Entanglement and Concurrence in the BCS State

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The study of entanglement of quantum states is now a central issue in the modern theory of quantum information [1]. Entanglement is not seen just as a sort of peculiar or curious property of multipartite quantum states, but more importantly, it has become a resource to achieve novel tasks, such as teleportation, quantum cryptography and other quantum transmission protocols surpassing the capabilities exhibited by their classical counterparts. Moreover, entanglement is also something of direct experimental importance since it amounts to interaction among parties: just to mention a simple instance of this, the application of the CNOT gate to a factorizable state \(|\Psi^\text{in}\rangle := 2^{-1/2}|0\rangle - |1\rangle \rangle \) produces one of the Bell states, namely, \(U_{\text{CNOT}}|\Psi^\text{in}\rangle = 2^{-1/2}|01\rangle - |10\rangle \rangle = |\Psi^-\rangle \). In this process, the output state is more difficult (and expensive) to realize than the initial state \(|\Psi^\text{in}\rangle \) because of the CNOT gate that implements entanglement. Therefore, to know whether a given purported state is entangled or not, as well as how much entangled it is, is of great importance both theoretically and experimentally.

In condensed matter theory, we are used to deal with quantum many-body states (or multiqubit states) in which their strong quantum correlations are responsible for novel properties or states of matter, like quantum liquids, or quantum phase transitions [2,3]. Example of strongly correlated states abound in these areas, for example, valence bond states are nothing but Bell states, and properties like entanglement swapping correspond to resonating valence bond (RVB) state configurations.

In low dimensional systems, like quantum spin chains and ladders, it is known that the effect of quantum fluctuations is stronger than in higher dimensions: the factorizable Neel state is a good starting point to describe the ground state of the antiferromagnetic Heisenberg model in \(D = 2\) or more dimensions, but it is unsuitable for \(D = 1\) where the Bethe ansatz solution is a complicated superposition (entangled) of single particle states. Thus, it is natural to ask whether the new ideas about qualifying and quantifying entanglement that have emerged in the field of quantum information can be helpful to describe the complicated patterns of behaviour exhibited by strongly correlated systems in condensed matter.

Recently, the entanglement properties of the one dimensional XY model in a transverse magnetic field have been analyzed in the vicinity of a quantum phase transition by Osterloh et al. [4] and Osborne and Nielsen [5]. In this model, entanglement shows scaling behaviour near the transition point and remains short ranged [6]. The quantification of entanglement is made with the entanglement measure known as entanglement of formation \(E(\rho)\), introduced by Bennett et al. [7] to describe the resources needed to create a given entangled bipartite state, either pure \(|\Psi\rangle\) or mixed \(\rho\) [8].

Generally, it is difficult to find closed mathematical expressions of \(E(\rho)\) solely in terms of \(\rho\), but for the special case of mixed states of bipartite qubit systems Wooters [9] found one such a formula. This formula makes use of what Wooters calls [10] a spin flip transformation, defined as

\[
|\tilde{\psi}\rangle := \sigma_y |\psi\rangle^* \quad (1)
\]

where \(\sigma_y := \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}\) is the Pauli matrix in the computational basis \(|0\rangle := |\uparrow\rangle, |1\rangle := |\downarrow\rangle\}. For a general state \(\rho\) of two qubits, the spin-flipped state is \(\tilde{\rho} := (\sigma_y \otimes \sigma_y) \rho^* (\sigma_y \otimes \sigma_y)\). When the state is pure \(\rho = |\psi\rangle \langle \psi|\), the entanglement of formation can be written as \(E(\rho) = \mathcal{E}(C(\psi))\), where the concurrence \(C\) is defined as

\[
C(\psi) := |\langle \psi |\tilde{\psi}\rangle| \quad (2)
\]

and \(\mathcal{E}(C) := h(\frac{1}{2}[1 + \sqrt{1 - C^2}]), h(x) := -x \log_2 x - (1 - x) \log_2 (1 - x)\), is a monotonically increasing function of \(C\) that ranges from 0 to 1 as the concurrence goes from 0 to 1.

In fact, Wooters proposes to use concurrence [10] as an entanglement measure in its own right. Here, we shall adhere to this proposal by studying the concurrence of a physically realizable state such as the BCS state [10]. There are very few cases where we have a solution to a quantum many-body problem in the form of an explicit wave function. The BCS theory of standard superconductors provides us with one of these examples. Specifically, the general quantum state representing a super-
conductor carrying a supercurrent at T=0 temperature is

$$|\text{BCS}_\theta\rangle := \prod_k (u_k + e^{i\theta} v_k c_k \langle k + Q, \uparrow | c_{-k - Q, \downarrow}\rangle |0\rangle$$  \hspace{1cm} (3)$$

where $|0\rangle$ denotes the zero-particle Fock state. In this state the electrons are created in Cooper pairs for the occupied states with quantum numbers $(k + Q, \uparrow; -k - Q, \downarrow)$. All these pairs have the same momentum $2kQ$. This pair momentum represents the finite supercurrent and it is usually very small. We shall concentrate in the static condensate of Cooper pairs with zero supercurrent $Q = 0$.

The parameters $u_k$ and $v_k$ represent the probability amplitudes of creating quasi-holes and quasi-electrons, respectively. They satisfy the following properties:

$$u_k^2 + v_k^2 = 1, \hspace{1cm} u_k, v_k \in \mathbb{R}; \hspace{0.5cm} k := |\mathbf{k}|$$  \hspace{1cm} (4)$$

The first condition comes from the normalization of the state $|\text{BCS}_\theta\rangle$, and they only depend on the modulus of $\mathbf{k}$. The phase factor $e^{i\theta}$ is arbitrary, but is the same for all Cooper pairs. In the macrocanonical BCS state $|\mathcal{E}\rangle$, the number of Cooper pairs $N$ is not a well defined quantity. By series expansion, the state can be thought of as an average over an ensemble of states $|N, Q\rangle$ with a definite number $N$ and pair momentum $2kQ$: $|\text{BCS}_\theta\rangle := \sum_N e^{iN\theta} AN|N, Q\rangle$, $\sum_N A_N^2 = 1$.

The advantage of having the explicit form of the ground state wave function is that we can compute any quantity needed for an entanglement measure. In particular, it is possible to compute the reduced density matrix $\rho(k_i, k_j)$ by tracing out over all Cooper pairs with momenta $\mathbf{k} \neq k_i, k_j$. This is a bipartite density matrix for which explicit formulas for the entanglement of formation also exist in terms of the concurrence $\mathcal{F}$. However, we notice that in the case of the macrocanonical BCS state, the matrix $\rho(k_i, k_j)$ corresponds precisely to the state formed by the product of two Cooper pairs with momenta $(\mathbf{k}_i, \mathbf{k}_j)$, namely, $[u_{k_i} |0\rangle + v_{k_i} |1\rangle] \otimes [u_{k_j} |0\rangle + v_{k_j} |1\rangle]$, where here $|0\rangle, |1\rangle$ denote states with zero and one Cooper pair, respectively. Then, the reduced density matrix leads to the same original problem we are dealing with, but with only two pairs.

Despite of this difficulty, it is still possible to use the concurrence to devise an entanglement probe for the macrocanonical BCS state? In principle it looks difficult since the BCS state is a many-body (multiqubit) state and it is known that concurrence fails to capture entanglement properties of multiqubit states. For example, it is known that any qutrit state can be entangled in two different ways $|\psi\rangle$: either as a $|\text{GHZ}\rangle := 2^{-1/2}(|000\rangle + |111\rangle)$ state or as a Werner $|\text{W}\rangle := 3^{-1/2}(|001\rangle + |010\rangle + |100\rangle)$ state. Both of them yield zero concurrence since $|\text{GHZ}\rangle = i2^{-1/2}(|000\rangle - |111\rangle)$ and $|\text{W}\rangle = i3^{-1/2}(|110\rangle + |101\rangle + |011\rangle)$. Thus, concurrence does not detect the existence of entanglement for qudits.

However, here we show that relying on physical grounds and motivated by the physical meaning of the concurrence, it is possible to give an entanglement measure for the BCS state based on the notion of concurrence. We do this in two steps.

In what follows, we shall study a many-body state $|\Psi\rangle$ which is a BCS ground state with $\theta = 0$:

$$|\Psi\rangle := |\text{BCS}_0\rangle := \prod_k (u_k + v_k c_k \langle k + Q, \uparrow | c_{-k - Q, \downarrow}\rangle |0\rangle$$  \hspace{1cm} (5)$$

This BCS state is the solution of minimum energy to a reduced Hamiltonian called pairing Hamiltonian $\tilde{H}$:

$$H_{\text{red}} := \sum_k 2c_k b_k^\dagger b_k - \sum_{k \neq k'} V_{k, k'} b_k^\dagger b_{k'}$$  \hspace{1cm} (6)$$

where $b_k^\dagger := c_{k, \uparrow} c_{-k, \downarrow}^\dagger$ and $b_k := c_{-k, \downarrow} c_{k, \uparrow}^\dagger$ are operators creating and annihilating Cooper pairs, respectively. The solution to this variational problem yields the following expressions for the probability amplitudes

$$u_k^2 = \frac{1}{2}(1 + \frac{\epsilon_k}{E_k}), \hspace{1cm} \frac{1}{2}(1 - \frac{\epsilon_k}{E_k}), \hspace{1cm} E_k = \sqrt{\epsilon_k^2 + \Delta_k^2}$$  \hspace{1cm} (7)$$

where $E_k$ is the energy of the quasi-particles (excitations), and $\Delta_k$ is called the gap function, which is determined by the self-consistent solution of the gap equation $\Delta_k = -\sum_{k'} \frac{\Delta_{k'}}{2E_{k'}} V_{k, k'}$. This solution represents a BCS superconductor or SC state.

In the first step, we extend the notion of concurrence to many-body states based on the physical interpretation of concurrence introduced by Wooters. Namely, for a spin $\frac{1}{2}$ particle the spin-flip operation $|\psi\rangle \mapsto -|\psi\rangle$ is the time-reversal operation. For two-qubit states, we can argue that concurrence can serve as an entanglement measurement directly form this definition, without resorting to its connection to $\mathcal{F}(C)$. The rationale goes as follows: as $|\tilde{\psi}\rangle$ is obtained from $|\psi\rangle$ by time inversion, we intuitively expect that if $|\tilde{\psi}\rangle$ is very much entangled, then $|\tilde{\psi}\rangle$ will be very similar to $|\psi\rangle$ thereby $C(\tilde{\psi}) \sim 1$. On the contrary, if $|\tilde{\psi}\rangle$ is factorized into two states then $|\tilde{\psi}\rangle$ will be very different from $|\psi\rangle$ and then $C(\psi) \sim 0$. When the given state is very entangled, the time-reversed state is very close to the original state and their overlap is very large.

Thus, it is reasonable to extend the notion of spin-flip operation by the time-reversal operation. Let us define the concurrence $C(\text{BCS})$ of the BCS state $|\Psi\rangle$ by means of the overlapping with its time-reversed state, namely,

$$C(\text{BCS}) := |\langle \Psi |\Psi\rangle|$$  \hspace{1cm} (8)$$

with
\[ |\text{BCS}\rangle_0 := U_T |\text{BCS}\rangle \] (9)

The action of the time-reversal operator \( U_T \) on position, momentum and spin variables is
\[
\begin{align*}
U_T r_i U_T^\dagger &= r_i \\
U_T k_i U_T^\dagger &= -k_i \\
U_T s_i U_T^\dagger &= -s_i
\end{align*}
\] (10)

In the second step, we realize that in the absence of a precise connection between entanglement of formation and concurrence beyond two-qubit states as the one provided by Wooters, we must define an entanglement measure with respect to a reference state for which we know that it has zero entanglement. The natural candidate for this is the Fermi Sea state \( |\text{FS}\rangle \) defined as
\[
|\text{FS}\rangle := \prod_{k \leq k_F} c_k^\dagger c_{k,F}^\dagger |0\rangle
\] (11)

Using (10), this state has maximum concurrence \( C(\text{FS}) = 1 \) despite being unentangled. Thus, we choose as our definition of entanglement what we shall call MEP macrocanonical entanglement of pairing \( E(\text{BCS}) \) defined as
\[
E(\text{BCS}) := \langle \text{FS}|\tilde{\text{FS}}\rangle - \langle \text{BCS}|\tilde{\text{BCS}}\rangle
\] (12)

With this definition the Fermi Sea state has zero entanglement. Now, we compute the MEP to check that it agrees exactly in the continuum limit \( \sum_k \to (\frac{2\pi}{\hbar})^3 \int d^3k \) with the following result
\[
C(\text{BCS}) = \left[ 1 + \left( \frac{n_2}{n_1} \right)^2 \right] \frac{2\pi}{\hbar} e^{n_2 \arctan \frac{n_2}{\Delta}}
\]

where \( n_1 := N(\epsilon_F)\hbar\omega_D \) and \( n_2 := N(\epsilon_F)\Delta \).

In Fig. we plot \( C_k(\text{BCS}) \) as a function of the energy \( \epsilon_k \) for several values of an homogeneous gap function \( \Delta_k := \Delta \). It clearly shows that the partial concurrences are different from 1 in the vicinity of the Fermi surface, and this region extends within an interval of the order of \( 2\Delta \). This is precisely the region where Cooper pairs are being formed. Thus, deviations of \( C_k(\text{BCS}) \) from 1 allows us to detect the onset of correlations between pairs of particles. In fact, when the gap vanishes the solution to \( u_k, v_k \) in (9) yields \( C_k(\text{BCS}) = 1, \forall k \), which agrees with the fact that it represents a normal metal with an uncorrelated (factorizable) ground state (4).

We can proceed even further and compute the total concurrence of the BCS state. It can be computed exactly in the continuum limit \( \sum_k \to (\frac{2\pi}{\hbar})^3 \int d^3k \) with the following result
\[
C(\text{BCS}) = \left[ 1 + \left( \frac{n_2}{n_1} \right)^2 \right] \frac{2\pi}{\hbar} e^{n_2 \arctan \frac{n_2}{\Delta}}
\]

Therefore, we find that the BCS concurrence depends on two adimensional quantities with a physical origin that we call the cut-off number \( n_1 \) and the gap number \( n_2 \). From (10) we see that this concurrence is always \( \leq 1 \), and the maximum value is attained when \( n_2 = 0 \) corresponding to the absence of superconductivity (and thus, no correlated pairs). In Fig. we plot the macrocanonical entanglement of pairing MEP (10).
to show how it depends on the numbers \(n_1\) and \(n_2\). We see that for a fixed value of \(n_1\) (and thus of the cut-off \(\omega_D\) and \(N(\epsilon_F)\)), the entanglement increases with \(n_2\) and in turn with the superconducting gap \(\Delta\) at \(T = 0\).

\[ E(BCS) = \int_{0}^{\infty} d\omega \alpha^2(\omega) N_{ph}(\omega)/\omega \]

where \(N_{ph}(\omega)\) is the phonon density of states and \(\alpha^2(\omega)\) is the electron-phonon coupling strength. In the weak coupling limit \(\lambda \ll 1\), it reduces to the BCS coupling parameter \(\lambda \approx N(\epsilon_F)V_0\).

From this table a clear picture emerges: as \(\lambda\) gets bigger, there is a large increase in the value of MEP, specially for the case of Eliashberg superconductors which have values of MEP about 3 orders of magnitude higher than in more conventional superconductors. For the group of elements Ru, Mo and Os that have similar values of \(\lambda\), their corresponding MEP values are also very close. Thus, we conclude that strongly coupled BCS superconductors are characterized by large MEP values. We find this reasonable since the effect of phonons is to enhance the electronic correlations [15]. This enhancement is also responsible of the higher \(T_c\) values in Table.

It might be possible that MEP could also be computed for other more complicated superconducting compounds such as heavy fermion materials, high-\(T_c\) cuprates, MgB\(_2\), fullerenes etc., with the purpose of having an indicator to distinguish them in different categories. Specially interesting could be the dependence of MEP with \(T\) as we approach the transition temperature \(T_c\) from the SC phase.

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| Superconductive Elements | \(\log_{10}(E(BCS))\) | \(\lambda\) | \(T_c\) (K) |
|--------------------------|-------------------------|--------|------------|
| **Transition SC Metals**  |                         |        |            |
| Hf                       | 7.557                   | 0.14   | 0.13       |
| Ru                       | 6.813                   | 0.38   | 0.49       |
| Mo                       | 6.381                   | 0.41   | 0.92       |
| Os                       | 6.290                   | 0.44   | 0.66       |
| **Eliashberg SC**        |                         |        |            |
| Nb                       | 3.549                   | 0.82   | 9.25       |
| Pb                       | 3.295                   | 1.55   | 7.20       |

TABLE I: A list of superconductive elements with their values of macrocanonical entanglement of pairing \(E(BCS)\), electron-phonon coupling constant \(\lambda\) and critical temperature \(T_c\).

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In general, time-reversal transforms a BCS state with $\theta$ into another with $\pi - \theta$.

[14] In general, time-reversal transforms a BCS state with $\theta$ into another with $\pi - \theta$.

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