Entanglement of Fermi gases in a harmonic trap

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Abstract. For both cases with and without interactions, bipartite entanglement of two fermions from a Fermi gas in a trap is investigated. We show how the entanglement depends on the locations of the two fermions and the total particle number of the Fermi gas. Fermions at the edge of trap have longer entanglement distance (beyond it, the entanglement disappears) than those in the center. We derive a lower limitation to the average overlapping for two entangled fermions in the BCS ground state, it is shown to be $\sqrt{Q/2M}$, a function of Cooper pair number Q and the total number of occupied energy levels M.

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As one of the most characteristic features of quantum systems, quantum entanglement lies at the heart of the difference between the quantum and classical multiparticle world. It is the phenomenon that enables quantum information processing and quantum computing [1,2]. Quantum entanglement is usually considered as existing between different degrees of freedom of two or more particles with mutual interactions, it is only recently that researchers have started to investigate entanglement in systems containing a large number of particles, in particular in a noninteracting Fermi gas [3–6]. Entanglement seems to play a crucial role in condensed matter systems, and has shown of relevance to thermodynamical quantities [7] such as the degeneracy pressure [8] and the number density of the gas [5], multipartite entanglement is also promising to make a breakthrough in solving unsolved problems such as high- T_c superconductivity [9].

Entanglement for noninteracting Fermi gases in a free space has already been studied [3–5]. It was found that all entanglement vanishes if the relative distance |r - r'| between electrons is greater than the entanglement distance $1/k_F$, where k_F denotes the Fermi momentum. In this situation, quantum entanglement is purely due to Fermi statistics and not due to any physical interactions. A natural question then arises, is this a general property of noninteracting Fermi gases? or it is special for the Fermi gas in a free space, and how the inter-particle interactions influence the entanglement?

In this paper, we will try to answer this question by studying the entanglement in noninteracting Fermi

gases in a harmonic trap, and examining the effect of inter-fermion interactions on the entanglement. As will be shown, bipartite entanglement measured by Wootters concurrence depends not only on the relative distance between the two fermions but also on the total number of particles in the gas, the larger the particle number of the gas N, the shorter the entanglement distance. The entanglement distance is no longer a constant $1/k_F$ (depending on the particle density) as in free space, it is related to locations of the two fermions. Our numerical simulations show that the entanglement distance is longer at the edge more than that at the center of trap. Further, we show the effect of interactions on the bipartite entanglement for the Fermi gas. The model adopted is the reduced BCS Hamiltonian, it is shown that the bipartite entanglement of BCS ground state depends on the overlapping of the time-reversed states, the minimum average overlapping is $\sqrt{Q/2M}$ depending on the ratio of Cooper pair number Q to the total number of occupied energy levels M. These results clearly establish the fact that entanglement should be taken into account when studying macroscopic observable, even if the system is in its ground state and the constituents of the system are not coupled with each other.

Suppose we have a collection of noninteracting fermions in harmonic traps. The Fermi gas may be electrons in a metal or ultracold atoms. Unless stated otherwise, we treat the Fermi gas in this paper as ultracold atoms, but the representation is applicable for all Fermi gases. At zero temperature, the atom gas is in its lowest energy configuration. All energy states are occupied up to the level M = N/2, where N is the total number of atom and assumed to be even (the case with odd number

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of particles will be discussed at the end of this paper). For simplicity, we consider throughout this paper a onedimensional harmonic trap. This condition is met if the trapping frequencies in the other directions are considerably large. The ground state of this system is

$$|\Psi_0\rangle = \prod_{n=1}^M b_{n\uparrow}^{\dagger} b_{n\downarrow}^{\dagger} |Vac\rangle, \qquad (1)$$

where $|Vac\rangle$ denotes the vacuum, and $b_{n\sigma}^{\dagger}(\sigma = \uparrow, \downarrow)$ creates an atom in state $\phi_n(x)$ with spin σ . We are interested in entanglement between two atomic spins at different locations. To solve this problem, the density matrix describing the spin state of two atoms at locations x and x' is needed. It can be defined by [3]

$$\rho_{ss';tt'} = \langle \Psi_0 | \psi_{t'}^{\dagger}(x') \psi_t^{\dagger}(x) \psi_{s'}(x') \psi_s(x) | \Psi_0 \rangle, \qquad (2)$$

where $\psi_t^{\dagger}(x)$ creates an atom of spin t at location x. This definition is reasonable, because the normalized second order correlation function can be considered as quantum states from the viewpoint of quantum measurement [6]. This density matrix also may be calculated by

$$\rho_{ss';tt'} = \operatorname{Tr}(|\Psi_0\rangle\langle\Psi_0|\cdot|st(x)\rangle\langle s't'(x')|), \qquad (3)$$

with $|st(r)\rangle$ standing for the two-atom state with spins s and t at location r. Writing $\psi_s(t)$ in terms of the annihilation operator $b_{n\sigma}$ and eigenfunctions $\phi_n(x)$ of the harmonic oscillator, we obtain the density matrix in the following form,

$$\rho_{ss';tt'} = N(x)N(x')\delta_{ts}\delta_{t's'} - \delta_{ts'}\delta_{t's}F^2(x,x'), \qquad (4)$$

where $F(x, x') = \sum_{\alpha}^{M} \phi_{\alpha}^{*}(x')\phi_{\alpha}(x) = F$, $N(x) = \sum_{\alpha} |\phi_{\alpha}(x)|^{2} = N_{x}$. Term *F* represents a sum over overlapping of the two atoms at locations *x* and *x'*, respectively. N(x) is the number density of atom at location *x*. In basis $\{|\uparrow\uparrow\rangle, |\downarrow\downarrow\rangle, |\downarrow\downarrow\rangle\}$, the density matrix takes the form,

$$\begin{aligned}
\rho_{12}(x,x') &= \frac{1}{4N_x N_{x'} - 2F^2} \\
\times \begin{pmatrix} N_x N_{x'} - F^2 & 0 & 0 & 0 \\ 0 & N_x N_{x'} & -F^2 & 0 \\ 0 & -F^2 & N_x N_{x'} & 0 \\ 0 & 0 & 0 & N_x N_{x'} - F^2 \end{pmatrix}, \quad (5)
\end{aligned}$$

where the subscript 1, 2 denotes the index of the two atoms. The entanglement of formation [10] measured by Wootters concurrence can be given by

$$C_{12}(x,x') = \frac{2}{|4N_x N_{x'} - 2F^2|} \max\left\{2F^2 - N_x N_{x'}, 0\right\}.$$
(6)

Obviously, the Wootters concurrence C_{12} is maximal when x = x' and it equals to 1. The corresponding entanglement state is the spin singlet $1/\sqrt{2}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$. With the relative distance between the two atoms increasing, F^2 behaves as a damping function of |x - x'|. As a consequence, the entanglement decays with |x - x'| increasing,



Fig. 1. (Color online) Wootters concurrence of two atoms located at x and x', respectively. The figure was plotted for 20 trapped atoms. $\alpha = \sqrt{m\omega/\hbar}$, m is the mass of atom, and ω is the trapping frequency.

this was shown in Figure 1, where the bipartite entanglement in a system with 20 atoms was plotted as a function of locations x and x'. The entanglement arrives at the maximum 1 at points |x - x'| = 0 and decays as atom separation increases from the Pauli exclusion principle. This can be understood as a result of more and more triplet states mixed in with the singlet. In contrast with the entanglement between two fermions in a free space, the entanglement between the two in a harmonic trap appears to be location dependent. It is clear from Figure 1 that the entanglement distance is longer for atoms at the edge of the trap than that at the center [11]. The reason for this is the following. The bipartite entanglement roughly depends on how and how many triplet state are mixed in with the singlet. At points |x - x'| = 0, there are no triplet states involved in from the Pauli exclusion, so the bipartite entanglement is maximal at these points. With the atom separation increasing, more triplet states are involved in, the two atom state is then a weighted sum over the singlet and triplet states, the weights depend on the locations of atoms. Because the overlapping of the wavefunction for atoms in the center is on average larger than that at the edge, the weights at the edge benefit the entanglement. The bipartite entanglement also depends on the total number of atoms, as shown in Figure 2, where one atom was located at 0.5α , $\alpha = \sqrt{m\omega/\hbar}$, m is the mass of atom, and ω stands for the trapping frequency. Clearly, the larger the number of atoms, the faster the damping of the bipartite entanglement. This results can be understood by considering F(x, x'), which represents a sum over the overlapping of atom states at x and x'. F(x, x') is proportional to the probability transfer of an atom from location x to x' (vice versa), it decreases with the atom number growing, and finally tends to the δ -function in the thermodynamical limit [12]. We would like to notice that the dependence of the entanglement on local particle density is involved. At first sight the entanglement decreases with



Fig. 2. (Color online) The bipartite entanglement as a function of the second atom's location x. (a–e) are for different total number of atoms. The number corresponding to (a), ..., (e) is 2, 4, 10, 14, 18, respectively.

the local particle density growing, however, this is not the case because F(x, x') depends on the local particle density through $\phi_{\alpha}(x)$ and $\phi_{\alpha}(x')$, too.

Up to now, we have not considered any interaction between the atoms. In the following, we study how the interaction influences the entanglement of the two atoms. For repulsive interactions, perturbation theory tells us that weak interactions modify the eigenvalues and the corresponding eigenfunctions of the free Hamiltonian, this results in a level shift to every eigenstate of the free Hamiltonian, and consequently there are more eigenfunctions participating in the summation for F, N_x , and $N_{x'}$. So, the damping in the dependence of entanglement on the relative distance would be faster than that without interactions. For attractive interaction, we will investigate the entanglement in trapped atoms by using the reduced BCS model. The reduced BCS Hamiltonian has received much attention as a result of effort to understand pairing correlations in nanoscale metallic system [13, 14]. We assume the model Hamiltonian in our consideration is [15],

$$H_{BCS} = \sum_{j=1}^{M} \varepsilon_j n_j - d\lambda \sum_{j,k}^{M} b_{j+}^{\dagger} b_{j-}^{\dagger} b_{k+} b_{k-}, \qquad (7)$$

where j, k = 1, ..., M represent a set of doubly degenerate single particle energy levels with energies ε_j and corresponding wavefunctions $\phi_j(x)$, λ is the dimensionless coupling, and d is the mean level spacing. $b_{j\pm}(b_{j\pm}^{\dagger})$ represents the annihilation (creation) operator for atoms at level j with the labels \pm referring to a pair of time-reversed states, and n_j was defined as $n_j = b_{j+}^{\dagger}b_{j+} + b_{j-}^{\dagger}b_{j-}$, which is the atom number operator for level j. The ground state entanglement (called ALC — average local concurrence) shared among different energy levels in this model was investigated in [16], it shown a simple relation between the ALC and the key order parameters in this model. The conventional BCS theory employs a grand canonical ensemble, by the Bogoliubov transformation $\gamma_{j1} =$ $u_j b_{j+} - v_j b_{j-}^{\dagger}$, $\gamma_{j0} = u_j b_{j-} + v_j b_{j+}^{\dagger}$, with $u_j^2 + v_j^2 = 1$, $4u_j^2 v_j^2 = \Delta^2/(\varepsilon_j^2 + \Delta^2)$, and $\Delta = \lambda d \sum_{j=1}^M \langle b_{j-} b_{j+} \rangle$, it gives

$$H_{BCS} = \sum_{j} \left[\varepsilon_j \left(u_j^2 - v_j^2 \right) - 2\Delta u_j v_j \right] \left(\gamma_{j1}^{\dagger} \gamma_{j1} + \gamma_{j0}^{\dagger} \gamma_{j0} \right) + \text{constant.}$$
(8)

In this situation, the pair of time-reversed states would play the same role as the spin in the discussion for free atoms, we hence consider entanglement between two atoms in the two time-reversed states + and -. The density matrix representing this entangled state can be represented by

$$\rho_{ss';tt'}^{BCS} = \text{Tr}(|BCS\rangle\langle BCS||st(x)\rangle\langle s't'(x')|), \qquad (9)$$

where $|BCS\rangle$ is the well-known ground state in the BCS model, $|BCS\rangle = \prod_{j=1}^{M} (u_j + v_j b_{j+}^{\dagger} b_{j-}^{\dagger}) |0\rangle$, s, t, s', t' = +, -. By the standard procedure, equation (9) yields,

$$\rho_{ss';tt'}^{BCS} = \left(\sum_{j} |v_j|^2\right)^2 \delta_{ts} \delta_{t's'} - \delta_{ts'} \delta_{t's} \times \operatorname{Re}(f(x, x')v^2(x, x')), \quad (10)$$

where

$$f(x, x') = \sum_{j} \phi_{j}(x)\phi_{j}^{*}(x'),$$

$$v^{2}(x, x') = \sum_{j} v_{j}^{2}\phi_{j}^{*}(x)\phi_{j}(x').$$
 (11)

Here, Re(...) denotes the real part of (...). In basis $\{|++\rangle, |+-\rangle, |-+\rangle, |--\rangle\}$, the density matrix in equation (9) follows,

see equation (12) below.

Here $f \equiv f(x, x')$ and $v^2 \equiv v^2(x, x')$. As well-known, $\sum_j v_j^2$ equals the total number of Cooper pairs Q in state $|BCS\rangle$, while f characterizes the overlapping of the two

$$\rho_{12}^{BCS}(x,x') = \frac{1}{4[\sum_{j} v_{j}^{2}]^{2} - 2\operatorname{Re}(fv^{2})} \begin{pmatrix} \sum_{j} v_{j}^{2} - \operatorname{Re}(fv^{2}) & 0 & 0 \\ 0 & \sum_{j} v_{j}^{2} - \operatorname{Re}(fv^{2}) & 0 \\ 0 & -\operatorname{Re}(fv^{2}) & \sum_{j} v_{j}^{2} - \operatorname{Re}(fv^{2}) \\ 0 & 0 & 0 & \sum_{j} v_{j}^{2} - \operatorname{Re}(fv^{2}) \end{pmatrix}$$
(12)

particles' wavefunctions. The state (12) is entangled iff the Peres-Horodecki condition [17] is met, i.e., $2\text{Re}(fv^2)$ – $Q^2 > 0$. Assume $\phi_j^*(x)\phi_j(x') = y$ independent of x, x^\prime and j, the Peres-Horodecki condition leads to |y|> $\sqrt{Q/2M}$ ($\sqrt{Q/2M} \le 1/\sqrt{2}$). This is the restriction to the overage overlapping for bipartite entanglement. With the assumption $\phi_i^*(x)\phi_j(x') = y$, it is easy to write down the concurrence corresponding to state (12) as $C_{12}^{BCS}(x,x') = \max\{\frac{(2|y|^2 - Q/M)}{(2Q/M - |y|^2)}, 0\}.$ The maximal entanglement $C_{12}^{BCS}(x,x') = 1$ is obtained at $|y|^2 = Q/M.$ For conventional BCS states, $\phi_j(x)$ may have the form of $e^{ip_j x}$, choose x = x', $|y| = 1 > 1/\sqrt{2}$. So two electrons in the conventional BCS state are entangled as long as the separation L is less than the entanglement distance determined by $|\phi_j^*(x)\phi_j(x+L)| = |y| = \sqrt{Q/2M}$. For atoms in a harmonic trap, we may write the wavefunctions $\phi_j(x)$ (j = 1, ..., M) as eigenvectors of the harmonic oscillator Hamiltonian. In the case of Q = M, i.e., all atoms are paired, the maximal entanglement that we may obtain in this system is less than 1, because $|\phi_i^*(x)\phi_j(x')| < 1$ for any j, x and x'. This is the difference in entanglement between interacting atoms in free space and in traps.

We now consider the case when the total number of particles is odd. Intuitively, for a large number (say, 2N + 1) of atoms, the bipartite entanglement would behave like that with 2N particles. This is the case indeed as will be shown. Let us first analyze the case without inter-particle interactions. Assume the (2N + 1)th atom is of spin up, the state of these 2N + 1 atoms may be written as $b^{\dagger}_{M+1\uparrow}|\Psi_0\rangle$, where $|\Psi_0\rangle$ was defined by equation (1) for the 2N particles. Following the calculation performed for equation (5), we find that the density matrix $\rho_{12}(x, x')$ can be divided into two parts, the first represents contributions from the 2N atoms, which takes the same form as in equation (5), and the second is a correction due to the (2N + 1)th atom. The elements of the second state σ are,

$$\sigma_{22} = 2N_x |\phi_{M+1}(x')|^2 + 2N_{x'} |\phi_{M+1}(x)|^2,$$

$$\sigma_{23} = -4F(x, x') \phi_{M+1}^*(x) \phi_{M+1}(x'), \qquad (13)$$

 $\sigma_{11} = \sigma_{22} + \sigma_{23}, \ \sigma_{22} = \sigma_{33}, \ \sigma_{32} = \sigma_{23}^*, \ \text{and the others}$ are zero. For a large system $(N \gg 1), \ |\phi_{M+1}(x)|^2 \ll N_x,$ and $|\phi_{M+1}(x)\phi_{M+1}(x')| \ll |F(x,x')|$. Therefore, the correction σ to the density matrix $\rho_{12}(x, x')$ can be neglected. However, this is not the case if the system only consists of few atoms, the correction due to the (2N+1)th atom should be taken into account to compute the bipartite entanglement. Note that exchanges of spin up with spin down do not change $|\Psi_0\rangle$, but $b^{\dagger}_{M+1\uparrow}|\Psi_0\rangle$. So matrix σ is of relevance to the spin of the (2N+1)th atom. But this does not affect the bipartite entanglement under consideration, i.e., the bipartite entanglement is independent of the spin of the (2N + 1)th atom. In the case of attractive interaction, the situation is similar if the BCS ground state is simply $b_{M+1\uparrow}^{\dagger}|BCS\rangle$. The situation becomes complicated when $b^{\dagger}_{M+1\uparrow}|BCS\rangle$ is not the ground state of the system [18]. In order to calculate the entanglement in BCS ground state, we have to find the

ground state first. Here, we analyze the effect of the unpaired atom on entanglement by a generalized BCS-like variational ansatz [18]. It uses a variational wavefunction $|BCS\rangle' = b_{M+1\uparrow}^{\dagger} \prod_{j=1}^{M} (u'_j + v'_j b_{j+}^{\dagger} b_{j-}^{\dagger})|0\rangle$ to minimize the kinetic energy cost of having the additional atom in level (M + 1). The variational parameters u'_j and v'_j must be found independently by minimizing $\mathcal{E} = \langle BCS|H|BCS\rangle'$. The results [18] showed that the additional unpaired atom can destroy pairing, and hence it decreases Q in our formulation. By the same analysis as in the case without inter-atom interactions, this change has negligible effects when $Q \gg 1$, but it should be taken into account when the number Q of pairs is small.

Before concluding, it is worth mentioning that bipartite (multipartite) entanglement as a properties of quantum systems depends on the definition of the two degrees (many degrees) that share the entanglement. Some properties of entanglement in the BCS model were studied in references [16, 19, 20], where the entanglement was defined among particles in different energy levels [16]. The entanglement presented in this paper is for two-fermion spins at different locations x and x', it characterizes two-fermion's correlation at the two locations.

In conclusion, we have shown that the bipartite entanglement in noninteracting fermions trapped in harmonic traps depend on particle number, relative distance and the locations of the two fermions. The entanglement distance which characterize the maximum separation of two entangled particles is longer at the edge of the trap than that at the center; the larger the number of trapped particles, the shorter the entanglement distance. For interacting Fermi system, we have adopted the reduced BCS model to study the entanglement in the BCS ground state. Reduced density matrix and Wootters concurrence have been presented, the restriction on the average overlapping y has been derived to be $\sqrt{Q/2M} < |y| \le \sqrt{Q/M}$, the lower limitation $\sqrt{Q/2M}$ corresponds to concurrence zero, while the upper one $\sqrt{Q/M}$ corresponds to maximal entangled states.

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coordinates and not just on their difference, is an consequence of the lack of translational symmetry in the harmonic trap.

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