Global entanglement and double occupancy in many-electron states

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The entanglement in many-electron states is investigated using a global entanglement measure, viz. average site mixedness. We have examined metallic states of noninteracting electrons, Nagaoka and Gutzwiller states of strongly-correlated electrons, and superconducting states. Un correlated metallic states at half filling seem to maximize entanglement, as these states optimize the number of holes, the number of doubly-occupied sites. Entanglement is calculated explicitly for Gutzwiller-projected many-electron states in one dimension, which have less entanglement as double occupancy is inhibited in these states. Entanglement in superconducting states, which tend to promote double occupancy, is calculated as a function of the energy gap, and found to be lower than the metallic state entanglement. There is a possibility of a regime with a nonzero single-site concurrence depending on the energy gap.

Quantum entanglement is perceived as a resource for quantum communication and information processing, and has emerged over the last few years as a major research area in various diverse fields such as physics, mathematics, chemistry, electrical engineering and computer science. There has been a wide-spread investigation of entanglement properties of the ground states and excited states of well-studied quantum spin models of the condensed matter physics like the Heisenberg-XY models, the transverse-field Ising model. Also, there has been an intense study of the dynamics of entanglement of these models, both from numerical and analytical approaches.

The spin-only states have several advantages; many entanglement measures have been successfully used to characterize and quantify the entanglement of many-spin states of lattices. Pair-wise entanglement or concurrence, which measures the entanglement of a given pair of spins in a many-spin state, has been widely studied both numerically and analytically. The global entanglement measure, which quantifies how entanglement is distributed and shared over various spatial parts of the lattice, has been studied. The reduced fidelity susceptibility measure has been studied to investigate the critical properties of spin systems. In contrast, the entanglement properties of general many-electron states, which combine both spin and orbital degrees of freedom, have not been studied extensively. In this article we will use a generalization of the global entanglement measure, viz. the average site mixedness, to quantify the entanglement between spatial parts of many-electron states on lattices.

Let us consider electrons either localized or hopping around on N lattice sites. The details of the interactions determine the exact many-electron ground state that we may like to study. Since the entanglement properties can be discussed entirely through the many-body state itself, we will refer to the interactions only through the structure of the state in this article. There are four states per site, implying a basis of $4^N$ states for the $N$–site lattice. A convenient basis states for any site is given by $|0\rangle$, $|1\rangle$, $|0\rangle$, $|1\rangle$; which correspond to no occupancy (or a hole), up-spin electron occupancy, down-spin electron occupancy, and double occupancy respectively. A general pure many-electron state for N sites can be written as,

$$|\psi\rangle = \sum_{\{a_1, a_2, \ldots, a_N\}} \phi_{a_1, a_2, \ldots, a_N} |a_1, a_2, \ldots, a_N\rangle,$$

where $a_i$ labels the basis states of site $i$ listed above. This state is characterized by $4^N$ complex-number amplitudes $\{\phi_{a_1, a_2, \ldots}\}$ for the basis states. The entanglement distribution in the state can be investigated using various reduced density matrices (RDM) constructed through partial traces over the density matrix of the system $\rho = |\psi\rangle\langle\psi|$. In general a RDM of a subsystem would correspond to a mixed state, implying an entropy for the subsystem, and a bipartite entanglement between the subsystem and the rest of the system, and also some amount of multi-party entanglement between the various sites of the subsystem. It is quite an uphill task to characterize and quantify the entanglement distribution in various partitions of the system.

In the context of many-electron states even two-site RMDs are difficult to work with and unravel the pair-wise entanglement, as the RDM is now 16-dimensional since no occupancy and double occupancy can occur. Here we will use the single-site RDMs, and use a generalization of the global entanglement measure, that has been used extensively in spin systems. The entanglement measure is given in terms of the single-site RDM $\rho_l$ as,

$$\varepsilon(\psi) = \frac{4}{3N} \sum_{l=1}^{N} (1 - Tr\rho_l^2).$$

In the above, the pre-factor is so chosen that if each site density matrix is maximally mixed (corresponding to all four eigenvalues being equal to 1/4), the entanglement measure equals unity. Since $1 - Tr\rho_l^2$ would be zero for a pure single-site RDM, the above measures average site mixedness or how entangled is a site with the rest of the system on an average. Though we are working with strictly local, single-site RDMs, the averaging process makes it a global measure. If a large number of sites
with nonzero measure are entangled with other sites, we get a nonzero entanglement.

Let us consider a quantum state with $N_e = nN$ number of electrons, where $n$ is the electron density. The state is further characterized by the densities of up and down spin electrons, with $N_\uparrow = n\uparrow N, N_\downarrow = n\downarrow N$ as the up and down spin electron numbers respectively. That is, we consider a quantum state with conserved densities of up and down spin electrons. Because of the conserved electron densities, the single-site RDM of site $i$ has a diagonal structure, using the site basis states as unoccupied, doubly-occupied, up-spin-only occupied, down-spin-only occupied states, it is given as

$$
\rho_i = \begin{pmatrix}
1 - n + d & 0 & 0 & 0 \\
0 & d & 0 & 0 \\
0 & 0 & n_\downarrow - d & 0 \\
0 & 0 & 0 & n_\uparrow - d
\end{pmatrix}.
$$

(3)

In the above $d$ is the probability of double occupancy, which related to the total number of doubly-occupied sites in the state as $Nd \equiv D = \sum n_\uparrow n_\downarrow$.

From the structure of the single-site RDM, we can infer a hierarchy of entanglement in many-electron states. The spin-only states $\{|\psi_1\rangle\}$, with every site being occupied by an electron with either up or down spin, correspond to the half-filled case of strongly-correlated electron states. Here, we have $d = 0, n = 1$, i.e. no double occupancy and no holes, effectively reducing the local Hilbert space to two, and the single-site RDM has only two eigenvalues. The maximum entanglement occurs when both these eigenvalues are same, i.e. $n_\uparrow = n_\downarrow = 1/2$. Thus we have from Eq.3,

$$
\varepsilon_{max}(\psi_1) = \frac{2}{3}.
$$

(4)

It should be pointed out that there will be many spin states with this entanglement $\varepsilon = 2/3$. In fact, all many-electron states with the total spin zero, no double occupancy, and no holes will satisfy this.

The second category comprises of states $\{|\psi_2\rangle\}$ with no doubly-occupied sites but a nonzero fraction of holes, $d = 0, n < 1$. Since the site Hilbert space now is three dimensional, we have three nonzero eigenvalues of the single-site RDM. These states correspond to low-lying states of a large-$U$ Hubbard model, or very strongly-correlated electron states with less than half filling electron density. Here, the maximum entanglement occurs for $1 - n = n_\uparrow = n_\downarrow = 1/3$, with the eigenvalues of RDM being equal to 1/3, we have

$$
\varepsilon_{max}(\psi_2) = \frac{8}{9}.
$$

(5)

Thus existence of holes increases the entanglement.

Finally, let us consider states with doubly-occupied sites as well. Maximum entanglement occurs if all the four eigenvalues of the RDM shown above are all equal, i.e. $d = 1/4, n_\uparrow = n_\downarrow = 1/2$. This corresponds to the half-filling case, except that doubly-occupied sites are allowed. Since the local Hilbert space dimension has been maximized to four, this gives the maximum entanglement, a global maximum,

$$
\varepsilon_{max}(\psi) = \varepsilon(d = 1/4, n_\uparrow = n_\downarrow = 1/2) = 1.
$$

(6)

In general there will be many such states with $\varepsilon = 1$, since the only criteria we used are the conserved electron densities and the spatial uniformity. However, it will be useful to analyze various physical states such as metallic states, strongly-correlated states, superconducting states etc. Below we will examined these qualitatively different states.

Let us consider the Nagaoka state$^{[13]}$, with $d = 0, N_e = N - 1$, which is the ground state of $U = \infty$ Hubbard model. This corresponds to a multiplet with the maximal total spin $S = S_{max} = N - 1/2$. However, all the states in the ground state multiplet need not have the same entanglement. Consider the ground state with $S^z = N - 1 - l$, i.e. $N_\uparrow = N - 1 - l, N_\downarrow = l$. The eigenvalues of the single-site RDM are $1/N, 0, 1 - (l + 1)/N, l/N$, giving an entanglement $\varepsilon(S^z = N - 1 - l) = \frac{8l}{3N}(1 - \frac{l}{N})$. It is easy to see that the maximum entanglement occurs for the state with $l = N - 1/2$, we have

$$
\varepsilon_{max}(\psi_{Nagaoka}) = \frac{2}{3}(1 + \frac{1}{N})^2.
$$

(7)

This illustrates that the presence of a hole increases the entanglement from 2/3, which is the maximum value for the case of half filling with infinite Hubbard interaction.

Let us now examine the behavior of the entanglement as a function of $d$, the average density of the doubly-occupied sites. A state with an optimal $d$ is the uncorrelated metallic state or Fermi ground state, which is constructed as a direct product of single-particle momentum states, $|F⟩ = \prod \epsilon_{k\uparrow} c_{k\uparrow}^\dagger |0⟩$. Each single-particle $k \leq k_F$ state is occupied by two electrons, and the electron density determines the Fermi wave vector $k_F$. In the site basis, the state does not have a direct product structure, thus exhibits entanglement. It is easy to see that in the Fermi ground state, the double occupancy is given by $d = n^2/4$, and $\varepsilon = 1$ for the case of half filling $n = 1$. A popular state that incorporates a double occupancy as the on-site correlation strength is varied is the Gutzwiller state$^{[14]}$, given as

$$
|g⟩ = \frac{1}{\sqrt{N}} \prod_{i=1}^{N} [1 - (1 - g)n_{i\uparrow} n_{i\downarrow}] |F⟩,
$$

(8)

where $N$ is a normalization factor, $g$ determines the amplitude for a state with double site occupancy. It is clear that $g = 1$ corresponds to the uncorrelated metallic state, where as the other extreme $g = 0$ corresponds to no double occupancy or strongest spin correlations, or to $U = \infty$ Hubbard model ground states. The double occupancy in the above state is related to the normalization factor,

$$
d(g) = \frac{1}{2N} \frac{\partial \log N}{\partial \log g}.
$$

(9)
which is not easy to calculate in general. In one dimension, it has been calculated by Metzner and Vollhardt,\[15\] which is not easy to calculate in general. In one dimension, it has been calculated by Metzner and Vollhardt,\[15\] we have

\[
d(g) = \frac{1}{2} \frac{g^2}{(1-g^2)^2} \bigl[-n(1-g^2) - \log(1-n(1-g^2))\bigr]. \tag{10}
\]

Using this, the entanglement is easily calculated, and is shown in Fig.1 as a function of the projection parameter $g$. It is seen that optimal entanglement occurs for the uncorrelated metallic state at $g = 1$ at half filling, and for small electron densities the entanglement at near $g \sim 0$ can be greater than the corresponding metallic case near $g \sim 1$, though, however, the actual amount is quite small compared to the global maximum at $n = 1, g = 1$. Thus, the tendency of inhibiting double occupancy, from the optimal metallic value of $d = n^2/4$, decreases in general the site mixedness or the global entanglement.

We now examine situations where it is energetically favorable to promote double occupancy, over and above the optimal metallic value. Superconducting states fit into this category, as the underlying attractive interaction mechanism tends to promote superconducting Cooper pairs of opposite spins and in a zero momentum state, which is equivalent to a promoting tendency for site double occupancy. Starting with the vacuum state $|0\rangle$, the superconducting state can be constructed as

\[
|s\rangle = \prod_k [u_k + v_k c_{k\uparrow} c_{-k\downarrow}] |0\rangle. \tag{11}
\]

Here, $c_{k\uparrow}$ creates an up-spin electron in a single-particle plane-wave state with energy $E_k = \hbar^2 k^2/2m$. $v_k$ is the amplitude for a Cooper pair to form, $u_k$ is fixed through the normalization $|u_k|^2 + |v_k|^2 = 1$ for every $k$. The Cooper pair probability is chosen as\[16\]

\[
|v_k|^2 = \frac{1}{2} \left( 1 - \frac{E_k - E_F}{\sqrt{(E_k - E_F)^2 + \Delta_k^2}} \right). \tag{12}
\]

An attractive interaction in a narrow energy range near the Fermi energy $E_F$, would imply that the gap is nonzero only in that energy range, $\Delta_k \approx \Delta_0, |E_k - E_F| \approx \hbar \omega_D$, where, $\omega_D$ is the Debye frequency or a suitable energy scale in general superconductors.

The single-site RDM is different from the displayed one in Eq.4, since the number of particles is not a conserved scale in general superconductors.

Start with the vacuum state $|0\rangle$, where, $\omega$ is the RDM or a suitable energy scale in general superconductors.

The signle-site RDM is different from the displayed one in Fig.4, since the number of particles is not a conserved variable under the pairing tendency as we argued earlier. Now, it is easy to calculate he global entanglement measure in the state, which is shown in Fig.2 as a function of the superconducting order parameter for a few values of $\hbar \omega_D/E_F$ and the electron density $n$. It can be seen from the plot, that for nonzero $\zeta$ (which means the double occupancy
is more than the optimal metallic value) the entanglement decreases, though only slightly for the half-filled case, about 15 per cent for smaller electron filling.

The promotion of double occupancy by explicit introduction of off-diagonal correlations can introduce an entanglement structure of different variety, viz. a single-site concurrence, similar to the two-site concurrence in spin-only states [10]. Two-site concurrence in spin systems is a measure of the entanglement between two sites in a many-spin state, viz. the bipartite entanglement between two spatial parts labeled by the two sites. Here, in the superconducting state, the one-site RDM can be viewed as a bipartite density matrix of two distinct spin parts. Let us rewrite the basis states of the RDM as

\[ | \uparrow \rangle = | \uparrow \rangle \otimes | \uparrow \rangle, \quad | \downarrow \rangle = | \downarrow \rangle \otimes | \downarrow \rangle. \]

Now the basis states have the bipartite direct-product structure of up-spin states and down-spin states. Naturally, one can ask how much entanglement is there between the up spin and the down spin (which are used to label the two distinct parts of the bipartite Hilbert space). Using the Wootters’ formula for the concurrence of the four-dimensional RDM, we have the single-site concurrence in the superconducting state as

\[ C_{\uparrow,\downarrow} = 2 \text{Max}(\zeta - | n/2 - d |, 0). \tag{15} \]

Thus, there is possibility of a nonzero on-site concurrence, depending on the pair order parameter, or the energy gap of the superconducting state. For example, we have \( C_{\uparrow,\downarrow} \neq 0 \), if \( \zeta(1+\xi) \geq \frac{1}{2}(1 - \frac{3}{2}) \). We have plotted the single-site concurrence calculated above in Fig.3 as a function of \( \Delta D/\hbar \), for a few representative values of the fermi energy and the electron filling.

In conclusion, we have examined the average impurity of the single-site reduced density matrix as a global entanglement measure in multi-electron systems. The maximum global entanglement occurs for the half filled uncorrelated metallic state, which optimizes densities of up and down electrons, the holes and the doubly-occupied sites, \( n_\uparrow = n_\downarrow = n_{\text{hole}} = d = 1/4 \). On-site density-density repulsive interactions, or strong spin correlations, tend to inhibit double occupancy, thus decrease the entanglement, as illustrated by Gutzwiller projection states. Superconductor states promote double occupancy, over and above the optimal value of the metallic states, but still the entanglement decreases. We have shown that there is possibility of a nonzero on-site concurrence in the superconducting states depending on the energy gap.

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