Multipartite entanglement in fermionic systems via a geometric measure

Pramod S. Joag

Department of Physics
University of Pune
Pune - 411007

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In Collaboration with:

Behzad Lari and P. Durganandini
Department of Physics
University of Pune
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In many situations involving interacting entangled quantum particles, the effects of their indistinguishability cannot be ignored. Interacting electrons in a system of quantum dots. All strongly correlated electron systems. Quantum Hall effect, Quantum phase transitions.
Local and non-local operations.
Antisymmetrization.
Different measures of entanglement.

Basically bipartite entanglement measures are suggested. Slater rank: Number of Slater determinants needed to expand an entangled state. (Schliemann)
Quantum correlations between modes. (Zanardi)
Maximum quantum correlations which can be extracted by means of local operations on modes from the two parts of the system. (Wiseman and Vaccaro)
We propose a geometric measure of entanglement for a pure state on $N$ indistinguishable fermions.

Main idea (Zanardi): The Fock space of a system of fermions is mapped to the isomorphic qubit or ‘mode’ space. We then obtain a geometric measure of entanglement in this mode space. The measure of $m$-partite entanglement is the Euclidean norm of the $m$-partite correlation tensor in the Bloch representation of the $N$-particle state. This correlation tensor has all the information of the genuine $m$-partite entanglement. This measure is shown to satisfy all the properties expected of a good entanglement measure.
$N$ spin $\frac{1}{2}$ fermions on a $L$ site lattice.
Number of single particle states $= 2L$.
Basis states for the Fock space $(F_{2L})$ in occupation number representation are $|n_1 n_2 \cdots, n_{2L}\rangle(n_i = 0, 1; i = 1, 2, \ldots, 2L)$.
No. of particles is conserved : We deal with the subspace of $F_{2L}$ corresponding to a fixed eigenvalue of the number operator $(F_N)$.

$$\dim(F_N) = \binom{2L}{N}$$

$$\dim(F_{2L}) = \sum_{N=0}^{2L} \binom{2L}{N} = 2^{2L} = \dim(\mathbb{C}^{\otimes 2L})$$

It is possible to construct isomorphism between $F_{2L}$ and $\mathbb{C}^{\otimes 2L}$ (2L qubit space).
The isomorphism we implement is

\[ |n_1 n_2 \cdots, n_{2L} \rangle \mapsto |n_1 \rangle \otimes |n_2 \rangle \otimes \cdots \otimes |n_{2L} \rangle \ (n_i = 0, 1 ; i = 1, 2, \ldots, 2L). \]

In the qubit space we associate \(|0\rangle \leftrightarrow |\uparrow \rangle\) and \(|1\rangle \leftrightarrow |\downarrow \rangle\). Note that this isomorphism maps separable states to separable states.

The subspace structure of the Fock space \(F_{2L} = \bigoplus_{N=0}^{2L} F_N\) is preserved under this isomorphism

\[ H_{2L} = (\mathbb{C}^2)^{\otimes 2L} = \bigoplus_{N=0}^{2L} H_{2L}(N) \]

\(H_{2L}(N)\) is the image of \(F_N\) under the isomorphism.
Next step is to transfer the action of the creation and annihilation operators on Fock space to the qubit space, under the isomorphism. We need the creation and annihilation operators $a$ and $a\dagger$ acting on a single qubit state,

$$a|0\rangle = 0, \quad a|1\rangle = |0\rangle$$
$$a\dagger|0\rangle = |1\rangle, \quad a\dagger|1\rangle = 0$$  \hspace{1cm} (1)

such that,

$$a_i \rightarrow I \otimes I \otimes \ldots \otimes a \otimes \ldots \otimes I$$

$$a_i\dagger \rightarrow I \otimes \ldots \otimes a\dagger \otimes \ldots \otimes I$$  \hspace{1cm} (2)
Here $a_i$ ($a_i^\dagger$) is the annihilation (creation) operator acting on Fock space $F_{2L}$, annihilating (creating) a fermion in $i$th mode. $I$ is the identity on single qubit space. The tensor product satisfying the correspondence in Eq. (?) must be consistent with the anti-commutation property of the Fock space creation and annihilation operators,

$$\{a_i, a_j^\dagger\} = \delta_{ij} \quad \{a_i, a_j\} = 0 = \{a_i^\dagger, a_j^\dagger\}$$
This requirement leads to the following action of the tensor product operators on the $2L$ qubit states

\[
(I \otimes I \otimes \cdots \otimes a(a^\dagger) \otimes \cdots \otimes I)(|n_1\rangle \otimes \cdots \otimes |n_i\rangle \otimes \cdots \otimes |n_{2L}\rangle) = (-1)^{\sum_{j=i+1}^{2L} n_j} (|n_1\rangle \otimes \cdots \otimes a(a^\dagger)|n_i\rangle \otimes \cdots \otimes |n_{2L}\rangle)
\]

Here $n_i \in \{0, 1\}$; $i \in \{1, 2, \ldots, 2L\}$ and $\sum_{j=i+1}^{2L} n_j$ is evaluated mod 2. Using the above Eq., it is straightforward to see that

\[
\{I \otimes I \otimes \cdots \otimes a(a^\dagger) \otimes \cdots \otimes I, I \otimes I \otimes \cdots \otimes a(a^\dagger) \otimes \cdots \otimes I\}(|n_1\rangle \otimes \cdots \otimes |n_i\rangle \otimes \cdots \otimes |n_{2L}\rangle) = 0
\]
and

$$\{ l \otimes l \otimes \cdots \otimes a \otimes \cdots \otimes l, \ l \otimes l \otimes \cdots \otimes a^\dagger \otimes \cdots \otimes l \}$$

\( \text{ith place} \)

\( \text{jth place} \)

\begin{equation}
\left( |n_1\rangle \otimes \cdots \otimes |n_i\rangle \otimes \cdots \otimes |n_j\rangle \otimes \cdots \otimes |n_{2L}\rangle \right) = (l \otimes \cdots \otimes l) \delta_{ij} \tag{5} \end{equation}

\( 2L \text{ factors} \)
fermions $\leftrightarrow$ spin $\frac{1}{2}$ fermions.

mode $\leftrightarrow$ single particle state.

$N$ fermions on $L$ sites $\leftrightarrow$ $2L$ mode system.

Two fermions on two sites $A, B$ constitute a four mode system with states $|A \uparrow\rangle, |A \downarrow\rangle, |B \uparrow\rangle, |B \downarrow\rangle$. 
We deal with entanglement between subsets forming a partition of a $2L$-mode fermionic system. We define entanglement measure for any such partition: no restriction on the no. and size of the partition. Local and non-local operations.
We assume that a partition equally divides $2L$ modes into $m = 2L/n$ subsets each containing equal no. of modes say $n$. $H_{2L}$ is divided into subspaces of dimension $d = 2^n$. The system then consists of $m$ qudits with $d = 2^n$.

We use the Bloch representation of $\rho = |\psi\rangle\langle\psi|$ namely,

$$\rho = \frac{1}{d^N} \{ I_d^\otimes m \} + \sum_{k \in \mathcal{N}} \sum s_{\alpha_k} \lambda^{(k)}_{\alpha_k} + \sum \sum t_{\alpha_k \alpha_{k_1}} \lambda^{(k_1)}_{\alpha_k} \lambda^{(k_2)}_{\alpha_{k_1}} + \cdots + \sum \sum \sum t_{\alpha_k \alpha_{k_1} \alpha_{k_2} \cdots} \lambda^{(k)}_{\alpha_k} \lambda^{(k_1)}_{\alpha_{k_1}} \lambda^{(k_2)}_{\alpha_{k_2}} \cdots + \cdots + \sum t_{\alpha_1 \alpha_2 \cdots} \lambda^{(1)}_{\alpha_1} \lambda^{(2)}_{\alpha_2} \cdots \lambda^{(m)}_{\alpha_N} \}$$
Definition of entanglement.

Let a $2L$ mode $N$ fermion system be partitioned by $m = 2L/n$ subsets, each containing $n$ modes. Then for this partition, we define the entanglement measure for a state $|\psi\rangle \in H_{2L}(N)$ by \[ \begin{align*} E &= ||\tau|| - ||\tau||_{\text{sep}} \end{align*} \]

where \[ \begin{align*} ||\tau|| &= \sqrt{\sum_{\alpha_1 \cdots \alpha_m = 1}^{d^2-1} t_{\alpha_1 \cdots \alpha_m}^2} \end{align*} \]

and $||\tau||_{\text{sep}}$ is $||\tau||$ for separable (product) $m$ qudit state \[ \begin{align*} ||\tau||_{\text{sep}} &= \left( \frac{d(d - 1)}{2} \right)^{m/2} \]
Consider a four mode system and the normalized state $|\psi\rangle \in H_4(2)$ defined as

$$|\psi\rangle = \frac{1}{\sqrt{6}} \{ i\alpha |1100\rangle + |1001\rangle + |0110\rangle + |0011\rangle + \beta |0101\rangle + |1010\rangle \}$$

where $\alpha, \beta$ are real. Note that $|\psi\rangle$ can be treated as a member of the Fock space $F_4(2)$ with the kets appearing in it being its basis states.
Consider the evolution of the system in state $|\psi\rangle \in F_4(2)$ via the Hamiltonian

$$H = f(a_1^{\dagger}a_4 + a_4^{\dagger}a_1) + q\hat{n}_1\hat{n}_2 + \Gamma\hat{n}_1 + \gamma\hat{n}_3 + \eta(a_1^{\dagger}a_2 + a_2^{\dagger}a_1)$$

acting on $F_4$. Here $f$ term is the interaction between two modes on different sites (inter-site interaction), $\eta$ term is the interaction between two modes on the same site (intra-site interaction). $\Gamma$ and $\gamma$ correspond to single mode on site $A$ and $B$ respectively. $q$ term involves number operators $\hat{n}_i = a_i^{\dagger}a_i$; $i = 1, 2$ for first two modes, on $A$ site. We have included all the different kinds of typical interactions encountered in condensed matter systems, respecting number super-selection rule.
After an infinitesimal unitary evolution via this Hamiltonian, the state $|\psi\rangle$ evolves to

$$|\psi'\rangle = |\psi\rangle - i\epsilon H|\psi\rangle$$  \hspace{1cm} (10)

By employing the mapping of annihilation and creation operators in Eq.(??) and Eq.(??) and that of Fock space basis states in Eq.(??), we get, for $|\psi'\rangle$
$|\psi'\rangle = \frac{1}{\sqrt{6}} \{(i\alpha + i\epsilon f + \alpha q\epsilon)|1100\rangle +$ 
$(1 - i\Gamma\epsilon - i\epsilon\eta\beta)|1001\rangle + (1 - i\gamma\epsilon - i\epsilon\eta)|0110\rangle +$ 
$(1 - i\epsilon f - i\epsilon\gamma)|0011\rangle + (\beta - \epsilon f \beta - i\epsilon\eta)|0101\rangle +$ 
$(1 + i\epsilon f - i\epsilon\Gamma - i\epsilon\gamma - i\epsilon\eta)|1010\rangle$
Now we find the entanglement for different partitions of this four mode system, using the geometric entanglement measure. We first partition four modes into four subsets, each containing one mode. This case gives genuine entanglement between four modes, which is more general than only the bipartite entanglement considered in the literature. For this case $d = 2$, so that $||\tau||_{sep} = 1$ and we get, for the genuine four mode entanglement,

$$E = ||\tau|| - 1 \quad (11)$$

where

$$||\tau|| = \sqrt{\sum_{i,j,k,l=1}^{3} t_{ijkl}^2} \quad (12)$$

with

$$t_{ijkl} = Tr[\rho \sigma_i \otimes \sigma_j \otimes \sigma_k \otimes \sigma_l] = \langle \psi |\sigma_i \otimes \sigma_j \otimes \sigma_k \otimes \sigma_l |\psi \rangle. \quad (13)$$

where $\{\sigma_i\} i = 0, 1, 2, 3$ are the generators of the $SU(2)$ group (Pauli operators).
The resulting entanglement in $|\psi'\rangle$ is

$$E_g(|\psi'\rangle) = \frac{1}{6} \left( -6 + \sqrt{88 + 64\alpha^2 + 32\beta + 64\beta^2 + 10\alpha^2\beta^2 + \beta^4} \right) - \frac{4 \left( 4f\alpha - 2q\alpha(1 + \beta) + f\alpha\beta(\alpha^2 - \beta^2) + 4\alpha\eta(1 + \beta) \right) \epsilon}{\left( -6 + \sqrt{88 + 64\alpha^2 + 32\beta + 64\beta^2 + 10\alpha^2\beta^2 + \beta^4} \right)} + O[\epsilon^2]$$

(14)

where the first term gives the entanglement $E(|\psi\rangle)$ for the state $\psi$ as defined in Eq. (??). For this partition, the operations on a single mode are the only local operations, while all others are non-local. Therefore, the terms $\Gamma\hat{n}_1$ and $\gamma\hat{n}_3$ are the only local interactions. Therefore, we expect that the four mode genuine entanglement should not depend on $\Gamma$ or $\gamma$ to the first order in $\epsilon$, which is the case, as seen from Eq.
Next, we consider the partition consisting of two subsets, each containing two modes on each site, \( \{ A \uparrow, A \downarrow \} \) and \( \{ B \uparrow, B \downarrow \} \) (site partition). Thus we have two subsystems with \( d = 4 \) corresponding to a \( SU(4) \otimes SU(4) \) qudit system. Further, \( n = 2 \) giving \( m = (2L/n) = 2 \) so that the geometric entanglement is

\[
E_s(|\psi\rangle) = ||\tau|| - 6
\]

(15)

where

\[
||\tau|| = 4 \sqrt{\sum_{j,k=1}^{15} K_{jk}^2}
\]

with

\[
K_{jk} = \langle \psi | \hat{\lambda}_j \otimes \hat{\lambda}_k | \psi \rangle
\]

where \( \hat{\lambda}_j \); \( j = 1, \ldots, 15 \) are the generators of \( SU(4) \).
The entanglement of $|\psi'\rangle$ in Eq.(??) is then given by

$$E_s(|\psi'\rangle) = \frac{1}{3} \left(-18 + \sqrt{208 + 136\alpha^2 + 9\alpha^4 - 32\beta + 104\beta^2 + 34\alpha^2\beta^2 + 9\beta^4}\right) - \frac{16(-f\alpha + f\alpha\beta(\alpha^2 - \beta^2 - 2))}{3(\sqrt{208 + 136\alpha^2 + 9\alpha^4 - 32\beta + 104\beta^2 + 34\alpha^2\beta^2 + 9\beta^4})} \epsilon + O[\epsilon^2]$$

According to the ‘site partition’, in addition to the operations on single modes, the operations on the pair of modes having the same site label are also local. Therefore, the resulting entanglement cannot change under the intra-site operations in the Hamiltonian, namely the $q$ term, the $\eta$ term and as before, $\Gamma$ and $\gamma$ terms. Thus, to the first order in $\epsilon$, the entanglement is expected to depend only on the non-local part of the Hamiltonian, that is, on the $f$ parameter. From Eq.(??) we see that this is the case.
We now consider some correlated fermionic lattice models and discuss multi-mode entanglement in these models using the geometric measure. The Hubbard dimer model is a simple model for a number of physical systems, including the electrons in a $H_2$ molecule, double quantum dots, etc [??]. The Hamiltonian can be written as

\[ H = -t \sum_{\sigma=\uparrow,\downarrow} \left( c_{A\sigma}^{\dagger} c_{B\sigma} + c_{B\sigma}^{\dagger} c_{A\sigma} \right) + U \sum_{j=A,B} \hat{n}_j^{\uparrow} \hat{n}_j^{\downarrow} \]  

(16)

where $A, B$ are the site labels and $\uparrow$ and $\downarrow$ are spin labels. $t$ is the hopping coefficient measuring hopping between two sites while conserving spin and $U$ quantifies Coulomb interaction between fermions on the same site. By varying $\left( \frac{U}{4t} \right)$ we can vary the relative contributions of hopping and Coulomb mechanisms.
The ground state of the system at zero temperature can be easily obtained as

$$|\psi_0\rangle = N \hat{G}_0 |\text{vac}\rangle$$

(17)

where $N = \langle \psi_0 | \psi_0 \rangle^{-1/2}$ is the normalization factor and

$$\hat{G}_0 = c_{A\uparrow}^\dagger c_{A\downarrow}^\dagger + c_{B\uparrow}^\dagger c_{B\downarrow}^\dagger + \alpha \left( \frac{U}{4t} \right) \left( c_{A\uparrow}^\dagger c_{B\downarrow}^\dagger - c_{A\downarrow}^\dagger c_{B\uparrow}^\dagger \right)$$

(18)

with $\alpha(x) = x + \sqrt{1 + x^2}$. By mapping to $H_{2L}$ via Eq.(??) we get,

$$|\text{vac}\rangle \rightarrow |0\rangle \otimes |0\rangle \otimes |0\rangle \otimes |0\rangle = |0000\rangle$$

(19)

while mapping between the operators, (Eq.(??) and Eq.(??)) gives

$$c_{A\uparrow}^\dagger \rightarrow a^\dagger \otimes l_2 \otimes l_2 \otimes l_2 \quad c_{A\downarrow}^\dagger \rightarrow l_2 \otimes a^\dagger \otimes l_2 \otimes l_2$$

$$c_{B\uparrow}^\dagger \rightarrow l_2 \otimes l_2 \otimes a^\dagger \otimes l_2 \quad c_{B\downarrow}^\dagger \rightarrow l_2 \otimes l_2 \otimes l_2 \otimes a^\dagger$$

(20)

The normalized ground state can be expressed in the qubit space as

$$|\psi_0\rangle = \frac{-1}{\sqrt{2(1 + \alpha^2)}} \left\{ |1100\rangle + |0011\rangle + \alpha |1001\rangle - \alpha |0110\rangle \right\}$$

(21)
The four-partite entanglement in any state $|\psi\rangle$ can be calculated by using Eqs.(??),(??),(??)) as,

$$E_g = ||\tau|| - 1 \quad (22)$$

where

$$||\tau|| = \sqrt{\sum_{i,j,k,l=1}^{3} t_{ijkl}^2} \quad (23)$$

with

$$t_{ijkl} = \langle \psi | \sigma_i \otimes \sigma_j \otimes \sigma_k \otimes \sigma_l | \psi \rangle. \quad (24)$$

The ground state entanglement can be then calculated to be

$$E_g = \frac{3}{(1 + \alpha^2)} \sqrt{1 + \frac{2}{9} \alpha^2 + \alpha^4 - 1} \quad (25)$$
We plot the four-partite entanglement as a function of $U$ and $t$ (Fig. 1(a)) and as a function of $\alpha$ (Fig. 1(b)). The entanglement is seen to monotonically increase as a function of $\alpha$, saturating at large values of $\alpha$ to the maximum value 2. The saturation to the maximum value can be obtained either for very large values of $U$ or very small values of $t$. We can interpret this result in the following way: since the total particle number is fixed to be 2, the four mode entanglement essentially measures the correlations between the spins. The entanglement increases as a function of $\alpha$ because the spin correlations increase with $\alpha$. 

(...) continued
Fig. 1) Four-partite entanglement for the Hubbard dimer (at half filling) as a function of $U$ and $t$ (a) and as a function of $\alpha$ (b).
Fig. 1) Four-partite entanglement for the Hubbard dimer (at half filling) as a function of $U$ and $t$ (a) and as a function of $\alpha$ (b).
We can also calculate the bipartite entanglement between sites $A$ and $B$ using the geometric measure Eqs.(??,??,??) considering the partitions to be $\{\{A \uparrow A \downarrow\}; \{B \uparrow B \downarrow\}\}$

$$E_s = ||\tau|| - ||\tau||_{sep}$$

where

$$||\tau|| = \sqrt{\sum_{i,j=1}^{15} t_{ij}^2}; \quad t_{ij} = \left(\frac{d}{2}\right)^2 \langle \psi | \hat{\lambda}_i \otimes \hat{\lambda}_j | \psi \rangle$$

and $||\tau||_{sep} = \left(\frac{d(d-1)}{2}\right)^{m/2}$. Here $\hat{\lambda}$s are the generators of $SU(4)$, there are $m = 2$ partitions (same as the number of sites) and each partition has dimension $d = 4$. This leads to an inter-site entanglement of the form
\[ E_s = \frac{2}{(1 + \alpha^2)} \sqrt{13\alpha^4 + 34\alpha^2 + 13 - 6} \]  

(28)

The bi-partite entanglement between sites \( A \) and \( B \) was calculated earlier using the von-Nueumann entropy \[ ? \]

\[ E_{VN} = \frac{1}{(1 + \alpha^2)} \left\{ \log_2 [2(1 + \alpha^2)] - \alpha^2 \log_2 \left[ \frac{\alpha^2}{2(1 + \alpha^2)} \right] \right\} \]  

(29)
We plot the inter-site entanglement (the von-Neumann entropy is also plotted for comparison) as a function of $\alpha$ in Fig.2. It is seen that both measures show qualitatively similar behavior, i.e, a monotonically decreasing entanglement as a function of $\alpha$ saturating at very large values of $\alpha$. The entanglement between the sites $A$ and $B$ decreases as a function of $\alpha$ because with increasing on-site repulsion $U$, the four dimensional local state space at each site gets reduced to a two dimensional local state space due to a suppression of charge fluctuations or in other words, as $\alpha \to \infty$ the $SU(4) \otimes SU(4)$ partition goes over to a $SU(2) \otimes SU(2)$ partition. We have explicitly checked that the entanglement obtained in the $\alpha \to \infty$ limit can be compared with that obtained for the $SU(2) \otimes SU(2)$ partition.
Fig. 2a) The bi-partite entanglement between sites A and B calculated with the geometric measure as a function of $\alpha$ for the Hubbard dimer at half filling. The corresponding von-Neumann entropy as a function of $\alpha$. 
Fig. 2b) The bi-partite entanglement between sites A and B calculated with the geometric measure as a function of $\alpha$ for the Hubbard dimer at half filling. The corresponding von-Neumann entropy as a function of $\alpha$. 