Quantum Entanglement in Fermionic Lattices

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The Fock space of a system of indistinguishable particles is isomorphic (in a non-unique way) to the state-space of a composite i.e., many-modes, quantum system. One can then discuss quantum entanglement for fermionic as well as bosonic systems. We exemplify the use of this notion –central in quantum information - by studying some e.g., Hubbard, lattice fermionic models relevant to condensed matter physics.

A big deal of attention have been recently devoted to the notion of quantum entanglement \[\text{[3]}.\] As a matter of fact this fashion is mostly due to the vital role that such notion is generally believed to play in Quantum Information Processing (QIP) protocols \[\text{[2]}.\] The definition of entanglement relies on the tensor-product structure of the state-space of a composite quantum system \[\text{[3]}.\]

On the other hand such a tensor product structure is not present in a large class of systems of major physical interest: ensembles of indistinguishable particles. Indeed in this case it is known – basically since the birth of quantum theory– that the state-space associated with a system of indistinguishable particles is constrained to be a subspace of the N-fold tensor product. Depending on the bosonic or fermionic nature of the subsystems one has to select the totally symmetric or antisymmetric subspace. This is an instance of a superselection rule \[\text{[3]}.\] i.e., a fundamental limitation on the possibility of preparing a given state.

We see therefore that the existence of quantum statistics \[\text{[3]}.\] makes the notion of entanglement problematic for systems of made of indistinguishable subsystems e.g., particles. Notice that, even if one allows for general \[\text{parastatistics [3]}.\] most of the product states \[\otimes_{i=1}^{N}|i\rangle\] do not belong to the physical state-space at all in that they do not have a proper transformation under permutations of \[\mathcal{S}_N\] i.e., they do not belong to an \[\mathcal{S}_N\text{-irrep [3]}.\]

Very recently some authors addressed the issue of entanglement (or more generally quantum correlations) in system of two fermions \[\text{[3]}.\] and bosons \[\text{[3]}.\] Their approach appears to be the natural generalization of the one used for the distinguishable particles.

In this paper we shall tackle the problem of the relation between entanglement and quantum statistics from a rather different perspective based on entanglement relativity as discussed in Ref. \[\text{[3]}.\] We shall mostly focus on the fermionic case \[\text{[3]}.\] In particular we shall analyze the local i.e., on-site, entanglement associated with simple fermionic models on a lattice.

Fermions and Qubits. Let us start be recalling basic kinematical facts about many fermion systems. Let \[h_L:=\text{span}\{|\psi_l\rangle\}_{l\in\mathbf{N}_L}, \quad (\mathbf{N}_L:=\{1,\ldots,L\})\] be an \(L\)-dimensional single particle state space. The labels in \(\mathbf{N}_L\) will be referred to as sites and the associated single-particle wavefunctions will be thought of as describing a (spatially) localized state. Accordingly the set of the \(l\)'s will be referred to as the lattice.

Let \(\mathcal{P}_L (\mathcal{P}^N_L)\) denote the whole (with \(N\) elements) family of subsets of \(\mathbf{N}_L\). For any \(A:=\{j_1,\ldots,j_N\}\in\mathcal{P}_L\) we define the anti-symmetrized state-vector

\[
|A\rangle := \frac{1}{\sqrt{N!}} \sum_{P\in\mathcal{S}_N} (-1)^{|P|} \otimes_{l=1}^{N} |\psi_{j_{P(l)}}\rangle.
\]

The \(|A\rangle\)'s are an orthonormal set. The state-space \(\mathcal{H}_L(N)\) associated with \(N\) (spinless) fermions with single-particle wavefunctions belonging to \(h_L\) is given by the totally anti-symmetric subspace of \(h^\otimes_{N}\) i.e., \(\mathcal{H}_L(N) := \text{span}\{|A\rangle / A \in \mathcal{P}^N_L\}\). The fermion number ranges from 0 to \(L\), the total Fock space is obtained as a direct sum of the fixed number subspaces i.e., \(\mathcal{H}_L = \bigoplus_{N=0}^{L} \mathcal{H}_L(N) = \text{span}\{|A\rangle / A \in \mathcal{P}_L\}\). From the well-known relation

\[
\dim\mathcal{H}_L = \sum_{N=0}^{L} \dim\mathcal{H}_L(N) = \sum_{N=0}^{L} \binom{L}{N} = 2^L,
\]

it follows that the fermionic Fock space is isomorphic to a \(L\)-qubits space, each qubit being associated with a site \([40]\). The latter isomorphism is realized by the the mapping

\[
\Lambda: \mathcal{H}_L \rightarrow (\mathcal{P}^L)\otimes \mathcal{H}_L: |A\rangle \rightarrow \otimes_{l=1}^{L} |\chi_A(l)\rangle,
\]

where \(\chi_A: \mathbf{N}_L \rightarrow \{0,1\}^{L}\) is the characteristic function of \(A\). Clearly \(\Lambda(|A\rangle)\) is nothing but a \(N\)-qubit basis state having in the \(j\)-th site a one (zero) if \(j \in A\) (\(j \notin A\)). The 0-particle state \(|0\rangle\) is mapped by \(\Lambda\) onto \( |0\rangle := |0\rangle \otimes \mathcal{H}_L\); thus latter vector is referred to as the vacuum.

In our considerations, once \(\mathcal{H}_L\) is endowed by \(\Lambda\) with a multi-partite structure, tensor products of individual single-particle spaces are not relevant anymore. To exemplify this point let us consider the case \(L = 3\). It is not difficult to see that all the states in \(\mathcal{H}_3(2)\), seen as elements of \(h^\otimes_3\), have the same entanglement. Indeed all of them can be written as \(|a\rangle \otimes |b\rangle - |b\rangle \otimes |a\rangle\), for suitable \(|a\rangle\) and \(|b\rangle\). On the other hand both the "separable" states \(|1\rangle \otimes |0\rangle\otimes |0\rangle\) and the "entangled" \(|0\rangle \otimes |1\rangle \otimes |0\rangle\) belongs to \(\Lambda(\mathcal{H}_3(2))\). This kind of puzzle is solved by observing that the entanglement of, say \(|a\rangle \otimes |b\rangle - |b\rangle \otimes |a\rangle\), is not physical. Indeed in the involved subsystems i.e., individual "labelled" particles, due to the very notion of indistinguishability, are physically not accessible.

This situation is just an illustration of the relativity of the notion of entanglement \([3]\). The latter crucially depends on the choice of a particular partition into physical subsystems. In this case "good" subsystems are associated with the set of single particle modes...
(labelled by $l \in \mathbb{N}_L$ whose occupation numbers are physical observables and not with the particles themselves. From this perspective one can have entanglement without entanglement. For instance a one-particle state e.g., $|0\rangle \otimes |1\rangle + |1\rangle \otimes |0\rangle$, can be – with respect to the partition into mode subsystems – entangled. It is important to stress that such kind of one-particle entanglement (or correlation), despite its paradoxical nature, has been recently proven to allow for quantum teleportation \cite{12}; therefore it has to be regarded as a genuine resource for QIP.

The Fock space $\mathcal{H}_L$, since it allows for a varying particle occupation, does not correspond generally to the state space of a physical system. For charged fermions coherent superpositions of vectors belonging to different particle number sectors are forbidden due to charge superselection rule \cite{3}. In this sense our qubits are unphysical. Only qubit states in the $\Lambda(\mathcal{H}_L(N))$ are associated with (N-particle) physical states. Accordingly not all the elements of $\text{End}(\mathcal{H}_L)$ correspond to physical observables: the latter span the subalgebra $\mathcal{F}$ of number conserving operators i.e., $\mathcal{F} := \{ X / [X, N] = 0 \} = \otimes N \text{End}(\mathcal{H}_L(N))$

**Local Entanglement.** Let $|\Psi\rangle \in \mathcal{H}_L(N)$ be the associated j-th local density matrix is given by $\rho_j := \text{Tr}_j|\Psi\rangle\langle\Psi|$ where $\text{Tr}_j$ denotes the trace over all but the j-th sites. For any $j \in \mathbb{N}_L$ one obtains a partition of $\mathcal{H}_L$ i.e., $\mathcal{C}^2 \otimes \mathcal{C}^2 \otimes \mathcal{L}^{(L-1)}$ therefore the entropy $S$ (von Neumann as well as linear) of $\rho_j$ is a measure of the entanglement of the j-th site with the remaining N – 1 ones.

Local entanglement is relative to the decomposition into subsystems i.e., sites, defined by mapping \cite{3} \cite{8}. One could consider different isomorphisms giving rise to inequivalent partitions in to “local” subsystems. This fact can be clearly seen by introducing creation and annihilation operators \{$c_j^{\dagger}$, $c_j$\}_{j=1}^L \subset \text{End}(\mathcal{H}_L)$, \{[a, b]± = $ab \pm ba$\} which satisfy canonical (anti) commutation relations for (fermions) bosons

$$[c_i, c_j]_{\pm} = 0, [c_i, c_j^\dagger]_{\pm} = \delta_{ij}, c_j |0\rangle = 0 (j \in \mathbb{N}_L).$$

Of course $\mathcal{H}_L = \text{span}\{\prod_{j=1}^L c_j^{\dagger} |n_1\rangle |n_2\rangle |n_3\rangle ... |n_L\rangle |0\rangle / n_1, n_2, n_3 ... n_L \in \mathbb{N}_\infty\}$. If $U$ is a $L \times L$ unitary matrix then it is well-known that the following (Bogoliubov) transformation

$$c_i \rightarrow \tilde{c}_i := \sum_{j=1}^L U_{ij} c_j, \ (i \in \mathbb{N}_L)$$

maps fermions (bosons) onto fermions (boson) giving rise to an automorphism of the observable algebra. Accordingly new occupation-number representations $\Lambda_U: \prod_{i=1}^L (c_i^{\dagger})^{n_i} |0\rangle \mapsto \otimes_{i=1}^L |n_i\rangle (n_i = 0, 1)$ are defined. Clearly entanglement is strongly relative to the decompositions associated with different $\Lambda_U$’s. Notice that even though automorphisms \cite{3} have a single-particle origin, they define non-local transformations of the Fock space onto itself. Indeed a mapping $W \in \mathcal{U}(\mathcal{H}_L)$ is local with respect the subsystem decomposition associated with $\Lambda_U$ iff $\Lambda_U \circ W \circ \Lambda_U^{-1} \in \prod_{i=1}^L \mathcal{U}(\mathcal{C})$.

As a particular, though quite relevant, case one can consider the Fourier transformation i.e., $U_{kj} := e^{i k_{j} x}, k := 2\pi (l - 1)/L, (l \in \mathbb{N}_L)$. The wave-vectors $k$ label the so-called reciprocal lattice ($\Lambda_U$ is denoted by $\Lambda'$) and represent physically modes delocalized over the spatial lattice. It is obvious that states that are entangled (non-entangled) with respect $\Lambda$ can be non non-entangled (entangled) with respect $\Lambda'$.

The situation we shall investigate in this paper is the following. Suppose $H \in \text{End}(\mathcal{H}_L)$ is a non degenerate (gran-canonical) hamiltonian and $H = \sum_m \epsilon_m |\psi_m\rangle \langle \psi_m|$ its spectral decomposition. If $\rho_j^m$ denotes the j-th local density matrix associated with the energy eigenstate $\epsilon_m$, one can compute the quantity

$$S_{1/\beta} := \frac{1}{Z_L} \sum_{m=1}^L e^{-\beta \epsilon_m} \sum_{j=1}^L S(\rho_j^m)$$

where $Z$ is the (gran-canonical) partition function i.e., $Z := \sum_{m=1}^L e^{-\beta \epsilon_m}$. Eq. (3) is the thermal expectation value of the local entanglement averaged over the whole lattice \cite{3}. In particular we will be interested in the limit $\beta \rightarrow \infty$ i.e., local entanglement $S_0$ in the ground state.

When energy spectrum shows degeneracies Eq (3) is no longer well-defined. We assume that there is a “natural” (see examples below) way to select a a complete set of commuting observables containing $H$, whose joint eigenvectors provide the $\epsilon_m$’s to be used in (3).

To begin with we observe that

$$\rho_j = |\psi_j\rangle \langle \psi_j| \otimes 1_j$$

where $n_i := c_i^\dagger c_i = |\psi_j\rangle \langle \psi_j| \otimes 1_j$ is the local occupation number projector. Indeed: $\langle 1_j | \rho_j | 1_j \rangle = \text{Tr}(\rho_j 1_j) = \langle \psi_j | \psi_j \rangle$ in the same way one obtains the other diagonal element of $\rho_j$. Moreover $\langle 0 | \rho_j | 0 \rangle = \text{Tr}(|\psi_j\rangle \langle \psi_j| c_j^\dagger c_j) = (|\psi_j\rangle \langle \psi_j| c_j^\dagger c_j) |\psi_j\rangle \langle \psi_j| = 0$, last equality is due to the fact that $|\psi_j\rangle$ is a particle number eigenstate i.e., an eigenstate of the operator $N := \sum_{j=1}^L c_j^\dagger c_j$.

**Itinerant Fermions.** We now consider free (spinless) fermions hopping in the lattice. The Hamiltonian is given by

$$H_{\text{Free}} = -t \sum_{j=1}^{L-1} (c_{j+1}^\dagger c_j + \text{h.c.}) - \mu \hat{N}$$

Introducing the Fourier fermionic operators $c_k := 1/\sqrt{L} \sum_j e^{i k_j} c_j$, it is a text-book exercise to prove that \cite{3} has eigenstates given by the $N$-particle vectors $|k\rangle := \prod_{m=1}^N c_{k_m} |0\rangle$, $k := (k_1, \ldots, k_N) \in \mathbb{R}^N$ with eigenvalues $\epsilon_k := -2t \sum_{k_m} \cos(k_m) - \mu N$.

The local density matrix is easily obtained by using Eq. (4) and the translational properties of the $|k\rangle$’s. If $T$ denotes the natural representation in $\mathcal{H}_L$.
of the cyclic permutations $i \mapsto i + 1 \mod L$ i.e., the translation operator, one has $T|\mathbf{k}\rangle = e^{i\sum_{m=1}^{N} k_m} |\mathbf{k}\rangle$. Therefore $\langle \mathbf{k}|n_\mathbf{k}\rangle = 1/L \sum_{i=1}^{L} \langle \mathbf{k}|n_i\rangle |\mathbf{k}\rangle = N/L =: n$. Whereby $E = 1/Z \sum_{N,L=0}^{\beta} S(N/L) e^{\beta N} Z(N/\beta) = 1/Z \text{Tr} (\hat{S}(N/L) e^{-\beta \hat{H}_{\text{free}}})$, in which $S(n) = -n \ln n - (1 - n) \ln(1 - n)$ and $Z(N/\beta) := \text{Tr}_{\mathcal{H}(N)} e^{-\beta (H + u N)}$ is the $N$-particle canonical partition function.

The fraction $p(N) := e^{\beta N} Z(N)/Z$ gives of course the probability of having any $N$-particle configuration. In the thermodynamical limit ($N, L \to \infty$, $N/L = \text{const}$) $p(N)$ becomes strongly peaked around the expectation value $N_0$ of $\hat{N}$. In this case local entanglement is simply given by the Shannon function $E \sim S(n_0)$, it readily displays an intuitive feature: local entanglement vanishes for the empty (fully filled) lattice being the unique associated state given the product $|0\rangle (\otimes |1\rangle)$; moreover $E$ is maximal at half-filling i.e., $n_0 = 1/2$. Notice that for the states $|\mathbf{k}\rangle$ entanglement associated with the $\Lambda^*$ partition is obviously zero.

**Spin 1/2 Fermions.** Here we consider the lattice models of spin 1/2 fermion model. We have then to introduce an extra dicothomic variable $\sigma = \uparrow, \downarrow$ to label the single-particle state-vectors. As usual fermionic operators corresponding to different $\sigma$’s always anti-commute. In this case it is convenient to consider the $2^L$-dimensional Fock space as isomorphic teh $L$-fold tensor power of four-dimensional space i.e., $\mathcal{H}_F \cong (\mathbb{C}^4 \otimes L$. The local state space is spanned by the vacuum $|0\rangle$ and the vectors

$$|1\rangle := c_{j\uparrow}^\dagger |0\rangle, |1\rangle := c_{j\downarrow}^\dagger |0\rangle, |1\rangle := c_{j\uparrow}^\dagger c_{j\downarrow}^\dagger |0\rangle. \quad (8)$$

The $\rho_j = \text{Tr}_\mathcal{F} |\Psi\rangle \langle \Psi|$ is now a $4 \times 4$ matrix. If the $N$-particle state $|\Psi\rangle$ is a) translational invariant, b) eigenstate of $S^z := \sum_{j=1}^{L} (n_{j\uparrow} - n_{j\downarrow})$, is easy to see that $\rho_j = 1/L \text{diag}(1 - N \uparrow - N \downarrow, N \uparrow, N \downarrow, N \downarrow)$ where $N_\sigma := \sum_{j=1}^{L} |\Psi| n_{j\sigma} (1 - n_{j\sigma}) |\Psi\rangle, (\sigma = \uparrow, \downarrow)$ is the number of lattice sites singly occupied by a $\sigma$ fermion and $N_i := \sum_{j=1}^{L} |\Psi| n_{j\uparrow} n_{j\downarrow} |\Psi\rangle$ is the number of doubly occupied sites. We see that local entanglement, in state $|\Psi\rangle$ is a function just of the occupation numbers $N_{\sigma}$, ($\alpha = \uparrow, \downarrow, \downarrow$, in particular it follows that Eq. (8) can be effectively computed for Hamiltonians commuting with the $N_{\alpha}$’s i.e., $E = \sum (N_{\alpha}) e^{\beta N} S(N_{\alpha}) Z(N_{\alpha})/Z$. An instance of this case is illustrated in the following.

**Supersymmetric Dimer.** We consider here a two-site i.e, a dimer, version of the so called supersymmetric EKS model [1-4]. For zero chemical potential i.e., half-filling the EKS Hamiltonian acts on the basis states as follows

$$H |\alpha\rangle \otimes |\beta\rangle = \{ -1 \}^{\text{parity}} |\beta\rangle \otimes |\alpha\rangle \quad (9)$$

where $|\alpha\rangle$ is the parity of the single-site state $|\alpha\rangle$ i.e., $|\uparrow\rangle = |\downarrow\rangle = 1/2, |0\rangle = |\uparrow\downarrow\rangle = 0$. Since $H$ is just a graded permutator the relations $[H, N_{\alpha}] = 0$ hold true. The state-space split according the $N_{\alpha}$’s configurations $\mathcal{H}_{\alpha} = \oplus (N_{\alpha}) \mathcal{H}(\{ N_{\alpha} \})$ and the Hamiltonian can be diagonalized within each sector. Notice that Eq. (11) is also invariant under a global particle-hole transformation i.e., $|\sigma\rangle \leftrightarrow | - \sigma\rangle, |0\rangle \leftrightarrow | \uparrow\downarrow\rangle$.

It is straightforward to check that $H$ admits four singlets non-entangled (the configurations $(0,0,0)$, $(2,0,0)$ along with their particle-hole conjugates) and six doublets $(1,1,0), (0,1,0)$ and conjugates and the self-conjugated $(1,1,0), (0,0,1)$ with entanglement ln 2. Moreover since $H^2 = \mathbb{1}$ one gets an energy spectrum given by $\{-1,1\}$, being both the eigenvalues 8-fold degenerated. Therefore $E = 12 \ln 2 \cosh \beta/16 \cosh \beta = 3/4 \ln 2$ : the local-entanglement (at half filling) is temperature independent.

This very simple result is due to the large symmetry group of the Hamiltonian (11). A more interesting case is obtained introducing a model in which a free parameter controls the competition between the localized and itinerant nature of the lattice fermions.

**Hubbard Dimer.** If $H_{\text{free}}^\sigma$ simply denotes Eq. (11) with extra spin index then Hubbard Hamiltonian reads (11)

$$H_{\text{Hubb}} = \sum_{\sigma = \uparrow, \downarrow} H_{\text{free}}^\sigma + U \sum_{j=1}^{L} n_{j\uparrow} n_{j\downarrow}. \quad (10)$$

The new local terms added account for the on-site interaction e.g., Coulomb repulsion, experienced by pairs of (opposite) spin fermions sitting on the same lattice site. By introducing the total fixed spin number operators $\hat{N}_{\sigma} := \sum_{j=1}^{L} n_{j\sigma}$ ($\sigma = \uparrow, \downarrow$) is easy to check that both of them commute with the Hubbard Hamiltonian (11). This implies that $H_{\text{Hubb}}$ can be separately diagonalized in each joint eigenspace $\mathcal{H}(N_{\uparrow}, N_{\downarrow})$ of the $N_{\sigma}$’s. In the the dimer case i.e, the dimer, one finds dim $\mathcal{H}(N_{\uparrow}, N_{\downarrow}) = \prod_{\sigma} \left( \begin{array}{c} 2 \\ N_{\sigma} \end{array} \right)$ ; then at most (for $N_{\uparrow} = N_{\downarrow} = 1$) one has to solve a four-dimensional diagonalization problem.

![FIG. 1. Entanglement of the Hubbard dimer ground state as a function of $U/4t$ for decomposition associated with real and reciprocal lattice.](image-url)
where \( \alpha_\pm(x) := x \pm \sqrt{1 + x^2} \), and the associated eigenvalue is given by \( E_0 = -2t \alpha_- \). The entanglement of the state (11) is easily studied as a function \( U/4t \). Using linear entropy as an entanglement measure one finds \( S_0(U/t) = 1 - \frac{1}{4}\sum \alpha_\sigma^2 = 1 - 1/2(\alpha_+^2 + 1)(\alpha_-^2 + 1)^{-2} \). Local entanglement is monotonically decreasing as a function of \( U/4t \). (Fig. 1). In particular one obtains the free limit \( S_0(0) = 3/4 \) and the strong coupling limit \( S_0(\infty) = 1/2 \) that correspond to ground states given by uniform superpositions of respectively four and two states [see Eq. (1)]. Of course the physical interpretation is quite simple: the higher the on-site repulsion \( U \) the more local charge fluctuations are suppressed and the smaller the number of available states. Eventually for infinite repulsion doubly occupied sites get decoupled and only spin fluctuations survive. In this regime Hubbard model is known to be equivalent to an anti-ferromagnetic Heisenberg model for spin 1/2 [10]. Ground state as well as thermal entanglement for this (and related) models have been quite recently studied [11].

It is instructive to write the dimer ground state \( \Psi_0 \) in terms of the Fourier operators \( c_\sigma^{(\pm)} := 1/\sqrt{2}(c_{\sigma \uparrow} \pm c_{\sigma \downarrow}) \) (\( \sigma = \uparrow, \downarrow \)), from Eq. (1) one finds

\[
G_0(\alpha) = \sum_{k=\pm} (1+ k \alpha_\pm) c^{(k)\dagger}_\uparrow c^{(k)\dagger}_\downarrow. \tag{12}
\]

With respect this reciprocal decomposition local entanglement is an increasing function of \( U/4t \). From the free case (\( \alpha_\pm = 1 \)), that is unentangled up to strong coupling (\( \alpha_\pm = \infty \)) which gives \( S_0(\infty) = 1/2 \) (see Fig. 1).

The example of the Hubbard dimer shows that -not surprisingly - entanglement is well-suited to analyze the interplay between itinerant and localized features of Hubbard Model (10): hopping term \( t \) (repulsion \( U \) ) term is responsible for entanglement in the real (reciprocal) lattice decomposition.

**Conclusions.** In this paper we discussed some issues related to entanglement in system of indistinguishable particle. For these systems quantum statistics applies and therefore their state-space is not naturally endowed with a tensor product structure.

Nevertheless mappings between their Fock spaces and multi-partite state-spaces can be established (the well-known occupation number representation) and then the usual definition of entanglement can be applied. For systems with \( L \) single particle states available the set of possible inequivalent decompositions into \( L \) subsystems (modes) is parametrized by the group \( U(L) \) of Bogoliubov transformations.

We focused on simple e.g., Hubbard, models of fermions on lattice studying how, as function of the model parameters, local entanglement varies both with respect to real and reciprocal lattice decomposition. Results suggest that this notion of entanglement is well suited to describe interplay between localization and itinerancy in these systems.

We believe that the approach pursued in this paper – besides to establish a connection between the field of Quantum Information Processing and condensed matter physics – can provide novel physical insights in the study of interacting ensembles of indistinguishable particles.

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