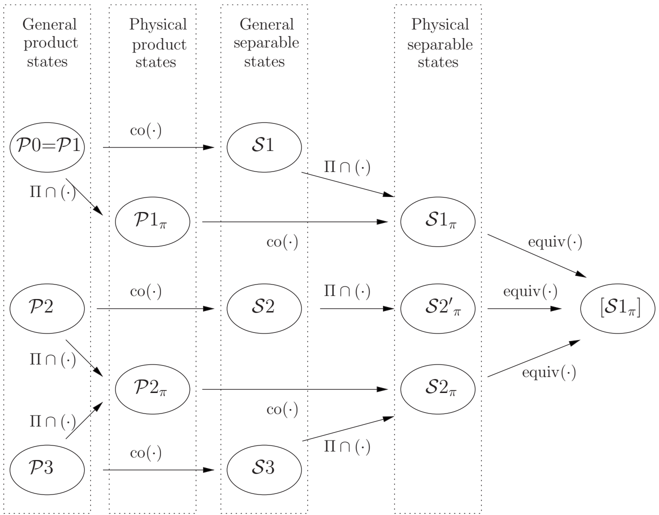

FIG. 1. Scheme of the construction of the different sets.

These contain both physical states, commuting with $\hat{P}$, and nonphysical ones. It can be shown that $\mathcal{S}3 \subset \mathcal{S}2 \subset \mathcal{S}1$.

The nonstrict inclusion $\mathcal{S}2 \subseteq \mathcal{S}1$ is immediate from the inclusion between product sets. The strict character can be seen by constructing an explicit example, as discussed in Appendix A 2. On the other hand, $\mathcal{S}3 \subset \mathcal{S}2$ was proved in [22].

B. Physical states

From the physical sets of product states we define the following sets of separable states:

$$\mathcal{S}1_\pi \coloneqq \mathrm{co}(\mathcal{P}1_\pi),$$

$$\mathcal{S}2_\pi \coloneqq \mathrm{co}(\mathcal{P}2_\pi).$$

Obviously, the corresponding $\mathcal{S}3_\pi \equiv \mathcal{S}2_\pi$. The inclusion relations among product states imply $\mathcal{S}2_\pi \subseteq \mathcal{S}1_\pi$. It is easy to see with an example that this inclusion is also strict. Table II summarizes the definitions and mutual relations of the various separability sets.

As shown in Fig. 1, we may take the physical states that satisfy the general definitions of separability introduced in the previous subsection, and hence use $\mathcal{S}i \cap \Pi$ as the definition of separable states. This yields the sets

$$\mathcal{S}1 \cap \Pi \equiv \mathcal{S}1_\pi,$$

$$\mathcal{S}2'_\pi \coloneqq \mathcal{S}2 \cap \Pi,$$

$$\mathcal{S}2 \cap \Pi \equiv \mathcal{S}2_\pi.$$

Only $\mathcal{S}2'_\pi$ is different from the separable sets defined above. Actually, given an $\mathcal{S}1$ state that commutes with $\hat{P}$, it is possible to construct a decomposition according to $\mathcal{S}1_\pi$ by taking the parity preserving part of each term in the original convex combination. Therefore $\mathcal{S}1 \cap \Pi \subseteq \mathcal{S}1_\pi$, while the converse inclusion is evident. For $\mathcal{S}3 \cap \Pi$, on the other hand, it was shown in [22] that any parity preserving state in $\mathcal{S}3$ has a decomposition in terms of only parity preserving terms, and is thus in $\mathcal{S}3_\pi$.

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

$$\mathcal{S}2_\pi \subset \mathcal{S}2'_\pi \subset \mathcal{S}1_\pi. \tag{8}$$

From the definitions, it is immediate that $\mathcal{S}2_\pi \subseteq \mathcal{S}2'_\pi$. The inclusion is strict because not every state $\rho \in \mathcal{S}2'_\pi$ has a decomposition in terms of products of even states (see example

TABLE II. The different sets of separable states and their relations. $\mathcal{S}2_\pi$ contains all states preparable by means of LOCC$_S$. $\mathcal{S}2'_\pi$ represents the usual definition of separability in Fock space, when no restriction from superselection rules is imposed. $\mathcal{S}1_\pi$ gives all convex combinations of states for which expectation values of products of locally measurable observables factorize. $[\mathcal{S}1_\pi]$ contains all states which are locally indistinguishable from $\mathcal{S}1_\pi$.

Set	Definition	Characterization	Relations	Example in 1×1
$[\mathcal{S}1_\pi]$	$[\mathcal{S}1_\pi]$	$\sum_{\alpha,\beta=e,o}\mathbb{P}^A_\alpha\otimes\mathbb{P}^B_\beta\rho\mathbb{P}^A_\alpha\otimes\mathbb{P}^B_\beta\in\mathcal{S}2'_\pi$		$\rho_{[\mathcal{S}1_\pi]}=\frac{1}{15}\begin{pmatrix}5&0&0&2\sqrt{5}\\0&3&3&0\\0&3&3&0\\2\sqrt{5}&0&0&4\end{pmatrix}\in[\mathcal{S}1_\pi]\backslash\mathcal{S}1_\pi$
			$\mathcal{S}1_\pi\subset[\mathcal{S}1_\pi]$	
$\mathcal{S}0_\pi$	$\mathrm{co}(\mathcal{P}0_\pi)$			For the 1×1 case, $\mathcal{S}1_\pi=\mathcal{S}2'_\pi$.
		$\rho=\sum_k\lambda_k\rho_k$, such that	$\mathcal{S}1_\pi=\mathcal{S}0_\pi$	Therefore examples of $\mathcal{S}1_\pi\backslash\mathcal{S}2'_\pi$ can
$\mathcal{S}1_\pi$	$\mathrm{co}(\mathcal{P}1_\pi)$	$\sum_{\alpha,\beta=e,o}\mathbb{P}^A_\alpha\otimes\mathbb{P}^B_\beta\rho_k\mathbb{P}^A_\alpha\otimes\mathbb{P}^B_\beta\in\mathcal{S}2'_\pi$		only be found in bigger systems, for
			$\mathcal{S}2'_\pi\subset\mathcal{S}1_\pi$	instance 2×2 modes.
$\mathcal{S}2'_\pi$	$\mathrm{co}(\mathcal{P}2)\cap\Pi$	$\rho=\sum_k\lambda_k\rho^k_A\otimes\rho^k_B$		$\rho_{\mathcal{S}2'_\pi}=\frac{1}{4}\begin{pmatrix}1&0&0&0\\0&1&1&0\\0&1&1&0\\0&0&0&1\end{pmatrix}\in\mathcal{S}2'_\pi\backslash\mathcal{S}2_\pi$
			$\mathcal{S}2_\pi\subset\mathcal{S}2'_\pi$	
$\mathcal{S}2_\pi$	$\mathrm{co}(\mathcal{P}2_\pi)$	$\mathbb{P}_e\rho\mathbb{P}_e\in\mathcal{S}2'_\pi$, $\mathbb{P}_o\rho\mathbb{P}_o\in\mathcal{S}2'_\pi$		$\rho\in\mathcal{S}2_\pi\Leftrightarrow\rho$ diagonal

$\rho_{\mathcal{S}2'_\pi}$ in Table II). The condition for $\mathcal{S}2_\pi$ is then more restrictive.

From the relation between product sets, $\mathcal{S}2 \subseteq \mathcal{S}1$, and $\mathcal{S}2'_\pi \subseteq \mathcal{S}1_\pi$. The strict inclusion can be shown by constructing an explicit example of a $\mathcal{P}1_\pi$ state without positive partial transpose (PPT) [23] in the 2×2-modes system.

The detailed proofs of the equivalences and inclusions above are shown in Appendix A 2.

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

$$\rho_1 \sim \rho_2 \quad \text{if} \quad \rho_1(A_\pi B_\pi) = \rho_2(A_\pi B_\pi) \quad \forall\ A_\pi \in \mathcal{A}_\pi, B_\pi \in \mathcal{B}_\pi,$$

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 $\mathcal{S}2_\pi$, i.e., $\rho = \Sigma_k \lambda_k \rho_A^k \otimes \rho_B^k$, where $[\rho_{A(B)}^k, \hat{P}_{A(B)}]=0$. Since the only locally accessible observables are local, parity preserving operators, i.e., quantities of the form $\rho(A_\pi B_\pi)$, 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 then given by the equivalence class of $\mathcal{S}2_\pi$ with respect to the equivalence relation above, $[\mathcal{S}2_\pi]$.

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

$$[\mathcal{S}i_\pi] \coloneqq \{\rho: \exists\ \tilde{\rho} \in \mathcal{S}i_\pi, \rho \sim \tilde{\rho}\}, \quad i = 1,2',2.$$

From the inclusion relation among the separability sets, $[\mathcal{S}2_\pi] \subseteq [\mathcal{S}2'_\pi] \subseteq [\mathcal{S}1_\pi]$. And, obviously, $\mathcal{S}i_\pi \subseteq [\mathcal{S}i_\pi]$.

On the other hand, any state $\rho \in [\mathcal{S}1_\pi]$ has also an equivalent state in $\mathcal{S}2_\pi$, so that

$$[\mathcal{S}2_\pi] = [\mathcal{S}2'_\pi] = [\mathcal{S}1_\pi].$$

This equivalence class includes then all the separability sets described in the previous subsection. However, it is strictly larger than all of them, as can be seen by the explicit example $\rho_{[\mathcal{S}1_\pi]}$ in Table II (see also Appendix A 2).

We have then defined four different sets of separable states, which can be now put in correspondence to the four classes of states mentioned in the Introduction.

(1) States preparable by local operations, subject to the restriction of parity conservation, and classical communication will be separable according to $\mathcal{S}2_\pi$.

(2) Any convex combination of product states in the Fock representation will be separable according to $\mathcal{S}2'_\pi$.

(3) Convex combinations of states for which all products of locally measurable observables factorize are separable as for $\mathcal{S}1_\pi$.

(4) Finally, $[\mathcal{S}2_\pi]$ contains the states such that all correlations that can be locally measured can also be produced by a separable state in any of the classes above.

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 [24] for a recent review) in order to decide whether a given state is in each of these sets.

The definition $\mathcal{S}2'_\pi$ corresponds to the separability in the sense of the tensor product, i.e., the standard notion [1], applied to parity preserving states.

As convex hull of $\mathcal{P}2 \cap \Pi$, the set $\mathcal{S}2_\pi$ 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 $\mathbb{P}_e \rho \mathbb{P}_e + \mathbb{P}_o \rho \mathbb{P}_o$ of any parity preserving state, we conclude that each block must have an independent decomposition in the sense of the tensor product. Therefore a state will be in $\mathcal{S}2_\pi$ iff both $\mathbb{P}_e \rho \mathbb{P}_e$ and $\mathbb{P}_o \rho \mathbb{P}_o$ are in $\mathcal{S}2'_\pi$.

A state ρ is in $\mathcal{P}0_\pi$ if its diagonal blocks are a tensor product,

$$\sum_{\alpha,\beta=e,o} \mathbb{P}_\alpha^A \otimes \mathbb{P}_\beta^B \rho \mathbb{P}_\alpha^A \otimes \mathbb{P}_\beta^B = \tilde{\rho}_A \otimes \tilde{\rho}_B \in \mathcal{P}2_\pi. \tag{9}$$

The set $\mathcal{S}1_\pi$ is characterized as the convex hull of $\mathcal{P}1_\pi \equiv \mathcal{P}0_\pi$, 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 $[\mathcal{S}1_\pi] \equiv [\mathcal{S}2_\pi]$ is completely defined in terms of the expectation values of observable products $A_\pi B_\pi$. These have no contribution from off-diagonal blocks in ρ, so the class can be characterized in terms of the diagonal blocks alone. Therefore a state is in $[\mathcal{S}1_\pi]$ iff

$$\sum_{\alpha,\beta=e,o} \mathbb{P}_\alpha^A \otimes \mathbb{P}_\beta^B \rho \mathbb{P}_\alpha^A \otimes \mathbb{P}_\beta^B \in \mathcal{S}2'_\pi. \tag{10}$$

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.

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 behavior when $N \to \infty$.

The criteria $\mathcal{S}2'_\pi$ and $\mathcal{S}2_\pi$ are stable when several copies of the state are considered.

$$\rho^{\otimes 2} \in \mathcal{S}2'_\pi \Leftrightarrow \rho \in \mathcal{S}2'_\pi,$$

TABLE III. Characterization of the sets for a 1×1-mode system.

General	$\rho=\begin{pmatrix}1-x-y+z & p & q & r\\ p^* & x-z & s & t\\ q^* & s^* & y-z & w\\ r^* & t^* & w^* & z\end{pmatrix}$
$\mathcal{P}1$	$z=xy$
$\mathcal{P}2$	$\rho=\rho_A\otimes\rho_B$, i.e., $\begin{cases} z=xy,\\ yp=(1-y)w,\\ xq=(1-x)t,\\ xyr=tw,\\ xys=tw^*\end{cases}$
$\mathcal{P}3$	$r=s=0$ $z=xy$ $\left\{\begin{matrix} q=t=0\\ (1-y)w=-yp\end{matrix}\right\}$ or $\left\{\begin{matrix} p=w=0\\ (1-x)t=xq\end{matrix}\right\}$
Π	$p=q=t=w=0$
$\mathcal{S}1_\pi$	$\lvert r\rvert^2\le(x-z)(y-z)$
$\mathcal{S}2'_\pi$	$\lvert s\rvert^2\le z(1-x-y+z)$
$\mathcal{S}2_\pi=\mathcal{S}3_\pi$	$r=s=0$
$[\mathcal{S}1_\pi]$	All $\rho\ge 0$

$$\rho^{\otimes 2}\in\mathcal{S}2_\pi\Leftrightarrow\rho\in\mathcal{S}2_\pi.$$

Moreover, it was shown in [15] that the entanglement cost of $\mathcal{S}2_\pi$ converges to that of $\mathcal{S}2'_\pi$, so that asymptotically both definitions are equivalent.

On the other hand, $\mathcal{S}1_\pi$ and $[\mathcal{S}1_\pi]$ do not show the same stability. It is possible to have a state $\rho\in\mathcal{S}1_\pi$ ($[\mathcal{S}1_\pi]$) such that $\rho^{\otimes 2}$ is not separable according to the same criterion. However, the opposite sense of the implication holds. As proved in Appendix A 3,

$$\rho^{\otimes 2}\in\mathcal{S}1_\pi\Rightarrow\rho\in\mathcal{S}1_\pi,$$

$$\rho^{\otimes 2}\in[\mathcal{S}1_\pi]\Rightarrow\rho\in[\mathcal{S}1_\pi].$$

It is also possible to prove that

$$\rho^{\otimes 2}\in[\mathcal{S}1_\pi]\Rightarrow\rho\text{ PPT}.$$

Therefore, a non-PPT state ρ is also nonseparable according to the broadest definition $[\mathcal{S}1_\pi]$ when one takes several copies. This is true, in particular, for distillable states [25,26]. 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 1×1 modes, as detailed in the following 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 III shows this characterization.

A generic state of a 1×1-mode system can be written in the Fock representation as

$$\rho=\begin{pmatrix}1-x-y+z & p & q & r\\ p^* & x-z & s & t\\ q^* & s^* & y-z & w\\ r^* & t^* & w^* & z\end{pmatrix},\qquad(11)$$

where x, y, z are real parameters, with the additional restrictions that ensure $\rho\ge 0$, which include $z\le x,y$, and $1+z\ge x+y$.

States in $\mathcal{P}1$ must satisfy a single relation between expectation values, namely, $\langle c_1c_2c_3c_4\rangle=\langle c_1c_2\rangle\langle c_3c_4\rangle$, which reads, in terms of the given parametrization, $z=xy$. This condition is also necessary for states in $\mathcal{P}2$ or $\mathcal{P}3$.

If a state is in $\mathcal{P}2$, it can be written as the tensor product of two one-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 III. Since $\mathcal{S}2$ corresponds to separability in the isomorphic qubit system, a state will be in $\mathcal{S}2$ iff it has PPT [27].

According to [22], a state in $\mathcal{P}3$ has zero expectation value for all observable products $A_{\#}B_{\#}$, and one of the restrictions of ρ to the subsystems is odd with respect to the parity transformation. In the 1×1 system, these conditions are fulfilled by states with one of two generic forms, shown in the table, which hence characterize product states $\mathcal{P}3$.

If we restrict the study to physical states, i.e., those commuting with $\hat{P}$, the density matrix has a block diagonal structure, as it can be written as the direct sum of two terms, which correspond to both parity eigenspaces. We use the conventional ordering of the number basis, where this block structure is not apparent, and the most general even 1×1 state can be written

$$\rho=\begin{pmatrix}1-x-y+z & 0 & 0 & r\\ 0 & x-z & s & 0\\ 0 & s^* & y-z & 0\\ r^* & 0 & 0 & z\end{pmatrix}.\qquad(12)$$

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) is in $\mathcal{P}1_\pi$ iff $z=xy$. Convex combinations of this kind of state will produce density matrices that fulfill $|s|^2\le z(1-x-y+z)$ and $|r|^2\le(x-z)(y-z)$, and thus have PPT. This shows that, for this small system, $\mathcal{S}1_\pi\equiv\mathcal{S}2'_\pi$.

The independent separability of both blocks of ρ, which determines separability according to $\mathcal{S}2_\pi$, requires that $r=s=0$, i.e., that the density matrix is diagonal in this basis.

Finally, the characterization (10) of $[\mathcal{S}1_\pi]$ applied to Eq. (11) yields the condition that the diagonal of ρ is separable according to the tensor product, so that all states of 1×1 modes of the form (12) are in $[\mathcal{S}1_\pi]$.

If we look at several copies of such a 1×1-mode system, it is possible to show that

$$\rho^{\otimes 2} \in [\mathcal{S}1_\pi] \Leftrightarrow \rho \in \mathcal{S}2'_\pi.$$

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

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

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

This Hamiltonian can be obtained as the Jordan-Wigner transformation of an XY spin chain with transverse magnetic field [28,29]. The Hamiltonian can be exactly diagonalized by means of Fourier and Bogoliubov transformations, yielding

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

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

We consider the thermal state $\rho = \frac{e^{-\beta H}}{\mathrm{tr}[e^{-\beta H}]}$, with inverse temperature β, 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, λ, γ, and β.

First we may study which values of the parameters result in entanglement between both modes according to each of the definitions. As mentioned above, for a two-mode system there is no distinction between the sets $\mathcal{S}1_\pi$ and $\mathcal{S}2'_\pi$. Moreover, any valid density matrix is, for this small system, in $[\mathcal{S}1_\pi]$. Therefore we look for the limits of the separability regions $\mathcal{S}2'_\pi$ and $\mathcal{S}2_\pi$ for a fixed value of the parameter λ. The results are shown in Fig. 2. For any given value of λ we find that $\mathcal{S}2_\pi$ corresponds to the horizontal axis of the plots, i.e., the reduced density matrix is in $\mathcal{S}2_\pi$ only if $\beta=0$. Therefore for all finite values of the temperature two adjacent fermions will be entangled according to this criterion. The region $\mathcal{S}2'_\pi$, on the contrary, changes with the parameters, as shown by the plots.

From a quantitative point of view, the entanglement with respect to $\mathcal{S}2'_\pi$ can be measured by the entanglement of formation [30],

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

With respect to $\mathcal{S}2_\pi$, it is natural to define the entanglement of formation conforming to parity conservation as

$$E_F^\pi(\rho) = \min_{\{i,\psi_i\}} \sum_i p_i E(\psi_i),$$

where the minimization is performed over ensembles all whose ψ_i have well-defined parity [14]. Both quantities can be calculated. The results as a function of the temperature β, for fixed values of λ and γ, are shown in Fig. 3. Consistently with the results in Fig. 2, there is always nonzero entanglement with respect to $\mathcal{S}2_\pi$, for $\beta \neq 0$. The entanglement of formation with respect to $\mathcal{S}2'_\pi$ is, for any other value of the temperature, strictly smaller, corresponding to the more restrictive definition of $\mathcal{S}2_\pi$. In fact, the explicit characterization of both sets in Table III shows that the condition for $\mathcal{S}2_\pi$ will only be satisfied if all the off-diagonal elements of the reduced density matrix vanish, which only happens when $\beta=0$. On the contrary, the characterization of $\mathcal{S}2'_\pi$ involves two simultaneous conditions on the same matrix elements, but positivity of the reduced density matrix ensures that only one of them can be violated at a time. For small values of β, both conditions can be satisfied, but the reduced density matrix starts to be entangled at a finite value of β when one of the inequalities is saturated. Due to the discontinuous definition of E_F, the transition from separable to entangled state is not smooth, as it would be expected.

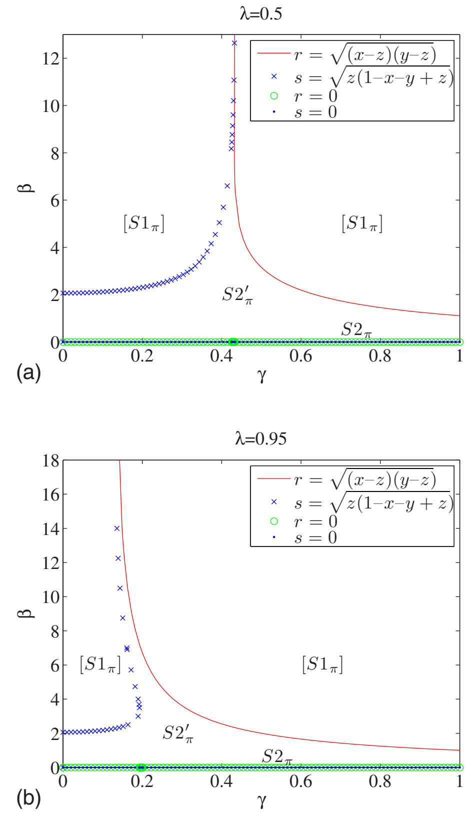

FIG. 2. (Color online) Regions of parameters that correspond to separable reduced density matrices of two neighboring fermions according to the different criteria. The different curves correspond to values of the parameters for which one of the conditions of separability (see Table III) is satisfied with equality. For a fixed value of λ [$\lambda=0.5$ for (a), $\lambda=0.95$ for (b)], the area at the bottom corresponds to values of β,γ for which the reduced density matrix is in $\mathcal{S}2'_\pi$. In both cases, the region of $\mathcal{S}2_\pi$ lies on the horizontal axis. Notice that for $\lambda=0.95$ there is a small range of values of $\gamma \lesssim 0.2$ for which the entanglement shows up when increasing the temperature, as illustrated quantitatively by the figure below.

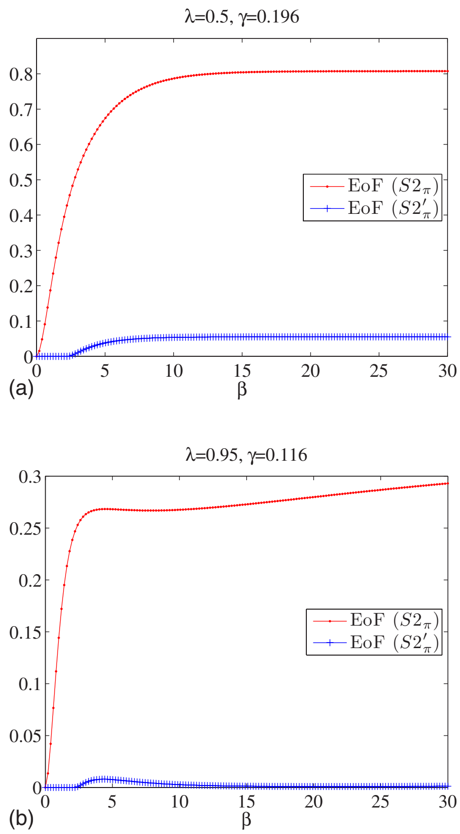

FIG. 3. (Color online) Entanglement of formation of the reduced density matrix of two neighboring fermions with respect to the sets $\mathcal{S}2_\pi$ (dots) and $\mathcal{S}2'_\pi$ (crosses), for fixed values of λ and γ, as a function of the inverse temperature.

VII. SUMMARY

In the previous sections we have studied various definitions of separability that are reasonable for a fermionic system in second quantization. The various possibilities arise from the anticommutation of fermionic operators and from the presence of the parity superselection rule.

The starting point is to analyze the different definitions of product states. We can think of four different definitions, which for physical states, i.e., those commuting with the parity operator, reduce to only two different sets: $\mathcal{P}2_\pi$, with states that are a product in the Fock representation, and $\mathcal{P}0_\pi$, containing the states whose locally measurable correlations can be reproduced by some state of $\mathcal{P}2_\pi$.

The various sets of separable states are constructed by taking the convex hull of the various sets of product states, an operation that may be performed before or after the application of the parity restriction, as summarized in Table IV. Finally we are left with four classes of separable states, which can be related to different physical capabilities of preparation or measurement of the states. $\mathcal{S}2_\pi$ represents states that can be prepared by $\text{LOCC}_\mathcal{S}$. $\mathcal{S}2'_\pi$ instead corresponds to the usual definition of separability in the Fock representation, and hence it contains states expressible as convex combinations of tensor products but not necessarily preparable by means of local operations. $\mathcal{S}1_\pi$ is constructed from the convex combinations of states such that the expectation values of all local observables factorize. Finally, states in $[\mathcal{S}1_\pi]$ are characterized by locally measurable correlations reproducible by a state that can be prepared locally. Table IV summarizes all the definitions and the relations among sets. We have also characterized the various sets in terms of the tensor product, so that the usual separability criteria can be applied to determine whether a state is or not in each of these classes.

TABLE IV. Summary of the different definitions of product and separable states.

Product states		Separable states		Equivalence classes
General	Physical	co(X)	Physical	
$\mathcal{P}0$		$\mathcal{S}0 := \text{co}(\mathcal{P}0)$	$\mathcal{S}0_\pi = \mathcal{S}0 \cap \Pi$	$[\mathcal{S}0_\pi]$
	$\mathcal{P}0_\pi := \mathcal{P}0 \cap \Pi$	$\mathcal{S}0_\pi := \text{co}(\mathcal{P}0_\pi)$		
$\mathcal{P}1$		$\mathcal{S}1 := \text{co}(\mathcal{P}1)$	$\mathcal{S}1_\pi = \mathcal{S}1 \cap \Pi$	$[\mathcal{S}1_\pi]$
	$\mathcal{P}1_\pi := \mathcal{P}1 \cap \Pi$	$\mathcal{S}1_\pi := \text{co}(\mathcal{P}1_\pi)$		
$\mathcal{P}2$		$\mathcal{S}2 := \text{co}(\mathcal{P}2)$	$\mathcal{S}2'_\pi := \mathcal{S}2 \cap \Pi$	$[\mathcal{S}2'_\pi]$
	$\mathcal{P}2_\pi := \mathcal{P}2 \cap \Pi$	$\mathcal{S}2_\pi := \text{co}(\mathcal{P}2_\pi)$	$\mathcal{S}2_\pi$	$[\mathcal{S}2_\pi]$
$\mathcal{P}3$		$\mathcal{S}3 := \text{co}(\mathcal{P}3)$	$\mathcal{S}3_\pi = \mathcal{S}3 \cap \Pi$	$[\mathcal{S}3_\pi]$
	$\mathcal{P}3_\pi := \mathcal{P}3 \cap \Pi$	$\mathcal{S}3_\pi := \text{co}(\mathcal{P}3_\pi)$		
		Relations between sets		
			$\mathcal{S}0_\pi = \mathcal{S}1_\pi$	$[\mathcal{S}0_\pi] = [\mathcal{S}1_\pi]$
$\mathcal{P}0 = \mathcal{P}1$	$\mathcal{P}0_\pi = \mathcal{P}1_\pi$	$\mathcal{S}0 = \mathcal{S}1$		
			$\mathcal{S}2'_\pi \subset \mathcal{S}1_\pi$	$[\mathcal{S}1_\pi] = [\mathcal{S}2'_\pi]$
$\mathcal{P}2$, $\mathcal{P}3 \subset \mathcal{P}1$	$\mathcal{P}2_\pi \subset \mathcal{P}1_\pi$	$\mathcal{S}2 \subset \mathcal{S}1$		
			$\mathcal{S}2_\pi \subset \mathcal{S}2'_\pi$	$[\mathcal{S}2'_\pi] = [\mathcal{S}2_\pi]$
$\mathcal{P}2 \neq \mathcal{P}3$	$\mathcal{P}2_\pi = \mathcal{P}3_\pi$	$\mathcal{S}3 \subset \mathcal{S}2$		
			$\mathcal{S}3_\pi = \mathcal{S}2_\pi$	$[\mathcal{S}2_\pi] = [\mathcal{S}3_\pi]$

When taking multiple copies of a state, the various sets behave differently. Whereas the definitions of $\mathcal{S}2_\pi$ and $\mathcal{S}2'_\pi$ are stable, the same is not true for $\mathcal{S}1_\pi$ or $[\mathcal{S}1_\pi]$. In the asymptotic regime, however, the differences among the various sets seem to disappear. In particular, $\mathcal{S}2_\pi$ and $\mathcal{S}2'_\pi$ become equivalent in the limit of a large number of copies. In the case of the smallest possible system of 1×1 modes, we have proved that the equivalence holds also for the larger classes. In the general case, multiple copies of ρ can be in $[\mathcal{S}1_\pi]$ only if the single copy is PPT. Therefore, any NPPT entangled state ρ (in particular, distillable states) will not become separable when taking several copies, even according to the broadest concept of separability, $[\mathcal{S}1_\pi]$.

Several questions remain open. Among them, the most relevant is whether all the classes of separable states collapse to a single one in the asymptotic regime.

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APPENDIX: DETAILED PROOFS

For the sake of clarity, we have compiled in this appendix the detailed proofs of all the inclusions and equivalences that appear in the text.

1. Product states

1.1. $\mathcal{P}0\equiv\mathcal{P}1$.

Proof. States in $\mathcal{P}0$ satisfy the restriction that

$$\rho(A_\pi B_\pi) = \tilde{\rho}_A(A_\pi)\tilde{\rho}_B(B_\pi)$$

for some product state $\tilde{\rho}$ and all parity conserving operators A_π, B_π. Since the only elements of ρ 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 $\tilde{\rho}=\tilde{\rho}_A\otimes\tilde{\rho}_B$.

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

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

where ρ' 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 $\rho'(A_\pi B_\pi)=\rho'(A_\pi)\rho'(B_\pi)$. On the other hand, an operator that is odd under parity has the form $A_{\not\pi}=\mathbb{P}^A_e A_{\not\pi}\mathbb{P}^A_o+\mathbb{P}^A_o A_{\not\pi}\mathbb{P}^A_e$. Therefore $\rho'(A_{\not\pi}B_{\not\pi})=0=\rho'(A_{\not\pi})\rho'(B_{\not\pi})$. Since ρ' commutes with parity, odd observables have zero expectation value. Therefore all the expectation values $\rho'(AB)$ factorize and ρ' can be written as a tensor product. ■

1.2. $\mathcal{P}2\subset\mathcal{P}1$.

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 $\tilde{A}_\pi\tilde{B}_\pi$ 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. The state

$$\rho_{\mathcal{P}1} = \frac{1}{16}\begin{pmatrix} 9 & 0 & 0 & -i \\ 0 & 3 & -i & 0 \\ 0 & i & 3 & 0 \\ i & 0 & 0 & 1 \end{pmatrix}$$

can be easily checked to be in $\mathcal{P}1_\pi$. For a 1×1-mode system, the conditions to be in $\mathcal{P}1$ reduce to a single equation (see Table III). In terms of the diagonal elements of the density matrix, this reads $\rho_{44}=(\rho_{22}+\rho_{44})(\rho_{33}+\rho_{44})$, trivially satisfied by $\rho_{\mathcal{P}1}$, which thus belongs to $\mathcal{P}1$. In particular, as the density matrix commutes with parity, $\rho_{\mathcal{P}1}\in\mathcal{P}1_\pi$. However, it is impossible to write the same state as a tensor product, and so $\rho_{\mathcal{P}1}\notin\mathcal{P}2_\pi$.

The previous example can be shown to be Gaussian. Actually, in the 1×1-mode system, the condition for a state to be Gaussian is given also by a single relation $i^2\,\mathrm{tr}(\rho c_1c_2c_3c_4)=\mathrm{Pf}(\Gamma)$, which in terms of the matrix elements and the parametrization in Table III reads $|r|^2-|s|^2=z-xy$. The previous example is easily seen to fulfill this condition, and is thus a Gaussian state. ■

1.3. $\mathcal{P}3\subset\mathcal{P}1$.

Proof. The inclusion $\mathcal{P}3\subseteq\mathcal{P}1$ is immediate from the definitions of both sets. The same example $\rho_{\mathcal{P}1}$ discussed in the previous paragraph can be used to show that the inclusion is strict. Observables of the form $A_{\not\pi}B_{\not\pi}$ have zero expectation value for all states in $\mathcal{P}3$ [22]. However, we can calculate, for instance, $\langle c_1c_3\rangle_{\rho_{\mathcal{P}1}}=i/4\neq 0$, so that $\rho_{\mathcal{P}1}\notin\mathcal{P}3$. ■

1.4. $\mathcal{P}2\neq\mathcal{P}3$.

Proof. The example

$$\rho_{\mathcal{P}2} = \frac{1}{4}\begin{pmatrix} 1 & 1 & -1 & -1 \\ 1 & 1 & -1 & -1 \\ -1 & -1 & 1 & 1 \\ -1 & -1 & 1 & 1 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}\otimes\frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix},$$

fulfills $\rho_{\mathcal{P}2}\in\mathcal{P}2$, but $\rho_{\mathcal{P}2}\notin\mathcal{P}3$ because it has nonvanishing expectation value for products of odd operators, in particular $\langle c_2c_3\rangle_{\rho_{\mathcal{P}2}}=i\neq 0$.

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

$$\rho_{\mathcal{P}3} = \frac{1}{6}\begin{pmatrix} 2 & 2 & 0 & 0 \\ 2 & 2 & 0 & 0 \\ 0 & 0 & 1 & -1 \\ 0 & 0 & -1 & 1 \end{pmatrix},$$

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

1.5. $\mathcal{P}2_\pi\subset\mathcal{P}1_\pi$.

Proof. The nonstrict inclusion is immediate from the result for general states 1.2. Actually, the same example $\rho_{\mathcal{P}1}$ is parity preserving and thus it also shows the nonequivalence of both physical sets. ∎

1.6. $\mathcal{P}2_\pi \equiv \mathcal{P}3_\pi$.

Proof. For every 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 $\rho(A_\pi B_\pi)=0$ [22]. 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 nonvanishing expectation values in these sets of states correspond to products of parity conserving local observables. It is then enough to check that

$$\rho(A_\pi B_\pi) = \rho(A_\pi)\rho(B_\pi) \Leftrightarrow \rho = \rho_A \otimes \rho_B .$$

Given the state ρ 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 $\sigma^{(1)}_{a_1} \otimes \cdots \otimes \sigma^{(m)}_{a_m}$.

Making use of the Jordan-Wigner transformation (2), 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

$$\rho \in \mathcal{P}2_\pi \Leftrightarrow \rho \in \mathcal{P}3_\pi .$$

This equivalence implies also that of the convex hulls, $\mathcal{S}2_\pi \equiv \mathcal{S}3_\pi$. ∎

Pure states

1.7. For pure states $\mathcal{P}1_\pi \Leftrightarrow \mathcal{P}2_\pi$.

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

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

where $\{|e_i\rangle\}$ ($\{|\varepsilon_i\rangle\}$) are mutually orthogonal states with $\hat{P}_A|e_i\rangle = +|e_i\rangle$ ($\hat{P}_B|\varepsilon_i\rangle = +|\varepsilon_i\rangle$) and $\{|o_i\rangle\}$ ($\{|\theta_i\rangle\}$) are mutually orthogonal states with $\hat{P}_A|o_i\rangle = -|o_i\rangle$ ($\hat{P}_B|\theta_i\rangle = -|\theta_i\rangle$).

The condition of $\mathcal{P}1_\pi$ 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

$$A_\pi = \sum_k A^e_k |e_k\rangle\langle e_k| + A^o_k |o_k\rangle\langle o_k| ,$$

$$B_\pi = \sum_k B^e_k |\varepsilon_k\rangle\langle \varepsilon_k| + B^o_k |\theta_k\rangle\langle \theta_k| .$$

On these observables the restriction reads

$$\left(\sum_i |\alpha_i|^2 A^e_i + \sum_i |\beta_i|^2 A^o_i\right)\left(\sum_i |\alpha_i|^2 B^e_i + \sum_i |\beta_i|^2 B^o_i\right) = \sum_i |\alpha_i|^2 A^e_i B^e_i + \sum_i |\beta_i|^2 A^o_i B^o_i .$$

Let us assume that the state Ψ 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 $A = A^e_1|e_1\rangle\langle e_1|$, $B = B^e_2|\varepsilon_2\rangle\langle\varepsilon_2|$, and applying the equality we deduce $|\alpha_1|^2 A^e_1 |\alpha_2|^2 B^e_2 = 0$, and thus $|\alpha_1||\alpha_2| = 0$, so that there can only be a single term in the $|e_i\rangle|\varepsilon_i\rangle$ sum. An analogous argument shows that also the sum of $|o_i\rangle|\theta_i\rangle$ must have at most one single contribution, for the state to be in $\mathcal{P}1_\pi$.

By applying the equality to operators $A = A^o_1|o_1\rangle\langle o_1|$ and $B = B^e_1|\varepsilon_1\rangle\langle\varepsilon_1|$ we also rule out the possibility that Ψ has a contribution from each sector. Then, if $\Psi \in \mathcal{P}1_\pi$, it has one single term in the Schmidt decomposition, and therefore it is a product in the sense of $\mathcal{P}2_\pi$. ∎

2. Separable states

2.1. $\mathcal{S}2 \subset \mathcal{S}1$ *and* $\mathcal{S}2'_\pi \subset \mathcal{S}1_\pi$.

Proof. The first (nonstrict) inclusion is immediate from the relation between product states 1.2. To see that both sets are not equal, we use again an explicit example. It is possible to construct a state in $\mathcal{P}1_\pi \subset \mathcal{S}1_\pi$, which has nonpositive partial transpose and is thus not in $\mathcal{S}2$. However, this has to be found in bigger systems than the previous counterexamples, as in a two-mode system the conditions for $\mathcal{S}1_\pi$ and $\mathcal{S}2'_\pi$ are identical, as shown in Table III.

We can use the following procedure to find a particular example. 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 $\rho_{\mathcal{S}1_\pi}$ in a 2×2 system such that $\rho_{\mathcal{S}1_\pi} \in \mathcal{P}1_\pi$ by construction, but its partial transposition with respect to the subsystem B, $\rho^{T_B}_{\mathcal{S}1_\pi}$, has a negative eigenvalue.

When taking the intersection with the set of physical states, the inclusion still holds, and it is again strict, since the counterexample $\rho_{\mathcal{S}1_\pi}$ is, in particular, in $\mathcal{P}1_\pi$. ∎

2.2. $\mathcal{S}1_\pi \equiv \mathcal{S}1 \cap \Pi$.

Proof. Obviously, $\mathcal{S}1_\pi \subseteq \mathcal{S}1 \cap \Pi$. To see the converse direction of the inclusion, we consider a state $\rho \in \mathcal{S}1 \cap \Pi$. By definition, ρ has a decomposition $\rho = \Sigma_i \lambda_i \rho_i$ with $\rho_i \in \mathcal{P}1$, but not necessarily in Π. We may split the sum into the even and odd terms with respect to the parity operator,

$$\rho = \rho_E + \rho_O := \sum_i \lambda_i \frac{1}{2}(\rho_i + \hat{P}\rho_i\hat{P}) + \sum_i \lambda_i \frac{1}{2}(\rho_i - \hat{P}\rho_i\hat{P}) .$$

The second term ρ_O gives no contribution to operators that commute with $\hat{P}$. Since ρ is physical, this term also gives zero contribution to odd observables, so that

$$\rho = \sum_i \lambda_i \frac{1}{2}(\rho_i + \hat{P}\rho_i\hat{P}) .$$

It only remains to be shown that each $\rho_{iE} := \frac{1}{2}(\rho_i + \hat{P}\rho_i\hat{P})$ is still a product state in $\mathcal{P}1_\pi$. But for parity commuting observables all the contributions come from the symmetric part of the density matrix, hence $\rho_i(A_\pi B_\pi)=\rho_{iE}(A_\pi B_\pi)$, and the condition for $\mathcal{P}1_\pi$ holds for ρ_{iE}. We have then found a convex decomposition of ρ in terms of product states, all of them conforming to the symmetry. The analogous relation for $\mathcal{S}2_\pi$ was shown in [22]. ■

2.3. $\mathcal{S}2_\pi \subset \mathcal{S}2'_\pi$.

Proof. Since $\mathcal{P}2_\pi = \mathcal{P}2 \cap \Pi$, taking convex hulls and intersecting again with Π implies that $\mathcal{S}2_\pi \subseteq \mathcal{S}2'_\pi$. 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

$$\rho_{\mathcal{S}2'_\pi} = \frac{1}{4}\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix},$$

which has PPT and thus belongs to $\mathcal{S}2'_\pi$, is not in $\mathcal{S}2_\pi$ (recall that for the 1×1 system, only density matrices which are diagonal in the number basis are in $\mathcal{S}2_\pi$). ■

2.4. $[\mathcal{S}1_\pi] \equiv [\mathcal{S}2'_\pi] \equiv [\mathcal{S}2_\pi]$.

Proof. From the relations $\mathcal{S}2_\pi \subset \mathcal{S}2'_\pi \subset \mathcal{S}1_\pi$ and the definition of the equivalence classes it is evident that $[\mathcal{S}2_\pi] \subseteq [\mathcal{S}2'_\pi] \subseteq [\mathcal{S}1_\pi]$. To show the equivalence of all sets it is enough to prove that any state $\rho \in [\mathcal{S}1_\pi]$ is also in $[\mathcal{S}2_\pi]$, i.e., that there exists a state in $\mathcal{S}2_\pi$ equivalent to ρ.

Given $\rho \in [\mathcal{S}1_\pi]$, there is a $\tilde{\rho} \in \mathcal{S}1_\pi$, i.e., $\tilde{\rho}=\Sigma\lambda_k\tilde{\rho}_k$ with each $\tilde{\rho}_k \in \mathcal{P}1_\pi$, producing identical expectation values for products of even operators $A_\pi B_\pi$. If we define

$$\rho'_k \coloneqq \sum_{\alpha,\beta=e,o} \mathbb{P}^A_\alpha \otimes \mathbb{P}^B_\beta \tilde{\rho}_k \mathbb{P}^A_\alpha \otimes \mathbb{P}^B_\beta,$$

it is evident that $\rho' \coloneqq \Sigma_k\lambda_k\rho'_k$ produces the same expectation values as $\tilde{\rho}$ for the relevant operators (see Proof 1.1). Therefore, $\rho \sim \rho'$. Moreover, $\rho'_k(A_\pi B_\pi)=0$ for all odd-odd products, hence $\rho'_k \in \mathcal{P}2_\pi\ \forall\ k$, and so $\rho' \in \mathcal{S}2_\pi$. ■

2.5. $\mathcal{S}1_\pi \subset [\mathcal{S}1_\pi]$.

Proof. The relation $\mathcal{S}1_\pi \subseteq [\mathcal{S}1_\pi]$ is immediate. As in previous paragraphs, we show the strict character of the inclusion with an explicit example. The state

$$\rho_{[\mathcal{S}1_\pi]} = \frac{1}{15}\begin{pmatrix} 5 & 0 & 0 & 2\sqrt{5} \\ 0 & 3 & 3 & 0 \\ 0 & 3 & 3 & 0 \\ 2\sqrt{5} & 0 & 0 & 4 \end{pmatrix}$$

is a valid density matrix for the 1×1-mode system, and thus it belongs to $[\mathcal{S}1_\pi]$ (see Table III). However, the partial transpose of $\rho_{[\mathcal{S}1_\pi]}$ is not positive (in particular, it violates the condition $|r|^2 \le (x-z)(y-z)$ from Table III), so that it is not in $\mathcal{S}1_\pi$. Again, this state can be seen to be Gaussian. ■

3. Multiple copies

3.1. $\rho^{\otimes 2} \in \mathcal{S}1_\pi \Rightarrow \rho \in \mathcal{S}1_\pi$.

Proof. An arbitrary state can be decomposed in two terms, $\rho=\rho_E+\rho_O$, where

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

and

$$\rho_O \coloneqq \sum_{\substack{\alpha,\beta,\gamma,\delta=e,o \\ (\alpha,\beta)\neq(\gamma,\delta)}} \mathbb{P}^A_\alpha \otimes \mathbb{P}^B_\beta \rho \mathbb{P}^A_\gamma \otimes \mathbb{P}^B_\delta.$$

For any state in $\mathcal{S}1_\pi$, there exists a decomposition $\rho_E=\Sigma_i\lambda_i\rho^i_E$, $\rho_O=\Sigma_i\lambda_i\rho^i_O$, such that $\rho^i_E+\rho^i_O \in \mathcal{P}1_\pi$. Let us consider two copies of a state such that $\tilde{\rho} \coloneqq \rho^{\otimes 2} \in \mathcal{S}1_\pi$. 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, $\rho=\rho_E+\rho_O=\Sigma_i\lambda_i\,\mathrm{tr}_2(\tilde{\rho}^i_E)+\Sigma_i\lambda_i\,\mathrm{tr}_2(\tilde{\rho}^i_O)$. Since $\tilde{\rho}^i_E$ was a tensor product, $\tilde{\rho}^i_E=\tilde{\rho}_{\tilde{A}}\otimes\tilde{\rho}_{\tilde{B}}$, with $\tilde{A}\equiv A_1A_2$, $\tilde{B}\equiv B_1B_2$, so is $\mathrm{tr}_2(\tilde{\rho}^i_E)$, and therefore $\rho \in \mathcal{S}1_\pi$. ■

3.2. $\rho^{\otimes 2} \in [\mathcal{S}1_\pi] \Rightarrow \rho \in [\mathcal{S}1_\pi]$.

Proof. Using the same decomposition as above, $\rho=\rho_E+\rho_O$, a state $\rho \in [\mathcal{S}1_\pi]$ satisfies $\rho_E \in \mathcal{S}2'_\pi$. If we consider $\tilde{\rho} \coloneqq \rho^{\otimes 2}=\tilde{\rho}_E+\tilde{\rho}_O$, the condition $[\mathcal{S}1_\pi]$ on the state of the two copies reads

$$\tilde{\rho}_E = \rho_E \otimes \rho_E + \rho_O \otimes \rho_O \in \mathcal{S}2'_\pi,$$

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 ρ_O is traceless, $\rho_E \in \mathcal{S}2'_\pi$, so that $\rho \in [\mathcal{S}1_\pi]$. ■

3.3. ρ non-PPT $\Rightarrow \rho^{\otimes 2} \notin [\mathcal{S}1_\pi]$.

Proof. We may restrict the proof to states such that $\rho \in [\mathcal{S}1_\pi]$. In another case, the implication follows immediately from the previous result (3.2). 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 Eq. (12) for the 1×1 case]

$$\rho = \begin{pmatrix} \rho_{ee} & 0 & 0 & C \\ 0 & \rho_{eo} & D & 0 \\ 0 & D^\dagger & \rho_{oe} & 0 \\ C^\dagger & 0 & 0 & \rho_{oo} \end{pmatrix}. \qquad \text{(A1)}$$

The diagonal blocks correspond to the projections onto simultaneous eigenspaces of both parity operators, $\rho_{\alpha\beta}=\mathbb{P}^A_\alpha \otimes \mathbb{P}^B_\beta \rho \mathbb{P}^A_\alpha \otimes \mathbb{P}^B_\beta$, whereas $C=\mathbb{P}^A_e\otimes\mathbb{P}^B_e\rho\mathbb{P}^A_o\otimes\mathbb{P}^B_o$ and $D=\mathbb{P}^A_e\otimes\mathbb{P}^B_o\rho\mathbb{P}^A_o\otimes\mathbb{P}^B_e$.

From the characterization (10) of separability, the state is in $[\mathcal{S}1_\pi]$ iff all the diagonal blocks $\rho_{\alpha\beta}$ are in $\mathcal{S}2'_\pi$. It is then enough to prove that the partial transpose of ρ is positive iff $\mathbb{P}^A_e\otimes\mathbb{P}^B_e\rho\otimes\rho\mathbb{P}^A_e\otimes\mathbb{P}^B_e$ has PPT. Nonpositivity of the partial transpose of ρ implies then the nonseparability (as $\mathcal{S}2'_\pi$) of one of the diagonal blocks of $\rho\otimes\rho$.

The partial transposition of the above matrix yields

$$\rho^{T_B}=\begin{pmatrix}\rho'_{ee} & 0 & 0 & D'\\ 0 & \rho'_{eo} & C' & 0\\ 0 & (C')^\dagger & \rho'_{oe} & 0\\ (D')^\dagger & 0 & 0 & \rho'_{oo}\end{pmatrix}, \quad (A2)$$

where $X':=X^{T_B}$, 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 $\tilde{\rho}_{ee}:=\mathbb{P}_e^A\otimes\mathbb{P}_e^B\rho\otimes\rho\mathbb{P}_e^A\otimes\mathbb{P}_e^B$,

$$\tilde{\rho}_{ee}=\begin{pmatrix}\rho_{ee}\otimes\rho_{ee} & 0 & 0 & C\otimes C\\ 0 & \rho_{eo}\otimes\rho_{eo} & D\otimes D & 0\\ 0 & D^\dagger\otimes D^\dagger & \rho_{oe}\otimes\rho_{oe} & 0\\ C^\dagger\otimes C^\dagger & 0 & 0 & \rho_{oo}\otimes\rho_{oo}\end{pmatrix}, \quad (A3)$$

whose partial transposition $(\tilde{\rho}_{ee})^{T_B}$ reads

$$\begin{pmatrix}\rho'_{ee}\otimes\rho'_{ee} & 0 & 0 & D'\otimes D'\\ 0 & \rho'_{eo}\otimes\rho'_{eo} & C'\otimes C' & 0\\ 0 & C'^\dagger\otimes C'^\dagger & \rho'_{oe}\otimes\rho'_{oe} & 0\\ D'^\dagger\otimes D'^\dagger & 0 & 0 & \rho'_{oo}\otimes\rho'_{oo}\end{pmatrix}. \quad (A4)$$

The matrices (A2) and (A4) 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 (A4), namely,

$$\begin{pmatrix}\rho'_{ee}\otimes\rho'_{ee} & D'\otimes D'\\ D'^\dagger\otimes D'^\dagger & \rho'_{oo}\otimes\rho'_{oo}\end{pmatrix}, \quad (A5)$$

and assume first that ρ'_{oo} is nonsingular. Applying a standard theorem in matrix analysis and making use of the fact that our $\rho\in[\mathcal{S}1_\pi]$, so that each diagonal block is PPT, we obtain that Eq. (A5) is positive iff

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

which holds iff

$$\rho'_{ee}\geq D'(\rho'_{oo})^{-1}D'^\dagger.$$

Reasoning in the same way for the second block of Eq. (A4), one gets that

$$(\tilde{\rho}_{ee})^{T_B}\geq 0\Leftrightarrow\rho^{T_B}\geq 0. \quad (A6)$$

The result holds also if the assumption of nonsingularity of ρ_{oo} (ρ_{oe} for the second block) is not valid. In that case, we may take ρ_{oo} diagonal and then, by positivity of $(\tilde{\rho}_{ee})^{T_B}$ (or ρ^{T_B} 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 ρ_{oo} (ρ_{oe}) is nonsingular. ■

3.4. For 1×1 *systems,* $\rho^{\otimes 2}\in[\mathcal{S}1_\pi]\Leftrightarrow\rho\in\mathcal{S}2'_\pi$.

Proof. One of the directions is immediate, and valid for an arbitrarily large system, since $\rho\in\mathcal{S}2'_\pi$ implies $\rho^{\otimes 2}\in\mathcal{S}2'_\pi\subset\mathcal{S}1_\pi\subset[\mathcal{S}1_\pi]$. On the other hand, if we take $\tilde{\rho}:=\rho^{\otimes 2}\in[\mathcal{S}1_\pi]$, then the diagonal blocks of this state are separable, in particular, $\mathbb{P}_e^{\tilde{A}}\otimes\mathbb{P}_e^{\tilde{B}}\tilde{\rho}\mathbb{P}_e^{\tilde{A}}\otimes\mathbb{P}_e^{\tilde{B}}\in\mathcal{S}2'_\pi$, which was calculated in Eq. (A3). For the case of 1×1 modes, with ρ given by Eq. (12), this block reads

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

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

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[32] Yet a different definition is based on a generalized notion of entanglement, which is relative to distinguished subspaces of observables [31].

[33] We use the notation LOCC_S for those operations which can be considered local in the presence of the superselection rule. In particular, when parity is conserved, local operations, on top of being defined by the partition of the system, must commute with the local parity operators $\hat{P}_A$ and $\hat{P}_B$.