Universal Subspaces for Local Unitary Groups of Fermionic Systems

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Abstract

Let $\mathcal{V} = \wedge^N V$ be the $N$-fermion Hilbert space with $M$-dimensional single particle space $V$ and $2N \leq M$. We refer to the unitary group $G$ of $V$ as the local unitary (LU) group. We fix an orthonormal (o.n.) basis $|v_1\rangle, \ldots, |v_M\rangle$ of $V$. Then the Slater determinants $e_{i_1,\ldots,i_N} := |v_{i_1} \wedge v_{i_2} \wedge \cdots \wedge v_{i_N}\rangle$ with $i_1 < \cdots < i_N$ form an o.n. basis of $\mathcal{V}$. Let $S \subseteq \mathcal{V}$ be the subspace spanned by all $e_{i_1,\ldots,i_N}$ such that the set $\{i_1, \ldots, i_N\}$ contains no pair $\{2k-1, 2k\}$, $k$ an integer. We say that the $|\psi\rangle \in S$ are single occupancy states (with respect to the basis $|v_1\rangle, \ldots, |v_M\rangle$). We prove that for $N = 3$ the subspace $S$ is universal, i.e., each $G$-orbit in $\mathcal{V}$ meets $S$, and that this is false for $N > 3$. If $M$ is even, the well known BCS states are not LU-equivalent to any single occupancy state. Our main result is that for $N = 3$ and $M$ even there is a universal subspace $W \subseteq S$ spanned by $M(M-1)(M-5)/6$ states $e_{i_1,\ldots,i_N}$. Moreover the number $M(M-1)(M-5)/6$ is minimal.

1 Introduction

Entanglement is at the heart of quantum information theory. It makes possible secure and high rate information transmission, fast computational solution of certain important problems, and efficient physical simulation of quantum phenomena [1,2]. The most fundamental property for any kind of study of entanglement is that it is invariant under local unitary (LU)
transformations. The celebrated Schmidt decomposition for bipartite pure states provides a canonical form for these states under LU, which makes possible a complete understanding of their entanglement properties. In particular, the entanglement measure is characterized by the entropy of Schmidt coefficients.

For multipartite systems, however, no direct generalization is possible. The study of entanglement for multipartite pure states is hence much more challenging than the bipartite case. Considerable efforts have been taken during the past decade. However no complete satisfactory theory can be reached as for the bipartite case \[2, 3\]. Still, the first step toward the understanding of multipartite entanglement is to study the orbits of pure quantum states under LU. Acin et al started from looking at the simplest nontrivial case of a three qubit system \[4, 5\]. They introduced the concept of local basis product states (LBPS), which are three-qubit product states from a fixed set of single particle orthonormal basis. They studied the property of subspaces spanned by LBPS such that every three-qubit pure state is LU equivalent to some states in such a subspace. This kind of subspace can hence be called ‘universal subspace’ \[4, 6\].

Acin et al. showed that five LBPS are enough to span a universal subspace for three qubits \[4\]. For one such choice given by \[\{\ket{000}, \ket{100}, \ket{101}, \ket{110}, \ket{111}\}\], they can further restrict the regions for the superposition coefficients such that it gives a canonical form in the canonical form. Generalizations to \(N > 3\) qubits are developed and it is found that a universal subspace needs to be spanned by \(2^N - N\) LBPS, and such a minimal set of LBPS are identified \[7\]. Unfortunately, this does not provide much saving compared to the \(2^N\)-dimensional Hilbert space. This is simply due to the fact the LU group is such a small group compared to the entire unitary group \(U(2^N)\).

Entanglement theory for identical particle systems has also been considerably developed during the past decade \[3, 8, 9, 10, 11, 12\]. Entanglement for identical particle systems cannot be discussed in usual way as for the distinguishable particle case. This is because the symmetrization for bosonic systems and antisymmetrization for fermionic systems for the wave functions may introduce ‘pseudo entanglement’ which is not accessible in practice. It is now widely agreed that non-entangled states are reasonably corresponding to the form \(\ket{v}^N\) for bosonic states \[11, 3, 12\] (there was indeed suggestion that non-entangled bosonic state corresponds to \(\ket{v_1} \lor \ket{v_2} \lor \cdots \lor \ket{v_N}\) \[10\], however most of the literatures accept \(\ket{v}^N\) and to the form of Slater determinants \(\ket{v_1} \land \ket{v_2} \land \cdots \land \ket{v_N}\) for fermionic states \[3, 12\].

For bipartite fermionic pure states, a direct generalization of Schmidt decomposition is available \[9\]. That is, every bipartite fermionic pure state is LU equivalent to a Slater decomposition \[\sum_i \lambda_i \ket{\alpha_i} \land \ket{\beta_i}\], where \[\langle \alpha_i | \alpha_j \rangle = \langle \beta_i | \beta_j \rangle = \delta_{ij}\] and \[\langle \alpha_i | \beta_j \rangle = 0\]. This thus allows a complete understanding of entanglement properties for bipartite fermionic pure states. Many interesting analogues to the bipartite distinguishable particle case have also been identified, such as concurrence and magic basis \[9, 12\]. The entanglement of formation (EOF) for mixed states has also been investigated for the single particle state Hilbert space of dimension four. In particular, a formula was identified \[9, 12\] and is similar to the known formula for two-qubit states by Wootters \[13\].
The generalization to more than two fermions has also been discussed [12]. However, similar to the distinguishable particle case, there is no Slater decomposition for multipartite fermionic system. Then it is more difficult to study their entanglement properties. The first step is still using the LU orbits. Due to particle-hole duality, in most cases one will need to have $M \geq 2N$ to obtain meaningful discussions, where $M$ is the dimension for the single particle state Hilbert space $V$. For examples with $M > 2N$, see the BCS states defined in Eq. (44). The reason is that the Pauli exclusion principle requires $M \geq N$, and the particle-hole duality gives equivalence between $N, M$ and $M - N, M$ systems. Also, it is even nontrivial to see whether a given fermionic pure state is unentangled (i.e. LU equivalent to a single Slater determinant), where one needs to check the Grassmann-Plücker relations (see e.g. p. A III.172 Eq. (84-(J,H)) in [14], Prop 11-32 in [15], and [12]).

In this paper, we take one further step beyond just the Grassmann-Plücker relations for the entanglement properties of multipartite fermionic pure states. We study the universal subspaces spanned by Slater determinants built from orthonormal local basis. So we can build a fermionic analogue of the universal subspace spanned by LBP$S$ in the distinguishable particle case. The obvious difficulty is the above-mentioned $M \geq 2N$ condition, for which one can no longer hope for any elementary method (e.g. linear algebra) as was useful in the $N$-qubit case. However, this difficulty, once overcome, might become an advantage given the relatively large LU group $U(M)$ compared to the entire unitary group on the $N$-particle fermion space $V = \wedge^N V$ which is of dimension $\binom{M}{N}$. In other words, one can ideally hope for a ‘saving’ of the dimension of $U(M)$, which is of the order $M^2$. That is, the best one can hope for the dimension of a universal subspace is of the order $\binom{M}{N} - M^2$ for $N > 2$.

Our focus will be mainly on the $N = 3$ case, where we show that such a saving of order $M^2$ is indeed achievable. Not only we want to find a universal subspace which mathematically achieves the order $\binom{M}{N} - M^2$, but also we want the universal subspace with a clear physical meaning. To obtain such a universal subspace, we introduce a configuration for the Slater determinants called single occupancy. This is typical in condensed matter physics for studying properties of strongly-correlated electron systems, for instance high temperature superconducting ground state of doped Mott insulator (see e.g. [16]).

Single occupancy fermionic states are also of interest in quantum information theory in recent years, as there exists a qubit to fermion mapping which is one to one between qubit states and single occupancy fermionic states. This mapping was used to show the QMA completeness of the fermionic $N$-representability problem, that is, the overlapping $N$-representability problem is hard even with the existence of a quantum computer [17, 30]. The same mapping was also used to disprove a 40-year old conjecture in quantum chemistry using methods of quantum error-correcting codes [18].

The physics considerations lead to the following picture. We illustrate this in Fig. 1. Suppose we have in total $K$ sites. At each site we have three possible states: 1) no spin (a hole, shown as a dot); 2) spin up (shown as arrow up); 3) spin down (shown as arrow down). Now suppose we have in total $N$ spins. Then there are in total $\binom{2K}{N}$ spin configurations (note that once the spin states are fixed, the holes are fixed). As an example, Fig. 2 shows the case $N = 3$ and $K = 4$, i.e. 3 spins in 8-dimensional space. Figure A is a single
occupancy configuration which has at most 1 spin on each site. A single occupancy state is a superposition of single occupancy configurations. Figure B is not a single occupancy configuration where site 1 is occupied by 2 spins (i.e. double occupancy on site 1). While the single occupancy configuration is defined for $M = 2K$ which is even, one can readily generalize the configuration to the case of odd $M$, leaving one single-particle spin state unpaired.

To be more precise, for the single particle Hilbert space $V$ of dimension $M = 2K$, which is a tensor product of the spatial part with dimension $K$ (with a fixed basis $|g_1\rangle, |g_2\rangle, \ldots, |g_K\rangle$, which each $|g_j\rangle$ highly localized on the $j$th site) and the spin part with dimension 2 (with a fixed basis $|\uparrow\rangle, |\downarrow\rangle$), then a single occupancy state is a Slater determinant where $|g_j\rangle \otimes |\uparrow\rangle, |g_j\rangle \otimes |\downarrow\rangle$ do not show up at the same time for any $j = 1, 2, \ldots K$. For instance, the single occupancy state shown in Fig. 2A can then be written as $(|g_1\rangle \otimes |\downarrow\rangle) \wedge (|g_2\rangle \otimes |\uparrow\rangle) \wedge (|g_4\rangle \otimes |\downarrow\rangle)$. However, the state given in Fig. 2B is $(|g_1\rangle \otimes |\uparrow\rangle) \wedge (|g_1\rangle \otimes |\downarrow\rangle) \wedge (|g_2\rangle \otimes |\uparrow\rangle)$, which is not single occupancy as both $|g_1\rangle \otimes |\uparrow\rangle, |g_1\rangle \otimes |\downarrow\rangle$ show up.

For a simplified notation, we can relabel the $2K$ single particle basis $\{|g_j\rangle \otimes |\uparrow\rangle, |g_j\rangle \otimes |\downarrow\rangle\}$ as $\{|2j-1\rangle, |2j\rangle\}$, for $j = 1, 2, \ldots, K$. The $M$ odd case is hence similar, just that one can correspond the first $M - 1$ basis states, denoted by $\{|2j-1\rangle, |2j\rangle\}$ to $\{|g_j\rangle \otimes |\uparrow\rangle, |g_j\rangle \otimes |\downarrow\rangle\}$ for $j = 1, 2, \ldots, (M - 1)/2$, and then the last ‘unpaired’ basis state $|M\rangle$ to $|g_{(M+1)/2}\rangle \otimes |\uparrow\rangle$, as the state $|g_{(M+1)/2}\rangle \otimes |\downarrow\rangle$ is ‘inaccessible’ by any of the $N$-fermions. Note that despite the choice of the labelling, the basis of the Hilbert space is fixed throughout the paper. This corresponds to a simple fact that the spatial sites are physically fixed.

Our main theorem of the paper proves that for $N = 3$, the single occupancy subspace $S$ (i.e. subspace of all single occupancy states) is universal. In other words, any $N = 3$ fermionic state is LU equivalent to a single occupancy state. Here by LU we mean that local unitary transformation on the entire $M$-dimensional single particle Hilbert, i.e. elements in
U(M), not only unitaries on the spatial part (or the spin part) of the wavefunction only. This definition of LU agrees with those used in quantum information community for fermionic systems (see, e.g. \[3, 12\]), which preserves entanglement properties, such as the spectra of reduced density matrices.

For \(M\) even, we can also obtain universal subspaces contained in \(S\) whose dimension is minimal. Our main tool is to apply Theorem 4.2 of \[6\] to the case of LU groups with representation on the \(N\)-fermion Hilbert space \(\mathcal{V} = \wedge^N V\). It should be emphasized that this application in our case is highly non-trivial. Indeed, after selecting a candidate for a universal subspace, one has to prove that the main condition of the theorem is satisfied. For small \(M\) this can be done by using a computer, but the proof that it can be applied for all \(M\) is hard to find. Finding a universal subspace of minimum dimension is much harder and we succeeded to find one which works for even \(M\). For the case when \(M\) is odd, one may conjecture that the candidate subspace described in Proposition 6 (see Eq. (31)) is universal but this has been verified only for \(M = 7, 9, 11\).

For the smallest non-trivial case of \(N = 3, M = 6\) where \(\text{Dim} \wedge^3 V = 20\), a direct application of our results gives universal subspaces with dimension 5. This is indeed a big saving. It is interesting to compare this result to Acin et. al’s result of three qubits, where they also have universal subspaces of dimension 5, which are spanned by LBPS. This may be related to the fact that, when \(M = 2N\), each qubit state corresponds to a single occupancy state based on the qubit to fermion mapping mentioned above. It should also be mentioned that, although it is not directly applicable, our work may shed light on the understanding of the N-representability problem \[19\], where the single particle eigenvalues are invariant under LU. Indeed, our universal subspace with dimension 5 for the case \(N = 3, M = 6\) gives an alternative proof of the N-representability equalities and inequalities in that case \[20, 21, 22, 23\].

To complete our study of single occupancy, we further prove that the single occupancy subspace is not universal for \(N > 3\), i.e. not all fermionic states are LU equivalent to a single occupancy state, though for fixed \(N\) almost all states are single occupancy in the large \(M\) limit. Our argument is based on dimension counting. For concrete examples, we show that for \(N\) even, BCS states are not LU equivalent to any single occupancy state. This is intuitive as BCS states are always ‘paired’ so they are most unlikely to be transformed with LU to something unpaired.

We organize our paper as follows. In Sec. 2, we provide preliminaries used throughout the paper. We formally define antisymmetric tensors, decomposable states (Slater determinants), LU operations, universal subspaces and single occupancy states. We also discuss the lower bound for dimension of universal subspaces. It sets the goal for later work. In Sec. 3, we consider universal subspaces for \(N = 3\). We prove our main theorem that for \(N = 3\), the single occupancy subspace \(S\) is universal, see Theorem 4. For \(M\) even, we can also obtain subspaces of \(S\) whose dimension is minimal, and explicit choice of Slater determinants for those subspaces are given. In Sec. 4, we try to generalize our theorem to the \(N > 3\) case but obtain a negative result. That is, we prove that the single occupancy subspace is not universal for any \(M \geq 2N\). So there always exist some states which are not LU equivalent.
to single occupancy states. For \( N \) even, we use BCS states as concrete examples of states that are not LU equivalent to any single occupancy states. Finally, a brief summary and discussion will be given in Sec. 5.

2 Preliminaries

2.1 Decomposable states and inner product

Let \( V \) be a complex Hilbert space of dimension \( M \) and \( \mathcal{H} = \otimes^N V \) the \( N \)th tensor power of \( V \). The inner product on \( V \) extends to one on \( \mathcal{H} \) such that

\[
\langle v_1, v_2, \ldots, v_N | w_1, w_2, \ldots, w_N \rangle = \prod_{i=1}^{N} \langle v_i | w_i \rangle.
\]

We denote by \( \wedge^N V \) the \( N \)th exterior power of \( V \), i.e., the subspace of \( \mathcal{H} \) consisting of the antisymmetric tensors. We refer to vectors \( | \psi \rangle \in \wedge^N V \) as \( N \)-vectors. We shall often identify the \( N \)-vectors with antisymmetric tensors by using the embedding \( \wedge^N V \to \mathcal{H} \) given by:

\[
| v_1 \rangle \wedge \cdots \wedge | v_N \rangle \to \sum_{\sigma \in S_N} \text{sgn}(\sigma) | v_{\sigma(1)} \rangle \otimes \cdots \otimes | v_{\sigma(N)} \rangle,
\]

where \( S_N \) is the symmetric group on \( N \) letters and \( \text{sgn}(\sigma) \) the sign of the permutation \( \sigma \). We say that an \( N \)-vector \( | \psi \rangle \) is decomposable if it can be written as

\[
| \psi \rangle = | v_1 \rangle \wedge \cdots \wedge | v_N \rangle
\]

for some \( | v_i \rangle \in V \). For brevity we may also write

\[
| \psi \rangle = | v_1 \wedge \cdots \wedge v_N \rangle
\]

when no confusion arises. Decomposable states are also called Slater determinant states or Slater determinants in physics. For the sake of brevity we shall mainly use the name of decomposable states. Unless stated otherwise, the states will not be normalized for convenience.

If \( W \) is a vector subspace of \( V \), then \( \wedge^N W \) is a vector subspace of \( \wedge^N V \). Given a \( | \psi \rangle \in \wedge^N V \), there exists the smallest subspace \( W \subseteq V \) such that \( | \psi \rangle \in \wedge^N W \). We shall refer to this subspace as the support of \( | \psi \rangle \). By Eq. (1), this is equal to the range of the reduced density matrix of any single particle of \( | \psi \rangle \). In the case when \( | \psi \rangle \neq 0 \) is decomposable, say \( | \psi \rangle = | v_1 \wedge \cdots \wedge v_N \rangle \), then its support is the subspace spanned by the vectors \( | v_i \rangle \), \( i = 1, \ldots, N \).

In general, an \( N \)-vector can always be written (not uniquely) as a sum of decomposable \( N \)-vectors. With this notation, the inner product in \( \wedge^N V \) is characterized by the fact that the inner product of two decomposable \( N \)-vectors \( | \varphi \rangle = | w_1 \wedge \cdots \wedge w_N \rangle \) and \( | \psi \rangle = | v_1 \wedge \cdots \wedge v_N \rangle \) is equal to the determinant of the \( N \times N \) matrix \( \langle w_i | v_j \rangle \). It is also equal to \( \frac{1}{N!} \langle \varphi | \psi \rangle \) where
the inner product is computed in the tensor space by using the identification given by Eq. (1). Hence, $|\varphi\rangle \perp |\psi\rangle$ when this determinant is zero.

The 2-vectors $|\psi\rangle \in \wedge^2 V$ are often identified with antisymmetric matrices of order $M$ via the isomorphism which assigns to any decomposable 2-vector $|\psi\rangle = |v \wedge w\rangle$ the matrix $|v\rangle(|w\rangle^T) - |w\rangle(|v\rangle^T)$. Under this isomorphism, the nonzero decomposable 2-vectors correspond to antisymmetric matrices of rank 2.

We shall use the well known exterior multiplication map from $\wedge^n V \times \wedge^n V$ into $\wedge^{N+n} V$, which is a complex bilinear map. Note that this map is identically zero if $N+n > M$. Let us also introduce the ‘partial inner product’ operations. Given an $n$-vector $|\varphi\rangle$ and an $N$-vector $|\psi\rangle$ with $n \leq N$, we can define their partial inner product $\langle \varphi|\psi\rangle \in \wedge^{N-n} V$. In other words, this is a map

$$\wedge^n V \times \wedge^n V \to \wedge^{N-n} V$$

which is antilinear in the first argument $|\varphi\rangle$ and complex linear in the second argument $|\psi\rangle$.

Thus, it suffices to write the definition in the special case when $|\varphi\rangle$ and $|\psi\rangle$ are decomposable, say $|\varphi\rangle = |w_1 \wedge \cdots \wedge w_n\rangle$ and $|\psi\rangle = |v_1 \wedge \cdots \wedge v_N\rangle$. In that case we have

$$\langle \varphi|\psi\rangle = \sum_{\sigma} \text{sgn}(\sigma) \left( \prod_{i=1}^n \langle w_i|v_{\sigma(i)} \rangle \right) |v_{\sigma(n+1)} \wedge \cdots \wedge v_{\sigma(N)}\rangle,$$

where the summation is over all permutations $\sigma \in S_N$ such that the sequence $\sigma(n+1), \ldots, \sigma(N)$ is increasing. This definition is a modification of the one given in [13, p. A III.166] for the partial bilinear inner product. We have omitted the overall factor $(-1)^{(n(n-1)/2}$, and replaced the bilinear inner product with the Hilbert space inner product. More importantly, it appears that there is an error (or misprint) in Bourbaki because the right hand side of their formula is not antisymmetric in the arguments $x_i^*$. We had to modify their formula by requiring that only the second one of their two sequences of $\sigma$-values is increasing. The Eq. (2) can be rewritten as

$$\langle \varphi|\psi\rangle = \sum_{\sigma} \text{sgn}(\sigma) \langle w_1 \wedge \cdots \wedge w_n|v_{\sigma(1)} \wedge \cdots \wedge v_{\sigma(n)} \rangle |v_{\sigma(n+1)} \wedge \cdots \wedge v_{\sigma(N)}\rangle,$$

where the summation now is over the permutations $\sigma \in S_N$ such that both sequences $\sigma(1), \ldots, \sigma(n)$ and $\sigma(n+1), \ldots, \sigma(N)$ are increasing.

If $n = 1$ then the formula reads as follows:

$$\langle w_1|\psi\rangle = \sum_{i=1}^N (-1)^{i-1} \langle w_1|v_i \rangle |v_1 \wedge \cdots \wedge v_{i-1} \wedge v_{i+1} \wedge \cdots \wedge v_N\rangle.$$

If we define the interior product $\iota(w)$ to be the linear map $\wedge^N V \to \wedge^{N-1} V$ which sends $|\psi\rangle$ to $\langle w|\psi\rangle$, then one can check that Eq. (2) can be rewritten as follows:

$$\langle \varphi|\psi\rangle = \iota(w_n) \circ \cdots \circ \iota(w_1)(|v_1 \wedge \cdots \wedge v_N\rangle).$$

By using the embedding (1), the partial inner product given by Eq. (2) is a positive scalar multiple of the inner product $\langle \varphi|\psi\rangle$ where both $|\varphi\rangle$ and $|\psi\rangle$ are viewed as antisymmetric tensors. Note that in the case $n = N$, the partial inner product in Eq. (2) is the same as the inner product on $\wedge^N V$ defined at the beginning of this section.
2.2 Local unitary equivalence

If \( A_i : V \rightarrow V, \ i = 1, \ldots, N, \) are linear operators, then their tensor product \( \bigotimes_{i=1}^N A_i \) will be identified with the unique linear operator on \( \mathcal{H} \) which maps

\[
|v_1\rangle \otimes |v_2\rangle \otimes \cdots \otimes |v_N\rangle \rightarrow A_1|v_1\rangle \otimes A_2|v_2\rangle \otimes \cdots \otimes A_N|v_N\rangle, \quad |v_i\rangle \in V, \quad (i = 1, 2, \ldots, N).
\]

If \( A_1 = A_2 = \cdots = A_N = A, \) then we shall write \( \bigotimes^N A \) or \( A^N \) instead of \( \bigotimes_{i=1}^N A_i \) and refer to \( \bigotimes^N A \) as the \( N \)th tensor power of \( A. \) If \( |\psi\rangle \in \wedge^N V \) then we also have \( \bigotimes^N A(|\psi\rangle) \in \wedge^N V. \) Consequently, we can restrict the operator \( \bigotimes^N A \) to obtain a linear operator on \( \wedge^N V, \) which we denote by \( \wedge^N A \) or \( A^{\wedge N}. \) We refer to \( \wedge^N A \) as the \( N \)th exterior power of \( A. \) Explicitly, we have

\[
\wedge^N A(|v_1 \wedge v_2 \wedge \cdots \wedge v_N\rangle) = |Av_1 \wedge Av_2 \wedge \cdots \wedge Av_N\rangle.
\]

The general linear group \( G := GL(V) \) acts on \( \mathcal{H} \) by the so called diagonal action:

\[
A \cdot (|v_1\rangle \otimes |v_2\rangle \otimes \cdots \otimes |v_N\rangle) = A|v_1\rangle \otimes A|v_2\rangle \otimes \cdots \otimes A|v_N\rangle, \quad A \in G, \quad |v_i\rangle \in V, \quad (i = 1, 2, \ldots, N).
\]

In other words, \( A \in G \) acts on \( \mathcal{H} \) as \( \bigotimes^N A. \) Similarly, we have the action of \( G \) on \( \wedge^N V \) where \( A \in G \) acts as \( \wedge^N A. \) For convenience we shall abbreviate both of these two actions by a ‘‘\( \cdot \)’’, i.e., we have

\[
A \cdot |v_1, \ldots, v_N\rangle = |Av_1, \ldots, Av_N\rangle, \quad (6)
\]

\[
A \cdot |v_1 \wedge \cdots \wedge v_N\rangle = |Av_1 \wedge \cdots \wedge Av_N\rangle. \quad (7)
\]

Both of these actions can be restricted to the unitary group \( U(V) \) of \( V. \)

We shall say that two \( N \)-vectors \( |\phi\rangle \) and \( |\psi\rangle \) are equivalent if they belong to the same \( G \)-orbit, i.e., \( |\psi\rangle = A \cdot |\phi\rangle \) for some \( A \in G. \) We shall also say that they are unitarily equivalent or LU-equivalent if such \( A \) can be chosen to be unitary. For example, any decomposable \( N \)-vector is unitarily equivalent to a scalar multiple of \( |1\rangle \wedge \cdots \wedge |N\rangle. \)

In practice, LU can be realized by a Hamiltonian

\[
H = \sum_{j=1}^{N} H_j, \quad (8)
\]

where \( H_j \) acts on the \( j \)th particle, \( H_j|v_1, \ldots, v_N\rangle = |v_1, \ldots, H_jv_j, \ldots, v_N\rangle. \) The evolution of the system is unitary, i.e.

\[
e^{-iHt} = \exp \left( \sum_{j=1}^{N} -iH_jt \right) = \bigotimes_{j=1}^{N} U_j, \quad (9)
\]

with \( U_j = e^{-iH_jt}. \) The Hamiltonian of the form Eq. (8) is usually called a single-particle Hamiltonian. For a fermionic system, we have \( H_1 = H_2 = \cdots = H_N = H, \) hence \( U_1 = U_2 = \cdots = U_N = U. \) Hence the evolution of the system is indeed the fermionic LU \( \wedge^N U. \)

In the case \( N = 2, \) we have the canonical form for unitary equivalence.
Lemma 1 If $N = 2$, then any 2-vector $|\psi\rangle$ is unitarily equivalent to $\sum_{i=1}^{k} c_i |2i-1\rangle \wedge |2i\rangle$ for some $c_1 \geq \cdots \geq c_k > 0$ and some integer $k \geq 0$. Moreover, the coefficients $c_i$ are uniquely determined by $|\psi\rangle$.

Proof. The first assertion follows easily from the antisymmetric version of Takagi’s theorem, see [15, Proposition 11.28]. To prove the second assertion, we denote by $K$ the antisymmetric matrix corresponding to $|\psi\rangle$. If $U$ is a unitary operator on $V$, then the 2-vector $U|\psi\rangle$ is represented by the antisymmetric matrix $UKU^T$. It follows that the Hermitian matrix $KK^*$ is transformed to $UKK^*U^\dagger$, and so its eigenvalues are independent of $U$. Since these eigenvalues are $-c_1^2, -c_2^2, \ldots, -c_k^2, 0, \ldots, 0$, the second assertion follows. 

It can be seen that the Slater decomposition for 2-vectors is essentially the same as the well-known Schmidt decomposition for bipartite pure states. While the later can be easily generalized to multipartite systems by regarding them as bipartite systems, the same method does not work for the former, because the two parties of the bipartite system would have different dimensions and this system cannot be antisymmetric.

We remark that this lemma provides a complete classification of $U(V)$-orbits on $\Lambda^2 V$. Let us also mention that the antisymmetric version of Takagi’s theorem used in the above proof was reproved recently in [10, Lemma 1]. However the authors missed to observe that this result can be used to construct the canonical form for bipartite fermionic states. Similarly, the symmetric version of Takagi’s theorem provides a canonical form for pure states of two bosons, which is rediscovered recently in [10, 11]. See also [25] where more advanced mathematical tools were used to solve this classification problem as well as its analogue for two bosons.

In the case when $V$ is 5-dimensional, there is also a simple canonical form for 3-vectors under unitary equivalence.

Corollary 2 If $\dim V = 5$ then every 3-vector $|\psi\rangle$ is unitarily equivalent to $(c_1 |1\rangle \wedge |2\rangle + c_2 |3\rangle \wedge |4\rangle \wedge |5\rangle$ for some $c_1 \geq c_2 \geq 0$. Moreover, the coefficients $c_1$ and $c_2$ are uniquely determined by $|\psi\rangle$.

Proof. It is well known that we can write $|\psi\rangle = |\varphi\rangle \wedge |v\rangle$ for some 2-vector $|\varphi\rangle$ and some $|v\rangle \in V$. Clearly we may assume that $||v|| = 1$ and that the support of $|\varphi\rangle$ is orthogonal to $|v\rangle$. Hence, by applying Lemma 1 we may assume that $|v\rangle = |5\rangle$ and $|\varphi\rangle = c_1 |1\rangle \wedge |2\rangle + c_2 |3\rangle \wedge |4\rangle$, $c_1 \geq c_2 \geq 0$. It remains to prove the uniqueness assertion. Note that $|\psi\rangle$ is decomposable if and only if $c_2 = 0$, in which case we have $c_1 = ||\psi||$. So, we may assume that $c_2 > 0$. Assume that we also have $U \cdot |\psi\rangle = |\psi'\rangle = |\varphi'\rangle \wedge |5\rangle$, where $|\varphi'\rangle = c'_1 |1\rangle \wedge |2\rangle + c'_2 |3\rangle \wedge |4\rangle$ and $c'_1 \geq c'_2 > 0$. Since $|5\rangle$ spans the kernel of the linear map $V \to \wedge^4 V$ sending $|x\rangle \to |\psi\rangle \wedge |x\rangle$ and the same is true for $|\psi'\rangle$, we deduce that $U|5\rangle = z|5\rangle$ where $z$ is some phase factor (see [15, Proposition 11.28]). We deduce that $|\varphi\rangle$ and $|\varphi'\rangle$ are unitarily equivalent, and the uniqueness assertion follows from Lemma 1. 

\[\blacksquare\]
2.3 Universal spaces and single occupancy states

Let $G$ be a connected compact Lie group and $V$ a real $G$-module. In other words, $V$ is a finite-dimensional real vector space and we have a linear representation $\rho$ of $G$ on $V$. For a vector subspace $W \subseteq U$, we say that $W$ is universal if every $G$-orbit in $V$ meets $W$ in at least one point. As an example consider the conjugation action of the unitary group $U(d)$ on the space of $d \times d$ complex matrices: $(A,X) \rightarrow AXA^{-1}$ where $A \in U(d)$. Then the well known Schur’s triangularization theorem can be simply expressed by saying that the subspace of upper triangular matrices is universal for this action. There are many other interesting examples of universal subspaces that occur in mathematics and physics. The first question one may ask about the universal subspaces is: what is the minimum dimension of a universal subspace? We can give a simple lower bound for this dimension. Denote by $\rho(\cdot)$ the stabilizer of $W$ in $G$, i.e., the subgroup of $G$ consisting of all elements $g \in G$ such that $\rho(g)$ maps $W$ onto itself. Then we have the following lower bound (see [6, Lemma 4.1]). If $W$ is a universal subspace then

$$\dim W \geq \dim V - \dim G/G_w,$$

where the dimension of the quotient space $G/G_w$ is equal to $\dim G - \dim G_w$. (All the dimensions here are to be interpreted as the dimensions of real manifolds.) A case of special interest is when $G_w$ contains a maximal torus, say $T$, of $G$. Then $G/T$ has even dimension, say $2m$, and we obtain the inequality $\dim W \geq \dim V - 2m$. Assume now that in fact $V$ is a complex vector space of dimension $d$, and so of real dimension $2d$, while $W$ is still assumed to be just a real vector subspace of $V$. If $W$ is universal, we must have $\dim W \geq 2(d - m)$.

In our application we shall take $V = \wedge^N V$, where $V$ is a complex Hilbert space of dimension $M$, and so $d = \begin{pmatrix} M \\ N \end{pmatrix}$. We also specify that $G = U(M)$ and so we have $m = \begin{pmatrix} M \\ 2 \end{pmatrix}$. In particular, for $N = 3$, the above inequality becomes $\dim_{\mathbb{R}} W \geq M(M - 1)(M - 5)/3$. If $W$ is also a complex subspace, we obtain that $\dim_{\mathbb{C}} W \geq M(M - 1)(M - 5)/6$.

In order to define the important notion of single occupancy states in a fermionic system, we partition the set of positive integers into pairs $\{2i - 1, 2i\}$, $i = 1, 2, \ldots$. We shall refer to these pairs as standard pairs. For any positive integer $i$ we denote by $\bar{i}$ the standard pair to which $i$ belongs. Thus, we have $\bar{i} = \{i, i + 1\}$ when $i$ is odd and $\bar{i} = \{i - 1, i\}$ when $i$ is even. We shall say that a finite sequence of positive integers $(i_1, i_2, \ldots, i_k)$ is a single occupancy sequence if the standard pairs $\bar{i}_1, \bar{i}_2, \ldots, \bar{i}_k$ are distinct.

Next we fix an o.n. basis $\{|i\rangle : i = 1, \ldots, M\}$ of the Hilbert space $V$. As explained below Fig. 2 each of our standard pairs $\bar{i}$ associated with basis vectors $\{|i\rangle, |i + 1\rangle\}$ for $i$ odd, then correspond to $\{|g_j\rangle \otimes |\uparrow\rangle, |g_j\rangle \otimes |\downarrow\rangle\}$, where $j = (i + 1)/2$. Similar for $i$ even, the standard pair $\bar{i}$ associated with basis vectors $\{|i - 1\rangle, |i\rangle\}$, then correspond to $\{|g_j\rangle \otimes |\uparrow\rangle, |g_j\rangle \otimes |\downarrow\rangle\}$, where $j = i/2$.

The $\begin{pmatrix} M \\ N \end{pmatrix}$ decomposable vectors $|i_1 \wedge \cdots \wedge i_N\rangle$, $1 \leq i_1 < \cdots < i_N \leq M$, form an o.n. basis of $\wedge^N V$. Hence, the dimension of the space $\wedge^N V$ is $\begin{pmatrix} M \\ N \end{pmatrix}$. If the sequence $(i_1, i_2, \ldots, i_N)$ is a single occupancy sequence then we shall say that $|i_1 \wedge \cdots \wedge i_N\rangle$ is a basic single occupancy $N$-vector (BSOV). Note that if $M$ is odd then $\overrightarrow{\mathcal{M}} = \{M, M + 1\}$ and so there is no state in $V$ that is paired with $|M\rangle$. Finally, we say that an $N$-vector $|\psi\rangle \in \wedge^N V$ is a single occupancy
vector (SOV), relative to the above o.n. basis, if it is a linear combination of the BSOVs. Thus, the set of all SOVs is a vector subspace (the SOV subspace) of $\wedge^N V$ and the set of BSOVs is an o.n. basis of this subspace. Clearly, this definition depends on the choice of the o.n. basis of $V$. A simple counting shows that the number of BSOVs is $2^N \binom{K}{N}$ if $M = 2K$ is even and $2^N \binom{K}{N} + 2^{N-1} \binom{K}{N-1}$ if $M = 2K + 1$ is odd. For the case $N = K$ and $M = 2K$, if one ensures single occupancy, then there are indeed only two possible states per site (spin up and spin down). In this case, any configuration has a natural correspondence to an $N$-qubit state.

Lemma 3 For $N = 2$, $M > 3$, any state is unitarily equivalent to an SOV.

Proof. This is a direct corollary of Lemma 1.

3 Universal subspaces for $N = 3$

3.1 The SOV-subspace is universal for $N = 3$

The main result of this section is that any tripartite antisymmetric state of dimension $M \geq 5$ is unitarily equivalent to a single occupancy state. Recall we say that a vector subspace $W \subseteq \wedge^3 V$ is universal if every $|\psi\rangle \in \wedge^3 V$ is unitarily equivalent to some $|\varphi\rangle \in W$. We denote the unitary group of $V$ by $U(V)$. If an o.n. basis of $V$ is fixed, we shall identify $U(V)$ with the group $U(M)$ of unitary matrices of order $M$.

Theorem 4 Let $V$ be a complex Hilbert space of dimension $M \geq 5$, $\{|i\rangle : i = 1, 2, \ldots, M\}$ an o.n. basis of $V$, and let $e_{ijk} = |i\rangle \wedge |j\rangle \wedge |k\rangle$. Then the SOV-subspace is universal, i.e., any 3-vector $|\psi\rangle \in \wedge^3 V$ is unitarily equivalent to an SOV.

Proof. The case $M = 5$ follows from Corollary 2. So, we shall assume that $M \geq 6$. We shall write $M = 2K$ when $M$ is even and $M = 2K + 1$ when $M$ is odd.

We apply [1] Theorem 4.2 to the problem at hand. Let us first explain what this theorem asserts in this concrete case. We consider the representation $\rho$ of $U(M)$ on the space $V := \wedge^3 V$. We denote by $T$ the maximal torus of $U(M)$ consisting of the diagonal matrices. Thus, if $x \in T$ then $x = \text{diag}(\xi_1, \ldots, \xi_M)$ where each $\xi_i$ is a complex number of unit modulus. Each basis vector $e_{ijk}$ is an eigenvector of $T$. Indeed, we have $x \cdot e_{ijk} := \rho(x)(e_{ijk}) = \xi_i \xi_j \xi_k e_{ijk}$.

A character, $\chi$, of $T$ is a continuous homomorphism into the circle group $S^1 := \{z \in \mathbb{C} : |z| = 1\}$. They form an abelian group under multiplication, but it is convenient to use the additive notation. This means that if $\chi'$ and $\chi''$ are characters of $T$, then their sum $\chi = \chi' + \chi''$ is defined by $\chi(x) = \chi'(x)\chi''(x)$. The map $\chi_i : T \to S^1$, defined by $\chi_i(x) = \xi_i$, is obviously a character of $T$. The group of all characters of $T$ is the free abelian group with basis $\{\chi_i : 1 \leq i \leq M\}$. By using this notation, we have $x \cdot e_{ijk} = (\chi_i + \chi_j + \chi_k)(x)e_{ijk}$ and we say that the character $\chi_{ijk} := \chi_i + \chi_j + \chi_k$ is the weight of the eigenvector $e_{ijk}$. An eigenvector which is fixed by $T$ would have weight 0, but in $V$ there are no such eigenvectors.

We embed the character group of $T$ into the polynomial ring $P := \mathbb{R}[x_1, \ldots, x_M]$ by sending $\chi_i \to x_i$ for each $i$. Let $I$ be the ideal of $\mathbb{R}[x_1, \ldots, x_M]$ generated by the elementary
symmetric functions $\sigma_1, \ldots, \sigma_M$ of the $x_i$. Let $\mathcal{B}$ be the o.n. basis of $\mathcal{V}$ consisting of all $e_{ijk}$. Denote by $\mathcal{B}_s$ the subset of $\mathcal{B}$ consisting of all BSOVs. Let $\mathcal{U}$ be a subspace of $\mathcal{V}$ spanned by a subset $\mathcal{B}' \subset \mathcal{B}$. We define its characteristic polynomial $f_\mathcal{U}$ to be the product of all linear polynomials $x_i + x_j + x_k$ taken over all triples $(i, j, k)$ such that $e_{ijk} \notin \mathcal{B}'$. Then [6] Theorem 4.2] asserts that the subspace $\mathcal{U}$ is universal if $f_\mathcal{U} \notin \mathcal{I}$.

To prove (a) we shall take $\mathcal{B}' = \mathcal{B}_s$. Consequently, we have $\mathcal{U}$ equals the SOV-subspace and the polynomial $q_0 := f_\mathcal{U}$ is given explicitly by the formula

$$q_0 = \prod_{i=1}^{K} \prod_{j \neq 2i-1, 2i} (x_{2i-1} + x_{2i} + x_j).$$

(11)

We shall need another important fact concerning the ideal $\mathcal{I}$. First observe that $\mathcal{I}$ is a homogeneous ideal, i.e., it is the sum of the intersections $\mathcal{I}_d := \mathcal{I} \cap \mathcal{P}_d$, where $\mathcal{P}_d$ is the subspace of $\mathcal{P}$ consisting of all homogeneous polynomials of degree $d$. We introduce an inner product $\langle \cdot | \cdot \rangle$ on $\mathcal{P}$ by declaring that the basis of $\mathcal{P}$ consisting of all monomials is an o.n. basis. In particular, $\mathcal{P}_d \perp \mathcal{P}_e$ if $d \neq e$. We denote by $S_M$ the symmetric group on $M$ letters which permutes the $M$ variables $x_i$ and point out that it preserves the above inner product on $\mathcal{P}$. The following polynomial of degree $\delta := M(M-1)/2$ (with the well known expansion)

$$p := \prod_{1 \leq i < j \leq M} (x_j - x_i) = \sum_{\sigma \in S_M} \text{sgn}(\sigma)x_{\sigma_1}^0x_{\sigma_2}^1x_{\sigma_3}^2 \cdots x_{\sigma_M}^{M-1},$$

(12)

will play an important role. Namely, for any $f \in \mathcal{P}_d$ we know that $f \in \mathcal{I}$ if and only if $\langle f | p \rangle = 0$, see [6] Theorem 4.2]. For $f, g \in \mathcal{P}$, we shall write $f \equiv g$ if $g - f \in \mathcal{I}$ and in that case we say that $f$ and $g$ are congruent modulo $\mathcal{I}$. Thus, if $f \equiv g$ then $\langle f | p \rangle = \langle g | p \rangle$. Note that the degree of $q_0$ is strictly less than $\delta$. For that reason we shall introduce the polynomial $q = \mu q_0$ of degree $\delta$, where $\mu = x_1x_3 \cdots x_{M-3}x_{M-1}$ if $M$ is even and $\mu = (x_1x_3 \cdots x_{M-2})^2$ if $M$ is odd. To prove (b) we shall prove that $q \notin \mathcal{I}$ (which implies that $q_0 \notin \mathcal{I}$).

From the formula (11), we obtain that

$$q_0 = \prod_{i=1}^{K} \sum_{j=0}^{M-2} (x_{2i-1} + x_{2i})^{M-2-j} \sigma_j^{(i)},$$

(13)

where $\sigma_j^{(i)}$ is the $j$th elementary symmetric function of the variables $x_k$ with $k \neq 2i-1, 2i$. (By convention, $\sigma_0^{(i)} = 1$ and $\sigma_{-1}^{(i)} = 0$.) By using the obvious recurrence formula $\sigma_j = \sigma_j^{(i)} + (x_{2i-1} + x_{2i})\sigma_{j-1}^{(i)} + x_{2i-1}x_{2i}\sigma_{j-2}^{(i)} \equiv 0$, we obtain that

$$\sigma_j^{(i)} \equiv (-1)^j \sum_{k=0}^{j} x_{2i-1}^{j-k} x_{2i}^k, \quad j = 0, 1, \ldots, M-2.$$  

(14)

It follows that

$$q_0 \equiv \prod_{i=1}^{K} \left( \sum_{j=0}^{M-2} (-1)^j (x_{2i-1} + x_{2i})^{M-2-j} \sum_{k=0}^{j} x_{2i-1}^{j-k} x_{2i}^k \right).$$

(15)

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We shall need the expansion
\[
\sum_{j=0}^{M-2} (-1)^j (x + y)^{M-2-j} \sum_{k=0}^j x^j y^k = \sum_{k=0}^{M-2} a_k^{(M)} x^{M-2-k} y^k,
\]
where \(x\) and \(y\) are commuting independent variables. Note that \(a_k^{(M)} = a_{M-2-k}^{(M)}\) for each \(k\), and \(a_0^{(M)} = a_{M-2}^{(M)} = 1\) for \(M\) even while \(a_0^{(M)} = a_{M-2}^{(M)} = 0\) for \(M\) odd. For convenience, we set \(a_{M-1}^{(M)} = 0\). We now distinguish two cases.

Case 1: \(M\) is even. By multiplying Eq. (13) by \(\mu\) and by using Eqs. (14) and (16), we obtain that
\[
q = \prod_{i=1}^{K} \sum_{k=0}^{M-2} a_k^{(M)} x_{2i-1}^{-1-k} x_{2i}^k.
\]
By setting \(s_{i,k} = a_k^{(M)} x_{2i-1}^{-1-k} x_{2i}^k + a_k^{(M)} x_{2i-1} x_{2i}^{M-1-k}\) for \(k = 0, 1, \ldots, K - 1\), we obtain that
\[
q = \prod_{i=1}^{K} (s_{i,0} + s_{i,1} + \cdots + s_{i,K-1}) = \sum_{f} \prod_{i=1}^{K} s_{i,f(i-1)},
\]
where \(f\) runs through all functions mapping the set \(\{0, 1, \ldots, K-1\}\) into itself. Let us denote by \(q_f\) the summand corresponding to \(f\). If \(f\) is not a permutation, then each monomial that occurs in the expansion of \(q_f\) will contain two variables with the same exponent, and so the inner product \(\langle q_f | p \rangle\) vanishes. If two of such functions, say \(f\) and \(g\) are permutations then there is an even permutation of the variables which sends \(q_f\) to \(q_g\). We deduce that \(\langle q_f | p \rangle = \langle q_g | p \rangle\), and so \(\langle q | p \rangle = K! \langle \text{id} | p \rangle\) where \(\text{id}\) is the identity permutation.

If the variables \(x_{2i-1}\) and \(x_{2i}\) do not occur in a polynomial \(r \in \mathcal{P}\), then by using the transposition which interchanges \(x_{2i-1}\) and \(x_{2i}\), we obtain that \(\langle x_{2i-1}^{-1-k} x_{2i}^k | p \rangle = - \langle x_{2i-1} x_{2i}^{M-1-k} r | p \rangle\), and so
\[
\langle s_{i,k} r | p \rangle = \langle a_{M-1-k}^{(M)} - a_k^{(M)} | x_{2i-1} x_{2i}^{M-1-k} r | p \rangle.
\]
Since \(q_{\text{id}} = s_{10}s_{21}s_{32} \cdots s_{K,K-1}\), we obtain that
\[
\langle q | p \rangle = K! \prod_{i=0}^{K-1} (a_{M-1-i}^{(M)} - a_i^{(M)}).
\]
By Lemma 5 below, we have \(\langle q | p \rangle \neq 0\).

Case 2: \(M\) is odd. The proof follows closely the one for Case 1 and we shall only briefly sketch the main steps. Recall that in this case \(a_0^{(M)} = a_{M-2}^{(M)} = 0\). By multiplying Eq. (13) by the new \(\mu\) and by using Eqs. (14) and (16), we obtain that
\[
q = \prod_{i=1}^{K} \left( \frac{2}{x_{2i-1}} \sum_{k=1}^{M-2} a_k^{(M)} x_{2i-1}^{-2-k} x_{2i}^k \right) = \prod_{i=1}^{K} \sum_{k=1}^{M-2} a_k^{(M)} x_{2i-1}^{-k} x_{2i}^k.
\]
By setting \( s'_{i,k} = a_k^{(M)} x_{2i-1}^k x_{2i}^k + a_{M-k}^{(M)} x_{2i-1}^k x_{2i}^{M-k} \) for \( k = 1, \ldots, K \), we have

\[
q = \prod_{i=1}^K (s'_{i,1} + s'_{i,2} + \cdots + s'_{i,K}) = \sum_{f} \prod_{i=1}^K s'_{i,f(i)},
\]

where \( f \) runs through all functions mapping the set \( \{1, 2, \ldots, K\} \) into itself. Let us denote by \( q_f \) the summand corresponding to \( f \). If \( f \) is not a permutation, then \( \langle q_f | p \rangle = 0 \). When \( f \) is a permutation, this inner product is independent of \( f \). Thus, \( \langle q | p \rangle = K! \langle q_{id} | p \rangle \) where \( q_{id} = s'_{11} s'_{22} s'_{33} \cdots s'_{K,K} \). By using a similar argument as in Case 1, we obtain that

\[
\langle q | p \rangle = K! \prod_{i=1}^K (a_{M-i}^{(M)} - a_i^{(M)}).
\]

By Lemma 5, \( \langle q | p \rangle \neq 0 \) which completes the proof. \( \Box \)

**Lemma 5** For any \( M > 4 \), let \( a_i^{(M)} \) be the coefficients defined by Eq. (16). Then

1. if \( M \) is even, then \( a_p^{(M)} \neq a_{M-1-p}^{(M)} \) for any \( p \),

2. if \( M \) is odd, then \( a_p^{(M)} \neq a_{M-1-p}^{(M)} \) for any \( p \).

**Proof.** Since the polynomial defining the coefficients \( a_i^{(M)} \) is symmetric, we have \( a_p^{(M)} = a_{M-2-p}^{(M)} \). By expanding this polynomial we obtain that

\[
\sum_{j=0}^{M-2} (-1)^j (x + y)^{M-2-j} \left( \frac{x^{j+1} - y^{j+1}}{x - y} \right)
\]

\[
= \sum_{j=0}^{M-2} (-1)^j \sum_{k=0}^{M-2-j} \binom{M-2-j}{k} x^{M-2-j-k} y^k \sum_{t=0}^j x^{j-t} y^t
\]

\[
= \sum_{j=0}^{M-2} \sum_{k=0}^{M-2-j} \sum_{t=0}^j (-1)^j \binom{M-2-j}{k} x^{M-2-t-k} y^{k+t},
\]

and so

\[
a_p^{(M)} = \sum_{k=0}^{p} \sum_{j=0}^{M-2-p} (-1)^{M-2-k-j} \binom{k+j}{k}
\]

\[
= \sum_{k=0}^{p} \sum_{j=0}^{M-2-p} (-1)^{M-2-k-j} \left( \binom{k+j-1}{k-1} + \binom{k+j-1}{k} \right) + (-1)^{M-2}
\]

\[
= \sum_{k=0}^{p-1} \sum_{j=0}^{M-2-(k+1)-j} (-1)^{M-2-k-j-1} \binom{k+j}{k} + \sum_{k=0}^{p} \sum_{j=0}^{M-3-p} (-1)^{M-2-k-(j+1)} \binom{k+j}{k} + (-1)^{M-2}
\]

\[
= a_p^{(M-1)} + a_p^{(M-1)} + (-1)^{M-2}.
\]
Then the values of $a_p^{(M)}$ can be easily computed, see Table 1.

| $M$ | $a_0^{(M)}$ | $a_1^{(M)}$ | $a_2^{(M)}$ | $a_3^{(M)}$ | $a_4^{(M)}$ | $a_5^{(M)}$ | $a_6^{(M)}$ |
|-----|-------------|-------------|-------------|-------------|-------------|-------------|-------------|
| 4   | 1           | 1           | 1           | 0           |             |             |             |
| 5   | 0           | 1           | 1           | 0           |             |             |             |
| 6   | 1           | 2           | 3           | 2           | 1           | 0           |             |
| 7   | 0           | 2           | 4           | 4           | 2           | 0           |             |
| 8   | 1           | 3           | 7           | 9           | 7           | 3           | 1           |

One may further observe that, for any even number $M$, $a_p^{(M)} \neq a_{M-1-p}^{(M)} \iff a_p^{(M)} \neq a_{p-1}^{(M-1)} + a_p^{(M-1)} \iff a_{p-2}^{(M-1)} \neq a_{p-1}^{(M-1)} + a_p^{(M-1)} \iff a_{p-2}^{(M-1)} \neq a_{M-1-p}^{(M-1)}$.

Therefore, the two parts in our lemma are indeed equivalent, hence we only need to focus on the case that $M$ is even.

For even $M = 2K > 4$ and $1 \leq p \leq M - 3$, we always have $a_0^{(M)} = 1$ and

$$a_p^{(M)} = a_{p-1}^{(M-1)} + a_p^{(M-1)} + 1 \tag{27}$$
$$a_p^{(M-2)} + a_{p-1}^{(M-2)} - 1 + a_p^{(M-2)} + a_p^{(M-2)} - 1 + 1 \tag{28}$$
$$a_p^{(M-2)} + 2a_{p-1}^{(M-2)} + a_p^{(M-2)} - 1. \tag{29}$$

We then show that $\{a_0^{(2K)}, a_1^{(2K)}, \ldots, a_{K-1}^{(2K)}\}$ is an increasing sequence. It is obviously true for $K = 3, 4$. Assume our claim is true for $K = K_0$, let’s look into the case $K = K_0 + 1$. We have $a_p^{(2K_0+2)} = a_p^{(2K_0)} + 2a_{p-1}^{(2K_0)} + a_p^{(2K_0)} - 1$ for any $1 \leq p \leq K_0$. Then $\{a_0^{(2K_0+2)}, a_1^{(2K_0+2)}, \ldots, a_{K_0+1}^{(2K_0+2)}\}$ is also an increasing sequence. Since $a_{K_0}^{(2K_0+2)} - a_{K_0-1}^{(2K_0+2)} = (a_0^{(2K_0)} + 2a_1^{(2K_0)} + a_0^{(2K_0)} - 1) - (a_0^{(2K_0)} + 2a_{K_0-2}^{(2K_0)} + a_{K_0-1}^{(2K_0)} - 1) = a_{K_0}^{(2K_0)} - a_{K_0-1}^{(2K_0)} - a_{K_0-2}^{(2K_0)} - a_{K_0-3}^{(2K_0)} - a_{K_0-4}^{(2K_0)} > 0$, the whole sequence $\{a_0^{(2K_0+2)}, a_1^{(2K_0+2)}, \ldots, a_{K_0}^{(2K_0+2)}\}$ is also an increasing sequence. This completes our proof. $\square$  

3.2 Universal subspaces of minimal dimensions

It follows from Proposition 10 that any subspace of $\wedge^3 V$ which is spanned by less than $M(M - 1)(M - 5)/6$ basic trivectors $e_{ijk}$ is not universal. It is natural to raise the question whether there exist universal subspaces spanned by exactly $M(M - 1)(M - 5)/6$ BSOVs. In the next proposition we show that this is indeed true when $M$ is even, and verify it for odd $M = 7, 9, 11$.

**Proposition 6** Let $V$ be a complex Hilbert space of dimension $M$ and let $e_{ijk} = |i\rangle \wedge |j\rangle \wedge |k\rangle$ for $1 \leq i < j < k \leq M$. 

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(a) If $M = 2K \geq 6$ is even, then the complex subspace spanned by all BSOVs $e_{ijk}$ except the $K$ of them with indexes

$$(1, 3, 6), (1, 4, 6) \quad \text{and} \quad (1, 2i - 3, 2i - 1) \quad 3 \leq i \leq K,$$

is a universal subspace of minimum dimension, $M(M - 1)(M - 5)/6$.

(b) If $M = 7, 9, 11$, then the complex subspace spanned by all BSOVs $e_{ijk}$ except the $M - 1$ of them with indexes

$$(1, 4, M), (2, 5, M) \quad \text{and} \quad (i, i + 2, M) \quad 1 \leq i \leq M - 3;$$

is a universal subspace of minimum dimension, $M(M - 1)(M - 5)/6$.

**Proof.** (a) We can write an arbitrary $|\psi\rangle \in \Lambda^3 V$ as $|\psi\rangle = \sum_{i,j,k} c_{ijk} e_{ijk}$ where the summation is over all triples $(i, j, k)$, $1 \leq i < j < k \leq M$. First, by Theorem 4 we may assume that the coefficients $c_{ijk} = 0$ whenever $e_{ijk}$ is not a BSOV. For $i \leq K$, denote by $U_i$ the subgroup of $U(M)$ which fixes all basis vectors $|j\rangle$ with $j \neq 2i - 1, 2i$. All subsequent LU transformations will be performed by using these subgroups, and so the above mentioned property of the coefficients $c_{ijk}$ will be preserved.

Second, we shall prove by induction that, by using only the $U_i$ operations, we can achieve our goal to make $c_{ijk} = 0$ also when $(i, j, k)$ is one of the triples $(1,3,6)$, $(1,4,6)$ or $(1,2i - 3, 2i - 1)$ with $3 \leq i \leq K$.

If $K = 3$, then $M = 6$. Note that the Hilbert space of 3-qubits can be isometrically embedded in this fermionic system as the subspace spanned by the BSOVs:

$$|i\rangle \otimes |j\rangle \otimes |k\rangle \rightarrow |i + 1\rangle \wedge |j + 3\rangle \wedge |k + 5\rangle, \quad i, j, k \in \{0, 1\}.$$  

The desired result then follows from the well known fact [5] that by performing LU transformations on any given pure state of three qubits one can make vanish any three coefficients (in the standard o.n. basis). This is because after the embedding, the three-qubit LU can be viewed as a special case of the fermionic LU, where we allow only the fermionic LU transformations given by block-diagonal unitary in $U(6)$ with three $2 \times 2$ blocks in $U(2)$.

Now let $K > 3$. By the induction hypothesis, we may assume that the coefficients $c_{ijk} = 0$ when $(i, j, k)$ is one of the triples $(1,3,6)$, $(1,4,6)$ or $(1,2i - 3, 2i - 1)$ with $3 \leq i < K$. We can choose $X \in U_K$ such that $X(c_{1,M-3,M-1}|M-1\rangle + c_{1,M-3,M}|M\rangle) \propto |M\rangle$. This means that the coefficient of $e_{1,M-3,M-1}$ in $X \cdot |\psi\rangle$ is 0. This completes the inductive proof.

(b) This proof is computational. All computations were performed by using Singular [26]. We just have to apply [6, Theorem 4.2] as explained in the proof of Theorem 4. The cases $M = 7$ and $M = 9$ were straightforward, and we omit the details. The values $\langle q|p\rangle$ that we computed for $M = 7, 9, 11$ are 48, 10368 and 12431232, respectively. In the case $M = 11$ we had first to eliminate the variable $x_{11}$ in order to avoid the problem of running out of memory. We shall describe this elimination procedure in general.

Thus, let $M \geq 7$ be an odd integer, and set $M = 2K + 1$. We define the polynomial ring $\mathcal{P}$, its ideal $\mathcal{I}$, and the inner product $\langle \cdot, \cdot \rangle$ of polynomials as in the proof of Theorem 4. The polynomials $g_0$ and $p$ will be the same as in that proof, see Eqs. (11) and (12). The
congruence of polynomials will be again modulo the ideal \( I \). We shall also use the coefficients \( a_k^{(M)} \), \( k = 0, 1, \ldots, M - 2 \), defined by the polynomial identity Eq. (10). (These coefficients are the same as the ones used in Lemma [5].) Other symbols that we are going to introduce, like \( \mu, q \) and \( s_{i,k} \) will have different meaning from the same symbols used in the proof of Theorem [4].

Since \( a_0^{(M)} = a_{M-2}^{(M)} = 0 \), from Eqs. (13) and (10) we obtain that

\[
q_0 \equiv \prod_{k=1}^{K} \sum_{i=1}^{M-3} \left( a_k^{(M)} x_{2i-1}^{M-2-k} x_{2i}^k \right)
= \prod_{k=1}^{K} s_{i,k} = \prod_{i=1}^{K} s_{i,f(i)},
\]

where \( f \) runs through all functions \( \{1, \ldots, K\} \to \{1, \ldots, K - 1\} \) and

\[
s_{i,k} = (x_{2i-1} x_{2i})^k \left( a_k^{(M)} x_{2i-1}^{M-2-k} + a_{M-2-k}^{(M)} x_{2i}^{M-2-k} \right)
= x_{2i-1} x_{2i} s'_{i,k}, \quad k = 1, \ldots, K - 1.
\]

Thus \( q_0 \equiv \sum_f q_f \) where \( q_f = x_1 x_2 \cdots x_{M-1} q'_f \) and \( q'_f = \prod_{i=1}^{K} s'_{i,f(i)} \). The characteristic polynomial of the subspace defined in part (b) is \( q = \mu q_0 \) where

\[
\mu = (x_1 + x_4 + x_M)(x_2 + x_5 + x_M) \prod_{i=1}^{M-3} (x_i + x_{i+2} + x_M),
\]

see (31). Hence, this subspace will be universal if we can prove that \( \langle q | p \rangle \neq 0 \).

By using the expansion (12), we deduce that \( \langle q | p \rangle = \langle \mu q_0 | p \rangle = \langle \mu' q_0 | p \rangle \) where \( \mu' \) is obtained from \( \mu \) by setting \( x_M = 0 \). After cancelling \( x_1 x_2 \cdots x_{M-1} \), we obtain \( \langle q | p \rangle = \langle q' | p' \rangle \), where \( q' = \mu' q'_0 \), \( q'_0 = \sum_f q'_f \) and the polynomial \( p' \) is defined by Eq. (12) with \( M \) replaced by \( M - 1 \). Hence \( x_M \) has been eliminated, it occurs in neither \( p' \) nor \( q' \). For \( M = 11 \), we were able to compute \( \langle q' | p' \rangle \). \( \square \)

We remark that in the case \( M = 6 \) any subspace spanned by 5 BSOVs is universal. However, in the case \( M = 7 \) the 6 BSOVs that we discard cannot be chosen arbitrarily, but there are several other good choices such as \((1, 5, 7), (2, 5, 7), (1, 3, 7), (2, 4, 7), (3, 5, 7), (4, 6, 7)\).

It should also be mentioned that, although it is not directly applicable, our work may shed light on the understanding of the N-representability problem [19], where the single particle eigenvalues are invariants under LU. For the \( N = 3, M = 6 \), let us consider a concrete example of the universal subspace with dimension 5, spanned by

\[
e_{235}, e_{145}, e_{136}, e_{246}, e_{135},
\]

where \( e_{ijk} = |i\rangle \wedge |j\rangle \wedge |k\rangle \).

In other words, any three-fermion pure-state with six single particle states is unitary equivalent to

\[
|\psi\rangle = ae_{235} + be_{145} + ce_{136} + de_{246} + ze_{135},
\]

where...
and the coefficients can be chosen as $a, b, c, d \geq 0, z \in \mathbb{C}$, and $\|\psi\|^2 = a^2 + b^2 + c^2 + d^2 + z^2 = 1$. Without loss of generality, we can further assume that $a \geq b \geq c$.

The one particle reduced density matrix $\rho_1$ of the state $\rho := |\psi\rangle\langle\psi|$, is given by (we choose the normalization $\text{Tr} \rho_1 = 3$

$$
\rho_1 = \begin{pmatrix}
    b^2 + c^2 + |z|^2 & az & 0 & 0 & 0 & 0 \\
    az^* & a^2 + d^2 & 0 & 0 & 0 & 0 \\
    0 & 0 & c^2 + a^2 + |z|^2 & bz & 0 & 0 \\
    0 & 0 & bz^* & b^2 + d^2 & 0 & 0 \\
    0 & 0 & 0 & 0 & a^2 + b^2 + |z|^2 & cz \\
    0 & 0 & 0 & 0 & cz^* & c^2 + d^2
\end{pmatrix}.
$$

We have $\rho_1 = R_a \oplus R_b \oplus R_c$, a direct sum of three $2 \times 2$ diagonal blocks. For $x = a, b, c$ let $D_x = \det R_x$.

Since $\text{Tr} R_x = 1$ and $R_x \geq 0$, we have $D_x \in [0, 1/4]$ and the eigenvalues of $R_x$ can be written as $\lambda_x$ and $1 - \lambda_x$ with $\lambda_x = (1 + \sqrt{1 - 4 D_x})/2 \in [1/2, 1]$. Let us denote the eigenvalues of $\rho_1$ arranged in decreasing order as $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_5 \geq \lambda_6$. Then $\lambda_i$ and $\lambda_{7-i}$ are the eigenvalues of the same block $R_x$ of $\rho_1$. Thus the following result is a direct corollary of Proposition 6.

**Corollary 7** If the $\lambda_i$s are arranged in decreasing order, then $\lambda_i + \lambda_{7-i} = 1$ for $i = 1, 2, 3$.

This hence gives an alternative proof for the $N$-representability equalities and inequalities in the case $N = 3, M = 6 \ [20, 21, 22, 23]$.

### 4 Universal Subspaces for $N > 3$

In this section we consider the generalization to $N > 3$. Note that for $N$ even the total number of configurations is $\binom{2K}{N}$, and that the number of basic single occupancy states is $2^N \binom{K}{N}$. Consider the ratio $r(N, K) = \left(\binom{2K}{N}/2^N \binom{K}{N}\right)$. We know that for any finite $N, K$, we have $r > 1$. If we fix $N$, we will have $\lim_{K \to \infty} r(N, K) = 1$. This means that the single occupancy states have measure 1 for large $K$, so one may hope that a similar result as for $N = 3$ might hold for $N > 3$ at least when $K$ is large. However we show that this is not the case.

#### 4.1 The SOV-subspace is not universal for $N > 3$

**Proposition 8** Let $M$ and $N$ be integers such that $M \geq 2N \geq 8$. Let $V$ be a complex Hilbert space of dimension $M$. Then there exist $|\psi\rangle \in \wedge^N V$ which are not equivalent to any SOV.

**Proof.** Write $M = 2K$ if $M$ is even and $M = 2K + 1$ if $M$ is odd. We fix an o.n. basis $\{|i\rangle : 1 \leq i \leq M\}$ of $V$. Let $V_i = \text{span}\{|2i-1\rangle, |2i\rangle\}$, $i = 1, \ldots, K$, and let $V_{K+1}$ be the
1-dimensional subspace spanned by $|M\rangle$ if $M$ is odd. Then the SOV-subspace, $S$, of $\wedge^N V$ is given by

$$S = \sum_{1 \leq i_1 < \cdots < i_N \leq M} V_{i_1} \wedge V_{i_2} \wedge \cdots \wedge V_{i_N}. \quad (37)$$

Let $G := \text{GL}(V)$ and let $f : G \times S \to \wedge^N V$ be the map sending $(A, |\psi\rangle) \to A \cdot |\psi\rangle$. Let $H$ be the subgroup of $G$ which leaves invariant each of the subspaces $V_i$. Since $S$ is $H$-invariant, we can form the algebraic homogeneous vector bundle $G*H W$ with projection map $p : G*H S \to G/H$ (see [27, section 4.8]). As the dimension of $G*H S$ is $D := \text{Dim} G + \text{Dim} S - \text{Dim} H$, we have

$$D = 4K(K-1) + 2^N\left(\frac{K}{N}\right), \quad (M \text{ even};)$$

$$D = 4K^2 + 2^N\left(\frac{K}{N}\right) + 2^{N-1}\left(\frac{K}{N-1}\right), \quad (M \text{ odd}). \quad (38)$$

Since $f$ factorizes through the canonical map $G \times S \to G*H S$, we have $\text{Dim} G \cdot S \leq D$. One can verify that $D < \binom{M}{N}$, see Lemma 9. Thus $G \cdot S$ must be a proper subset of $\wedge^N V$. $\square$

**Lemma 9** For the dimension $D$ defined by Eq. (38), we have $D < \binom{M}{N}$.

**Proof.** We first prove the assertion for even $M$, i.e., that

$$f(M, N) := \binom{M}{N} - 2^N\left(\frac{K}{N}\right) > 4K(K-1) \quad (39)$$

when $M = 2K \geq 2N \geq 8$. We use induction on $N$. One can easily verify $f(M, 4) > 0$. Suppose $f(M, N) > 0$ holds for some $N$ and that $M \geq 2N + 2$. The inductive step follows from the identity

$$(N+1) (f(M, N+1) - f(M, N)) = (M-2N-1) f(M, N) + N \cdot 2^N\left(\frac{K}{N}\right). \quad (40)$$

which is easy to verify. Indeed, it implies that $f(M, N+1) > f(M, N)$.

Next we show the assertion for odd $M = 2K + 1 \geq 2N$ and $N \geq 4$. For $N = 4$, we have

$$D - \binom{M}{4} = 4K^2 + 2^4\left(\frac{K}{4}\right) + 2^3\left(\frac{K}{3}\right) - \left(\frac{2K+1}{4}\right)$$

$$< 4K + \left(\frac{2K}{4}\right) + 2^3\left(\frac{K}{3}\right) - \left(\frac{2K+1}{4}\right) = 2K(3-K) < 0, \quad (41)$$

where the first inequality is from Eq. (39). For $N > 4$, we have

$$D - \binom{M}{N} = 4K^2 + 2^N\left(\frac{K}{N}\right) + 2^{N-1}\left(\frac{K}{N-1}\right) - \left(\frac{2K+1}{N}\right)$$

$$< 4K^2 + \left(\frac{2K}{N}\right) - 4K(K-1)) + \left(\frac{2K}{N-1}\right) - 4K(K-1)) - \left(\frac{2K+1}{N}\right)$$

$$= 4K(2-K) < 0, \quad (42)$$

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where the first inequality is from Eq. (39). So the assertion is true for odd \( M \). This completes the proof.

To conclude this subsection, we give the lower bound for the dimension of universal subspaces.

**Proposition 10** Let \( V \) be a complex Hilbert space of dimension \( M \) and \( \{ |i\rangle : i = 1, 2, \ldots, M \} \) an o.n. basis of \( V \). Let \( W \) be a complex subspace of \( \wedge^N V \) spanned by some basis vectors \( |i_1 \wedge i_2 \wedge \cdots \wedge i_N\rangle, i_1 < i_2 < \cdots < i_N \). If \( \dim W < \binom{M}{N} - \binom{M}{2} \) then \( W \) is not universal (for the diagonal action of \( U(M) \)).

**Proof.** Let \( U(M) \) be the unitary group of \( V \), identified with the group of unitary matrices of order \( M \) by using the basis \( \{ |i\rangle \} \). Let \( f : U(M) \times W \rightarrow \wedge^N V \) be the restriction of the action map \( U(M) \times \wedge^N V \rightarrow \wedge^N V \). Since \( W \) is spanned by the basis vectors, it is invariant under the action of the maximal torus \( T \) of \( U(M) \) consisting of the diagonal unitary matrices. We can form the equivariant vector bundle \( U(M)^*TW \). The map \( f \) factorizes through the canonical map \( U(M) \times W \rightarrow U(M)^*TW \), and so we have

\[
\dim(U(M) \cdot W) \leq \dim(U(M)^*TW) = M(M - 1) + 2d,
\]

where \( d \) is the complex dimension of \( W \). As \( d < \binom{M}{N} - \binom{M}{2} \), we obtain that \( \dim(U(M) \cdot W) < 2\binom{M}{N} = \dim_\mathbb{R}(\wedge^N V) \). Hence, \( U(M) \cdot W \) must be a proper subset of \( \wedge^N V \), i.e., \( W \) is not universal.

We do not know that whether the bound \( \binom{M}{N} - \binom{M}{2} \) is sharp for universal spaces of general \( N > 2, M \). For \( N = 3 \) and \( M \) even, the bound is sharp by Proposition 6 (a).

**4.2 BCS states are not LU-equivalent to single occupancy states**

We construct a concrete example that is not LU-equivalent to any SOV, i.e. the BCS states. The BCS states are named after Bardeen, Cooper and Schrieffer for their 1957 theory using the states to build microscopic theory of superconductivity [28]. Here we consider the finite dimensional version of the BCS state \( |\psi_{N,M}\rangle \), which is an \( N \)-fermion state, i.e. \( |\psi_{N,M}\rangle \in \wedge^N V \) with \( \dim V = M \), where both \( N \) and \( M \) are even (see e.g. [29]). The \( M \) states are ‘paired’ in a sense: say as \( \{1, 2\}, \{3, 4\}, \ldots, \{M - 1, M\} \). In each pair, the two states are either both ‘occupied’ by a pair of fermions or both ‘empty’. The BCS state is an equal weight superposition of all those ‘paired’ states. Intuitively, BCS states are ‘always double occupancy’, so that they should be among the ‘hardest’ ones to be transformed by LU to some single occupancy state.
We list a few BCS states:

\[ |\psi_{2,M}\rangle = \sum_{i=1}^{K} |2i - 1\rangle \wedge |2i\rangle, \]
\[ |\psi_{4,M}\rangle = \sum_{i_1 < i_2} |2i_1 - 1\rangle \wedge |2i_1\rangle \wedge |2i_2\rangle \wedge |2i_2 - 1\rangle, \quad (44) \]
\[ \vdots \]
\[ |\psi_{N,M}\rangle = \sum_{i_1 < \cdots < i_{N/2}} |2i_1 - 1\rangle \wedge |2i_1\rangle \wedge \cdots \wedge |2i_{N/2} - 1\rangle \wedge |2i_{N/2}\rangle, \quad (45) \]

where the \( i_k \in \{1, \ldots, K\} \).

We shall use exterior multiplication and partial inner products with the BCS states, e.g., \( |a\rangle \wedge |\psi_{N,M}\rangle \) or \( \langle a|\psi_{N,M}\rangle \) where \( |a\rangle \in V \). To simplify this computation, let \( U_1, \ldots, U_K \) be \( 2 \times 2 \) unitary matrices with \( \det U_i = 1 \). So \( U = \bigoplus_{i=1}^{K} U_i \) is a \( M \times M \) unitary matrix. One can verify that

\[ \wedge^2 U |2i - 1\rangle \wedge |2i\rangle = |2i - 1\rangle \wedge |2i\rangle, \quad (46) \]

where \( i = 1, \ldots, K \). Hence we obtain the stabilizer formulas

\[ \wedge^N U |\psi_{N,M}\rangle = |\psi_{N,M}\rangle. \quad (47) \]

Consequently, in the expressions \( |a\rangle \wedge |\psi_{N,M}\rangle \) and \( \langle a|\psi_{N,M}\rangle \), after an LU transformation we may assume that \( |a\rangle \) is a linear combination of the \( |2i - 1\rangle \), \( i = 1, \ldots, K \).

By Lemma 3, if \( N = 2 \) then any BCS state is LU-equivalent to some SOV. In Theorem 12 we will show that this is not the case for \( N \geq 4 \). For this purpose we give a general criterion of deciding whether a state is LU-equivalent to an SOV. We shall denote by \( \rho_{12} \) the bipartite reduced density matrix of \( \rho \).

**Lemma 11** Let \( |\psi\rangle \in \wedge^N V \), \( \dim V = M \geq 2N \), be an antisymmetric state and let \( \rho = |\psi\rangle \langle \psi| \). Then \( |\psi\rangle \) is LU-equivalent to an SOV if and only if there is an o. n. basis \( |a_1\rangle, \ldots, |a_M\rangle \) of \( V \) such that \( \rho_{12}(|a_{2k-1}\rangle \wedge |a_{2k}\rangle) = 0 \) for all \( i \) with \( 2i \leq M \).

**Proof.** **Sufficiency.** By replacing \( |\psi\rangle \) with an LU-equivalent state, we may assume that \( |a_i\rangle = |i\rangle \) for all \( i \). We can write

\[ |\psi\rangle = \sum_{i_1 < \cdots < i_N} c_{i_1, \ldots, i_N} |i_1 \wedge \cdots \wedge i_N\rangle. \quad (48) \]

If \( i_1 = 2s - 1 \) and \( i_2 = 2s \), the hypothesis implies that \( |2s - 1\rangle \wedge |2s\rangle \in \ker \Tr_{3,\ldots,N} |\psi\rangle \langle \psi| = \ker \rho_{12} \). So the coefficient \( c_{i_1, \ldots, i_N} = 0 \). Similarly, \( c_{i_1, \ldots, i_N} = 0 \) if \( \{2s - 1, 2s\} \subseteq \{i_1, \ldots, i_N\} \) for some \( s \). So \( |\psi\rangle \) is a single occupancy state.

**Necessity.** Suppose \( |\psi\rangle \) is LU-equivalent to a single occupancy state \( |\varphi\rangle \), i.e., \( |\psi\rangle = \wedge^N U |\varphi\rangle \) with a unitary \( U \). By definition of SOV we have \( \langle \varphi|(|2s - 1\rangle \wedge |2s\rangle) = 0 \). This is
equivalent to \( \langle (2s - 1) \wedge (2s) \rangle \sigma(2s - 1) \wedge (2s) \rangle = 0 \), where \( \sigma = |\varphi\rangle\langle\varphi| \). By tracing out all but the first two systems, we obtain \( \langle (2s - 1) \wedge (2s) \rangle \sigma_{12}((2s - 1) \wedge (2s)) = 0 \). It follows that \( (2s - 1) \wedge (2s) \in \ker \sigma_{12} \). Thus, the assertion holds with \( |a_i\rangle = U|i\rangle \) for all \( i \). This completes the proof.

Note that the proof can be easily extended to the case in which LU is replaced by the diagonal action \( \wedge^N V \) where \( V \) is invertible. Now we prove the main result on BCS states.

**Theorem 12** Let \( M = 2K \) and \( N \) be even integers with \( K \geq N \geq 4 \). Then the BCS state \( |\psi_{N,M}\rangle \) is not LU-equivalent to any SOV.

**Proof.** We start with the case \( N = 4 \). Suppose \( |\psi_{4,M}\rangle \) is LU-equivalent to an SOV. By Lemma 11 there is a nonzero decomposable 2-vector \( |\varphi\rangle = |a\rangle \wedge |b\rangle \) such that the partial inner product \( \langle \varphi|\psi_{4,M}\rangle = 0 \). By the simplification mentioned beneath Eq. (47), we may assume that \( |a\rangle = \sum_{j=1}^{K} a_{2j-1}|2j-1\rangle \), \( a_1 = 1 \), and \( |b\rangle = \sum_{j=2}^{M} b_j|j\rangle \). As a special case of formula (2) we have

\[
\langle a \wedge b|v_1 \wedge v_2 \wedge v_3 \wedge v_4 = \sum_{1 \leq i < j \leq 4} (-1)^{i+j-1}\langle a \wedge b|v_i \wedge v_j)|v_k \wedge v_l\rangle,
\]

where \( \{i,j,k,l\} = \{1,2,3,4\} \) and \( k < l \). Recall from subsection 2.3 that \( \overline{t} = \{i, i-1\} \) when \( i \) is even and \( \overline{t} = \{i, i+1\} \) when \( i \) is odd. For convenience, we shall write \( \overline{t} < \overline{j} \) if \( i < j \) and \( \overline{i} \neq \overline{j} \). By using the formulae in Eqs. (19) and (14), we conclude that

\[
\langle a \wedge b|i \wedge j\rangle = 0 \quad \text{if} \quad \overline{t} < \overline{j},
\]

where \( i, j \in \{1, \ldots, M\} \). By setting \( i = 1 \) in Eq. (50), we conclude that \( b_j = 0 \) for \( j > 2 \) and so \( |b\rangle \propto |2\rangle \). Next, by setting \( i = 2 \) in Eq. (50), we conclude that also \( a_j = 0 \) for \( j > 1 \) and so \( |a \wedge b\rangle \propto |1 \wedge 2\rangle \). As \( \langle 1 \wedge 2|\psi_{4,M}\rangle \neq 0 \), we have a contradiction. Thus \( |\psi_{4,M}\rangle \) is not LU-equivalent to an SOV.

Next, we use the induction on \( N \) to show that there is no nonzero decomposable 2-vector \( |\varphi\rangle = |a \wedge b\rangle \) such that the partial inner product \( \langle \varphi|\psi_{N,M}\rangle = 0 \). By Lemma 11 this implies that the BCS state \( |\psi_{N,M}\rangle \) is not LU-equivalent to any SOV.

Since we have already verified the first case, \( N = 4 \), let us assume that the assertion holds for \( |\psi_{N-2,M}\rangle \) with \( N \geq 6 \) and \( M \geq 2(N-2) \). Suppose there is a nonzero decomposable 2-vector \( |\varphi\rangle = |a \wedge b\rangle \) such that \( \langle \varphi|\psi_{N,M}\rangle = 0 \) with \( M \geq 2N \). Let

\[
|a\rangle = \sum_{j=1}^{M} a_j|j\rangle := |\alpha\rangle + \sum_{j=M-1}^{M} a_j|j\rangle,
\]

\[
|b\rangle = \sum_{j=1}^{M} b_j|j\rangle := |\beta\rangle + \sum_{j=M-1}^{M} b_j|j\rangle.
\]

Since \( \langle \varphi|\psi_{N,M}\rangle = 0 \), we have

\[
0 = \langle M-1 \wedge M|\langle \varphi|\psi_{N,M}\rangle\rangle = \langle \varphi\rangle \left( \langle (M-1) \wedge M|\psi_{N,M}\rangle \right)
\]

\[
= \langle \varphi|\psi_{N-2,M-2}\rangle = \langle \alpha \wedge \beta|\psi_{N-2,M-2}\rangle.
\]
As \( M - 2 > 2(N - 2) \), the induction hypothesis implies that \( \langle \alpha \wedge \beta \rangle = 0 \). Thus \( |\alpha\rangle \) and \( |\beta\rangle \) are linearly dependent. Consequently, we may assume that \( |\beta\rangle = 0 \), and moreover that \( |b\rangle = |M\rangle \) and that all \( a_{2i} = 0 \). Then by expanding the left hand side of \( \langle a \wedge b | \psi_{N,M} \rangle = 0 \), we obtain a contradiction similarly as in case \( N = 4 \). So there is no nonzero decomposable 2-vector \( |\varphi\rangle \) such that \( \langle \varphi | \psi_{N,M} \rangle = 0 \). This completes the proof by induction. \( \square \)

5 Summary and Discussion

We have discussed universal subspaces for local unitary groups of fermionic systems. We have shown that for \( N = 3 \), the SOV-subspace is universal. Furthermore, for \( M \) even, we can always find a universal subspace, contained in the SOV-subspace, whose dimension is equal to the lower bound \( M(M - 1)(M - 5)/6 \). Although our main tool is a natural application of Theorem 4.2 in [3], which can be used in small dimensions to construct universal subspaces by computers, the analytical proof we obtained for the general case is far from trivial. In fact, some special features of polynomials are used, which do not generalize to settle the odd \( M \) case.

We have also shown that, for \( N > 3 \), not all fermionic states are LU-equivalent to a single occupancy state. Our argument is based on dimension counting. For \( M \) even, we give BCS states as concrete examples that are not LU equivalent to any single occupancy state. This is intuitive as BCS states are always paired so they are most unlikely to be transformed with LU to something unpaired. Given that for fixed \( N \) almost all states are single occupancy in the large \( M \) limit, the BCS states are also among the ‘measure zero’ states.

We wish our results shed light on further study of entanglement properties on fermionic system, as well as other properties of fermionic states such as the N-representability problem (as we discussed for the \( N = 3, M = 6 \) case). We also leave some open questions. One of them is to understand the achievability of the dimension lower bound for \( N = 3 \) and \( M \) odd, or for even the case of general \( N > 2, M \), which is worth further investigation.

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