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# Fermionic entanglement in itinerant systems

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## Abstract

We study pairwise quantum entanglement in systems of fermions itinerant in a lattice from a second-quantized perspective. Entanglement in the grand-canonical ensemble is studied, both for energy eigenstates and for the thermal state. Relations between entanglement and superconducting correlations are discussed in a BCS-like model and for  $\eta$ -pair superconductivity.

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## 1. Introduction

The concept of quantum entanglement [1] is believed to play an essential role in quantum information processing (QIP) [2]. As a consequence much effort has been devoted to the characterization of entanglement [3]. The very definition of entanglement relies on the tensor product structure of the state-space of a composite quantum system. Unfortunately, due to quantum statistics, such a structure does not appear in an obvious fashion for systems of indistinguishable particles, i.e. bosons or fermions. Indeed for these systems, in view of the (anti)symmetrization postulate, one has to restrict to a subspace of the  $N$ -fold tensor product of the single particle spaces. Such a subspace, e.g., the totally anti-symmetric one, does not have a naturally selected tensor product structure. It turns out that the notion of entanglement is affected for systems of indistinguishable particles by some ambiguity.

Since it is of direct relevance to several implementation proposals for QIP, e.g., quantum-dots based, this issue has been very recently addressed in the literature [4–10]. A quantum computation model was proposed [11] by using  $L$  local fermionic modes (LFMs)—sites which can be either empty or occupied by a fermion. Moreover, the use of quantum statistics for some QIP protocols has been analysed [12].

Along the same line of realizing a bridge between quantum information science and conventional many-body theory, entanglement in magnetic systems has been discussed [13–17]. In particular, entanglement in both the ground state [13, 14] and thermal state [15–17] of a spin-1/2 Heisenberg spin chain has been analysed in the literature. In this

situation the system state is given by Gibb's density operator  $\rho_T = \exp(-H/kT)/Z$ , where  $Z = \text{tr}[\exp(-H/kT)]$  is the partition function,  $H$  the system Hamiltonian,  $k$  is Boltzmann's constant which we henceforth will take equal to 1 and  $T$  is the temperature. As  $\rho(T)$  represents a thermal state, the entanglement in the state is called *thermal entanglement* [15]. Finally, the intriguing issue of the relation between entanglement and quantum phase transition [18] has been addressed in a few quite recent papers [19, 20].

In this paper we will explore the relations between entanglement and (super)conducting correlations by following the spirit of [7]. It is important to stress that due to the lack of measure of genuine many-body entanglement, we restrict ourselves to pairwise entanglement in this paper. Note that in this approach *the subsystems are given by modes and not by particles*. This is therefore an essentially *second-quantized* approach [23].

In section 2 basic definitions are given and the mapping scheme between LFMs and qubits introduced in [7] is briefly recalled. In section 3 the entanglement in both eigenstates and thermal state is studied for free fermions hopping in a lattice. In section 4 the relations between pairwise entanglement and superconducting correlations are discussed for two types of superconductivity, BCS-like superconductivity [21] and the so-called  $\eta$ -pair superconductivity [22]. Section 5 contains the conclusions.

## 2. Lattice fermions

Let us start by recalling some basic facts about (spinless) fermions on a lattice. In the second-quantized picture the basic objects are the creation and annihilation operators  $c_l^\dagger$  and  $c_l$  of the  $l$ th LFM. They satisfy the canonical anti-commutation relations

$$[c_i, c_j]_+ = 0 \quad [c_i, c_j^\dagger]_+ = \delta_{ij}. \quad (1)$$

The Hilbert space naturally associated with the  $L$  LFMs, known as Fock space  $\mathcal{H}_F$ , is spanned by  $2^L$  basis vectors  $|n_1, \dots, n_L\rangle := \prod_{l=1}^L (c_l^\dagger)^{n_l} |0\rangle$  ( $n_l = 0, 1 \forall l$ ).

From the above occupation-number basis it should be evident that  $\mathcal{H}_F$  is isomorphic to the  $L$ -qubit space. This is easily seen by defining the mapping [7]

$$\Lambda := \prod_{l=1}^L (c_l^\dagger)^{n_l} |0\rangle \mapsto \bigotimes_{l=1}^L |n_l\rangle = \bigotimes_{l=1}^L (\sigma_l^+)^{n_l} |0\rangle \quad (2)$$

where  $\sigma_l^+$  is the raising operator of  $l$ th qubit. This is a Hilbert-space isomorphism between  $\mathcal{H}_F$  and  $\mathbb{C}^{\otimes L}$ . By means of this identification one can discuss entanglement of fermions by studying the entanglement of qubits. Clearly this entanglement is strongly related to the mapping (2) and is by no means unique. By defining new fermionic modes by automorphisms of the algebra defined by equation (1) one gives rise to different mappings between  $\mathcal{H}_F$  and  $\mathbb{C}^{\otimes L}$  with an associated different entanglement. This simple fact is one of the manifestations of the relativity of entanglement [24].

It is useful to see how the mapping (2) looks on the operator algebra level. From the relation  $c_l^\dagger |n_1, \dots, n_L\rangle = \delta_{n_l,0} (-1)^{\sum_{k=1}^{l-1} n_k} |n_1, \dots, n_{l-1}, 1, n_{l+1}, \dots, n_L\rangle$ , it follows that

$$c_l^\dagger \mapsto \sigma_l^+ \prod_{k=1}^{l-1} (-\sigma_k^z) \quad (3)$$

where  $\sigma_k^z$  is the  $z$  component of the usual Pauli matrices for the  $k$ th qubit. This algebra isomorphism is quite well known in the condensed matter literature and is referred to as the Jordan–Wigner transformation [25]. Note that the inverse of equation (3) is given by  $\sigma_l^+ \mapsto c_l^\dagger \prod_{k=1}^{l-1} \exp(i\pi c_k^\dagger c_k)$ . We see that due to the *non-local* character of the mapping

$\Lambda(\Lambda^{-1})$ , even simple fermionic (spin) models can be transformed into non-trivial spin (fermionic) models. On the other hand, the fermionic states such as  $\prod_k c_k^\dagger |0\rangle$  are clearly mapped by  $\Lambda$  onto product qubit states.

It is important to keep in mind that for charged and/or massive fermions, the Fock space is *not* the state-space of any physical system. Indeed, at variance with massless neutral particles, e.g., photons, only eigenstates of  $\hat{N} = \sum_{l=1}^L c_l^\dagger c_l$  are allowed *physical* vectors and, for the same reason, only operators commuting with  $\hat{N}$  could be physical observables. This of course is nothing but a *superselection rule*, i.e.  $\mathcal{H}_F = \bigoplus_{N=0}^L \mathcal{H}_F(N)$ , that does not allow for linear superposition of states corresponding to different charge/mass eigenvalues [26].

Despite the above considerations, we note that in some situations one is led to attribute to the whole Fock space some physical meaning. This happens for systems in a symmetry broken phase. For example, in superconductivity and superfluidity the order parameter corresponds to an expectation value of an operator connecting different  $N$ -sectors. It follows that the associated mean-field Hamiltonian does not commute with  $\hat{N}$ .

Of course one can argue that this kind of violation occurs on a level that does not have any deep physical significance, after all the mean-field approach is just a variational one aimed at producing a good approximation to physical expectation values. According to this view, therefore, the properties, e.g., entanglement, of the ansatz states should not to be taken too seriously. Nevertheless, we think that this issue has some interest and the relations between pairwise entanglement and superconductivity will be provided before the conclusions.

### 3. Itinerant systems

Let us now consider free spinless fermions in a lattice. The Hamiltonian is given by

$$H = -t \sum_{l=1}^L (c_l^\dagger c_{l+1} + c_{l+1}^\dagger c_l) - \mu \sum_{l=1}^L c_l^\dagger c_l \quad (4)$$

with the periodic boundary condition. Here  $t$  represents the hopping integral between sites and  $\mu$  is the chemical potential.

It is known that the eigenvalue problem of  $H$  can be solved by a discrete Fourier transformation (DFT)

$$c_l = \frac{1}{\sqrt{L}} \sum_{k=1}^L \omega^{lk} \tilde{c}_k \quad (5)$$

where  $\omega = \exp(i2\pi/L)$ . After the DFT, the Hamiltonian (4) becomes

$$H = -2t \sum_{k=1}^L \cos(2\pi k/L) \tilde{c}_k^\dagger \tilde{c}_k - \mu \hat{N} \quad (6)$$

where  $\hat{N} = \sum_{k=1}^L \tilde{c}_k^\dagger \tilde{c}_k = \sum_{l=1}^L c_l^\dagger c_l$  is the total fermion number operator. From equation (6), we immediately obtain the eigenvectors

$$|\mathbf{k}_N\rangle = \tilde{c}_{k_1}^\dagger \tilde{c}_{k_2}^\dagger \dots \tilde{c}_{k_N}^\dagger |0\rangle \quad \mathbf{k}_N = (k_1, k_2, \dots, k_N) \in \mathbf{Z}^N \quad (7)$$

and the corresponding eigenvalues

$$E_{\mathbf{k}_N} = \sum_{l=1}^N (\epsilon_{k_l} - \mu) \quad \epsilon_{k_l} = -2t \cos(2\pi k_l/L). \quad (8)$$

Associated with the new fermionic modes  $\tilde{c}_k$  there is a tensor product structure for the Fock space. The latter is defined by the mapping

$$\Lambda_{\text{DFT}} := \prod_{k=1}^L (\tilde{c}_k^\dagger)^{n_k} |0\rangle \mapsto \bigotimes_{k=1}^L |n_k\rangle. \quad (9)$$

Obviously since the eigenstates  $|\mathbf{k}_N\rangle$  are products with respect to the tensor product structure due to  $\Lambda_{\text{DFT}}$  the entanglement in the eigenstates (7) is always zero. However, entanglement associated with map  $\Lambda$  may exist in the eigenstates. For instance, the concurrence  $C = 2/L$  for any pair of fermions when  $N = 1$ . The corresponding eigenstates are called W states [16, 27, 28].

### 3.1. Entanglement in the eigenstates

In order to make an analysis of the entanglement of our spinless fermions we will use the notion of concurrence [29]. This is a simple measure for two qubits that allows us to quantify the entanglement between *any* pair of fermions by our mapping.

We define the reduced density matrix associated with the first and second LFMs as  $\rho^{(12)} \in \text{End}(\mathbb{C}^4)$ . Note that the Hamiltonian is translation invariant, therefore entanglements between nearest-neighbour fermions are identical. Due to the fact that  $[\hat{N}, H] = 0$ , the reduced density matrix has the following form:

$$\rho^{(12)} = \begin{pmatrix} u & & & & \\ & w_1 & z & & \\ & z^* & w_2 & & \\ & & & & v \end{pmatrix}. \quad (10)$$

The nonvanishing relevant matrix elements of  $\rho^{(12)}$  are given by ( $\langle \cdot \rangle$  denotes the expectation value over  $\rho$ ),

$$u = 1 - 2\langle \hat{N} \rangle / L + \langle \hat{n}_1 \hat{n}_2 \rangle \quad v = \langle \hat{n}_1 \hat{n}_2 \rangle \quad z = \langle c_1^\dagger c_2 \rangle. \quad (11)$$

The concurrence of  $\rho^{(2)}$  is then given by [13]

$$C = 2 \max\{0, |z| - \sqrt{uv}\}. \quad (12)$$

As the matrix elements  $w_1$  and  $w_2$  do not appear in the concurrence (12), their expressions are not given in this paper. From equations (11) and (12) it follows that, in order to obtain the concurrence, we need to compute the *correlation functions*  $\langle \hat{n}_1 \hat{n}_2 \rangle$  and  $\langle c_1^\dagger c_2 \rangle$  and the mean fermionic number  $\langle \hat{N} \rangle$ . For the eigenstate  $|\mathbf{k}_N\rangle$ , after direct calculations<sup>3</sup>, we obtain

$$u = (n - 1)^2 - |S_{\mathbf{k}_N}|^2 \quad v = n^2 - |S_{\mathbf{k}_N}|^2 \quad z = S_{\mathbf{k}_N} \quad (13)$$

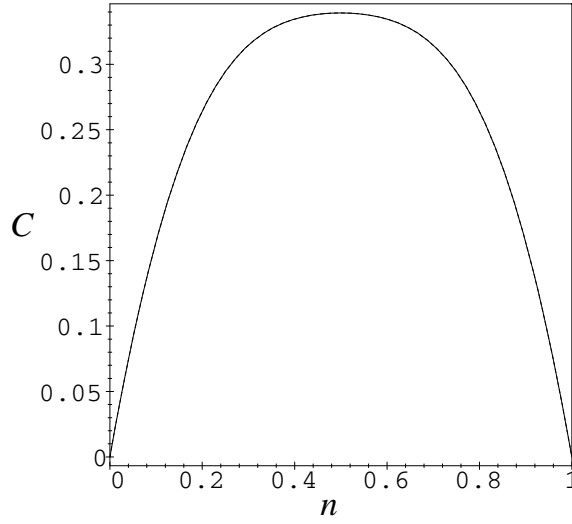
where  $n = N/L$  is the filling and

$$S_{\mathbf{k}_N} = L^{-1} \sum_{l=1}^N \omega^{k_l} = L^{-1} \sum_{l=1}^N e^{ik_l 2\pi/L}. \quad (14)$$

By combining equations (12) and (13) one gets the concurrence between two LFMs,

$$C = 2 \max \left\{ 0, |S_{\mathbf{k}_N}| - \left[ \left[ (n - 1)^2 - |S_{\mathbf{k}_N}|^2 \right] \left[ n^2 - |S_{\mathbf{k}_N}|^2 \right] \right]^{1/2} \right\} \quad (15)$$

<sup>3</sup> From equation (5) we can express the operators  $\hat{n}_1 \hat{n}_2$  and  $c_1^\dagger c_2$  in terms of Fourier fermionic creation and annihilation operators. Then the relation  $\langle c_{k_1}^\dagger c_{k_2} c_{k_3}^\dagger c_{k_4} \rangle = (\delta_{k_1, k_2} \delta_{k_3, k_4} - \delta_{k_1, k_4} \delta_{k_3, k_2}) n_1 n_2 + \delta_{k_3, k_2} \delta_{k_1, k_4} n_1$  is used where the averages are taken in the eigenstate  $|\mathbf{k}_N\rangle$ .



**Figure 1.** The concurrence as a function of the filling  $n$  in an infinite lattice.

which is determined only by the filling and the correlation function  $\langle c_1^\dagger c_2 \rangle = S_{\mathbf{k}_N}$ . This latter quantity is obviously related to the ‘itinerancy’ of the state, i.e. how fermions propagate. It follows that the concurrence (15) contains direct information about the conducting properties of the given quantum state.

From equation (15) one can directly see that there exists entanglement if the correlation function  $z$  and the filling factor  $n$  satisfy the equation  $|z|^4 - 2(n^2 - n + 1)|z|^2 + (n^2 - n)^2 < 0$ . Then we obtain that there exists pairwise entanglement between two LFM in the eigenstates if  $|z|^2$  is in the range  $n^2 - n + 1 - \sqrt{2n^2 - 2n + 1} < |z|^2 < n^2 - n + 1 + \sqrt{2n^2 - 2n + 1}$ . In the case of  $N = 1$ ,  $|S_{\mathbf{k}_N}| = n = 1/L$ , and therefore  $C = 2/L$  [16, 27, 28]. For  $L = 2$ , this state is maximally entangled. In the trivial case  $N = 0$ , there is no entanglement at all. Now we consider the case  $N = L$ , i.e. the lattice is fully filled. Now  $|S_{\mathbf{k}_N}| = 0$ , and hence  $C = 0$ . For the half filling ( $n = 1/2$ ),  $u = v$  and equation (15) reduces to  $C = 2 \max \{0, |S_{\mathbf{k}_N}| + |S_{\mathbf{k}_N}|^2 - 1/4\}$ . Then the entanglement exists if and only if  $(\sqrt{2} - 1)/2 < |S_{\mathbf{k}_N}| \leq 1/2$ .

Now we consider the ground state  $|G\rangle$  of the system. It is obtained by filling the lowest single particle energy levels. By taking, for simplicity,  $N$  odd one has  $|G\rangle = c_{k_0}^\dagger \prod_{n=1}^{N/2-1} c_{k_n}^\dagger c_{-k_n}^\dagger |0\rangle$  ( $k_n = 2\pi n/L$ ). From this definition it follows that  $S_G = L^{-1}(1 + 2\Re \sum_{n=1}^{N/2-1} \omega^n) = 2L^{-1}[\cos(\pi(N/2 - 1)/L) \sin((N/2 - 1)/L) / \sin(\pi/L) - 1]$ ; now taking the limit  $L \mapsto \infty$ ,  $N/L \mapsto n$ , the resulting expression is given by

$$S_G(n) = \frac{1}{\pi} \sin(\pi n) \quad (16)$$

where we have used  $\lim_{L \rightarrow \infty} L \sin(\pi/L) = \pi$ . Moreover, from the inequality  $S_G \geq n(1 - n)$  it follows that the second argument of the max function in equation (15) is always non-negative and we can get rid of the maximization. the concurrence then becomes

$$C = 2\{\sin(\pi n)/\pi - [(n - 1)^2 - \sin^2(\pi n)/\pi^2]^{1/2}[n^2 - \sin^2(\pi n)/\pi^2]^{1/2}\} \quad (17)$$

in the infinite lattice. Figure 1 shows the concurrence as a function of the filling  $n$  in the infinite lattice. We see that the entanglement becomes maximal at half filling for two neighbouring

fermions, and the entanglement is symmetric with respect to the point of half filling. At the point of half filling the concurrence simply becomes  $C = 2/\pi + 2/\pi^2 - 1/2 \approx 0.339262$ . The property of symmetry can also be seen directly from equation (17) as the concurrence is invariant if we make the transformation  $n \mapsto 1 - n$ .

For zero chemical potential, i.e. half filling, there exists a direct relation between the concurrence and the ground state energy density  $\epsilon_0$ . Indeed, from translational symmetry of the Hamiltonian one has  $\langle c_1^\dagger c_2 \rangle = -1/2tL \langle H \rangle = -1/2t\epsilon_0(n)$ , where we have used even the reality of  $\langle c_1^\dagger c_2 \rangle$ . This relation, which can be extended to finite temperature as well, is in a sense remarkable in that it connects entanglement with a thermodynamical quantity that depends on just the partition function of the system. The latter is determined just by the Hamiltonian spectrum, whereas computing concurrence also requires, in general, knowledge of the eigenstate. This kind of connection between entanglement and thermodynamical quantities has been discussed even for spin chains, both zero [13] and finite temperature [30].

### 3.2. Thermal entanglement

In this section we extend our analysis to the entanglement at a finite temperature. The state of fermions at thermal equilibrium is described by the following Gibbs grand-canonical state:

$$\rho_T = \frac{1}{Z} \sum_{\mathbf{k}_N} \exp(-\beta E_{\mathbf{k}_N}) |\mathbf{k}_N\rangle \langle \mathbf{k}_N| \quad (18)$$

where  $\beta = 1/kT$ ,  $k$  is Boltzmann's constant, and the partition function  $Z$  is given by

$$Z = \sum_{\mathbf{k}_N} \exp(-\beta E_{\mathbf{k}_N}) = \prod_{k=1}^L [1 + e^{-\beta(\epsilon_k - \mu)}]. \quad (19)$$

The average occupation number  $\langle n_k \rangle$  is given by

$$\langle n_k \rangle_T = \frac{1}{e^{\beta(\epsilon_k - \mu)} + 1} \quad (20)$$

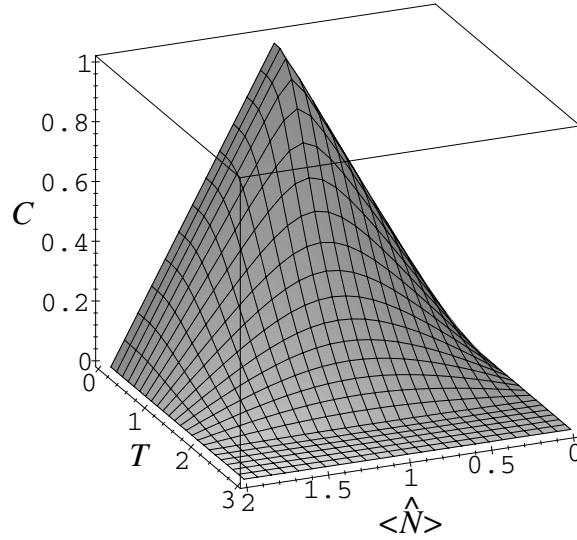
which is the Fermi–Dirac distribution. The expectation value  $\langle \hat{N} \rangle$  is then easily obtained as  $\langle \hat{N} \rangle = \sum_{k=1}^L \langle n_k \rangle$ .

The reduced density matrix  $\rho_T^{(12)}$  associated with  $\Lambda_{\text{DFT}}$  will be a  $4 \times 4$  diagonal matrix. Then from equation (12), the concurrence is zero for any pair of LFMs. So we will discuss the entanglement associated with the map  $\Lambda$ . The form of the reduced density matrix in the state  $\rho_T$  is then given by equation (10) and the concurrence is given by equation (12). Now we need to calculate the correlation functions in equation (11) for the state  $\rho_T$ . The result is readily obtained from equation (13) by replacing the eigenvalues of the  $n_k$  with the corresponding thermal averages:

$$\langle c_1^\dagger c_2 \rangle = L^{-1} \sum_{k=1}^L \omega^k \langle n_k \rangle \quad \langle n_1 n_2 \rangle = \langle \hat{N} \rangle^2 / L^2 - |\langle c_1^\dagger c_2 \rangle|^2. \quad (21)$$

Then the exact expression for the concurrence is given by the combination of equations (11), (12) and (21). Note that the concurrence is thus obtained in an analytical form for arbitrary  $N$ . To exemplify this result let us first consider the simple case of  $L = 2$ . For two sites, from equations (11), (12) and (21), the concurrence is given by

$$C = \frac{\max\{0, \sinh(2\beta|t|) - 1\}}{\cosh(\beta\mu) + \cosh(2\beta t)} \quad (22)$$



**Figure 2.** The concurrence as a function of the temperature and the mean fermion number for  $L = 2$  and  $t = 1$ .

**Table 1.** The concurrence for three special values of mean fermion number.

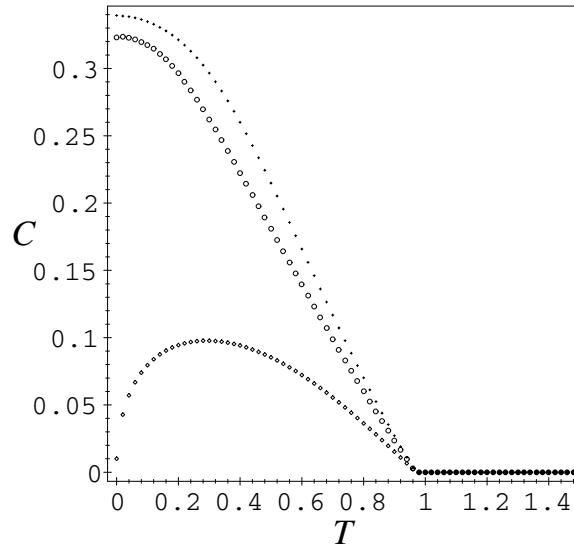
$\langle \hat{N} \rangle$	$\mu$	$C$
0	$-\infty$	0
1	0	$\max \left[ \frac{\sinh(2\beta t) - 1}{\cosh(2\beta t) + 1}, 0 \right]$
2	$\infty$	0

which is similar to the concurrence in a thermal state of the two-qubit  $XX$  model [16]. For three special values of  $\langle \hat{N} \rangle$ , we have table 1, from which we see that there is no entanglement when the chemical potential is  $\mp\infty$  (the corresponding mean fermion numbers are 0 and 2). The entanglement is maximal when  $\mu = 0$  and other parameters are fixed. The mean fermion number is simply given by

$$\langle \hat{N} \rangle = \frac{e^{\beta\mu} + \cosh(2\beta t)}{\cosh(\beta\mu) + \cosh(2\beta t)} \quad (23)$$

from which we obtain  $\mu = \beta^{-1} \ln\{(2 - \langle \hat{N} \rangle)^{-1} \{ \cosh(2\beta t)(\langle \hat{N} \rangle - 1) + [\cosh^2(2\beta t)(\langle \hat{N} \rangle - 1)^2 + 2\langle \hat{N} \rangle - \langle \hat{N} \rangle^2]^{1/2} \}$ . From this relation and equation (22) one can calculate the concurrence as a function of temperature and the mean fermion number  $\langle \hat{N} \rangle$ . This function is represented in figure 2. We observe that the entanglement becomes maximal when the mean fermion number is 1 for fixed temperature  $T$ . Let us first comment on the  $n \mapsto 1 - n$ , or in view of equation (22) equivalently  $\mu \mapsto -\mu$ , symmetry of the function  $C$ . This fact can be understood from equation (12). Clearly the only thing to check is that  $|z(t, \mu)| = |z(t, -\mu)|$ . This latter statement easily follows by the use of particle-hole transformation, i.e.  $c_j \leftrightarrow c_j^\dagger$  ( $j = 1, \dots, L$ ), realizing  $z(t, -\mu) \mapsto z(-t, -\mu)$  along with the unitary mapping  $c_j \mapsto (-1)^j c_j$  that, for bi-partite lattices, changes the sign of  $t$ . Another important feature is the existence of a threshold temperature, above which the entanglement disappears. Remarkably this threshold





**Figure 3.** The concurrence as a function of the temperature for different  $\mu$ :  $\mu = 0.1$  (crosses),  $\mu = 1.0$  (circles), and  $\mu = 2.0$  (diamonds). The parameter  $L = 100$ .

temperature is independent of the mean fermion number. This phenomenon is related to the independence of an external magnetic field displayed by the associated spin model [15, 16].

For large  $L$ , we plotted in figure 3 the concurrence as a function of temperature for different  $\mu$ . We observe that the threshold temperature is independent of  $\mu$ . Moreover, it is worth noting that for sufficiently high  $\mu$ , i.e. filling, one has a non-monotonic behaviour of the concurrence as a function of  $T$ . Indeed we see that the entanglement can initially *increase* as the temperature is raised. This phenomenon is due to the fact that the chemical potential in fermionic systems plays a role analogous to the external magnetic field  $B_z$  for spin systems [15]. When  $B_z$  is large enough the ground state is given by a product state (all the spins aligned), hence entanglement in the thermal state is due to the excited eigenstates. Of course for  $T$  large enough one always get  $C = 0$  in that the Gibbs state is approaching the maximally mixed state.

#### 4. Entanglement and superconductivity

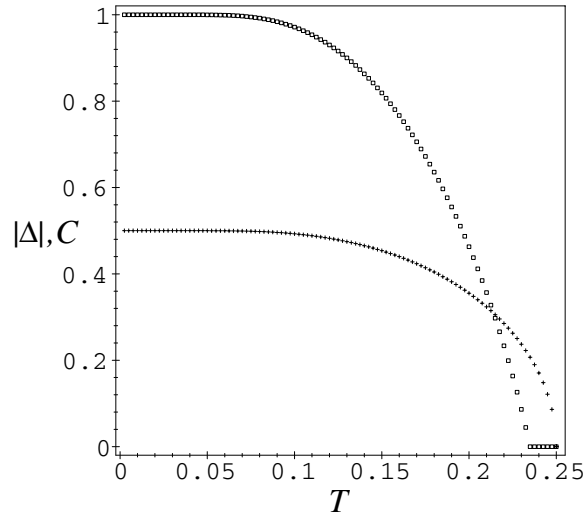
In this section we discuss fermionic entanglement in simple superconducting systems and explore the relations between entanglement and superconducting correlations. Let us first consider a BCS-like, i.e. mean-field model.

##### 4.1. BCS-like superconductivity

The following BCS-like Hamiltonian describes the pairing between fermions carrying momentum  $k$  and  $-k$ ,  $H = \sum_k H_k$ ,

$$H_k = \epsilon_k(n_k + n_{-k} - 1) + \Delta_k c_k^\dagger c_{-k}^\dagger + \bar{\Delta}_k c_k c_{-k}. \quad (24)$$

The quantities  $\Delta_k = |\Delta_k| e^{i\phi_k}$  are order parameters of conductor–superconductor phase transitions. They are determined by the self-consistent relations  $\Delta_k = \langle c_k c_{-k} \rangle$ , and



**Figure 4.** The order parameter (crosses) and the concurrence (boxes) as a function of the temperature. The parameter  $\epsilon_k = 0$ .

above a critical temperature they vanish, thus signalling the absence of superconducting correlation.

The structure of equation (24) clearly suggests that the relevant tensor-product structure of this problem is given by  $\mathcal{H}_F \cong \otimes_k (h_k \otimes h_{-k})$ , where  $h_k := \text{span}\{(c_k^\dagger)^\alpha |0\rangle / \alpha = 0, 1\}$ . Moreover, it is very simple to check that for any  $k$ , the operators  $J_k := n_k + n_{-k} - 1$ ,  $J_k^+ := c_k^\dagger c_{-k}^\dagger$ ,  $J_k^- := c_{-k} c_k$  span an  $su(2)$  Lie-algebra. The states  $|\alpha\alpha\rangle := |\alpha\rangle_k \otimes |\alpha\rangle_{-k}$  ( $\alpha = 0, 1$ ) realize a spin-1/2 representation of such an algebra. Therefore, the Hamiltonian (24), which it is equivalent to a spin-1/2 particle in an external magnetic field along the  $x$  direction, is readily diagonalized. For example, if we define  $\theta_k := \tan^{-1} |\Delta_k|/\epsilon_k$ , the ground state is given by  $\otimes_k |-\rangle_k$  where

$$|-\rangle_k := \cos(\theta_k/2) |00\rangle_k - e^{i\phi_k} \sin(\theta_k/2) |11\rangle_k. \quad (25)$$

It corresponds to the eigenvalue  $E_{k-} = -E_k$ . Here  $E_k = \sqrt{\epsilon_k^2 + |\Delta_k|^2}$ . The self-consistent equation for the  $\Delta_k$  reads

$$|\Delta_k| = \frac{\sinh(\beta E_k) \sin(\theta_k)}{2[\cosh(\beta E_k) + 1]}. \quad (26)$$

The concurrence associated with the thermal state  $\rho_k(\beta) := \exp(-\beta H_k)/Z$  is given by

$$C = \frac{\max\{0, \sinh(\beta E_k) \sin(\theta_k) - 1\}}{\cosh(\beta E_k) + 1}. \quad (27)$$

In the limit  $T \rightarrow 0$ , the concurrence becomes  $\sin(\theta_k)$  which is just the concurrence of the ground state  $|-\rangle_k$ . By solving these equations the numerical results are given in figure 4. One can see that the concurrence goes to zero at a temperature slightly *lower* than the superconductor critical one. Since in the temperature range  $[0, T_c]$  the function  $\Delta_k(T)$  is invertible one can express the concurrence as a function of the order parameter only. This is illustrated in figure 5 which shows that it is necessary to have a certain amount of superconducting correlation

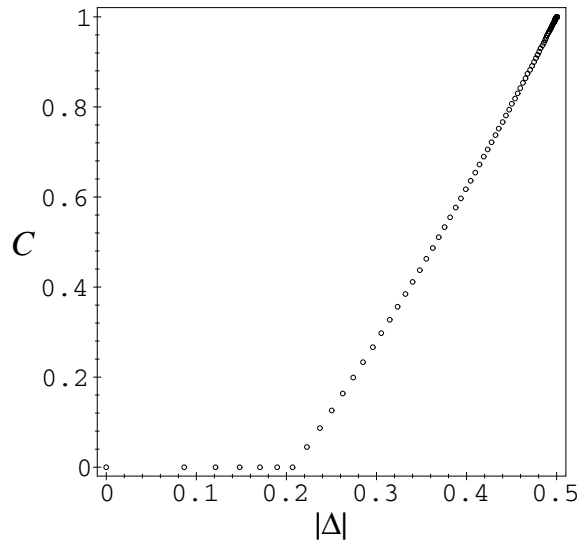


Figure 5. The concurrence against the order parameter. The parameter  $\epsilon_k = 0$ .

in order to have a pairwise entangled thermal state. Note that we set  $\epsilon_k = 0$ , which in a grand-canonical picture ( $\epsilon_k \mapsto \epsilon_k - \mu$ ) corresponds to half filling<sup>4</sup>.

We would like to observe now that a *non* mean-field Hamiltonian formally analogous to (24) plays an important role in the excitonic proposal for QIP by Biolatti *et al* [31]. In that case the fermionic bilinear terms  $c_k^\dagger c_{-k}^\dagger$  are replaced by  $X_i := c_l^\dagger d_m^\dagger$  ( $i := (l, m)$ ) where  $c_l^\dagger$  ( $d_m^\dagger$ ) creates an electron (hole) in the  $l$ th ( $m$ th) state of the conduction (valence) band of a semiconductor. The order parameter  $\Delta_k$  becomes a (independently controllable) coupling to an external laser field. The excitonic index  $l$  can be associated with  $L$  different, spatially separated, quantum dots; this implies that  $l \neq l' \Rightarrow [X_l, X_{l'}] = 0$ . Let  $|0\rangle$  denote the particle-hole vacuum (ground state of the semiconductor crystal). Since  $X_l^2 = 0$  one immediately sees that the ‘excitonic Fock space’  $\text{span}\{\prod_l X_l^{n_l} |0\rangle / n_l = 0, 1\}$  is isomorphic to a  $L$  qubit space [23]. This example shows that one can consider spaces allowing for a varying number of ‘particles’ that nevertheless are fully legitimate quantum state-spaces. No super-selection rule violation (possibly due to spontaneous symmetry-breaking) has to be invoked. Next we consider another kind of *non* mean-field superconductivity, i.e. the  $\eta$ -pair superconductivity.

#### 4.2. $\eta$ -pair superconductivity

Yang [22] discovered a class of eigenstates of the Hubbard model which have the property of off-diagonal long-range order (ODLRO) [32], which in turn implies the Meissner effect and flux quantization [33]. Let us begin by introducing the  $\eta$ -operators

$$\eta = \sum_{j=1}^L c_{j\uparrow} c_{j\downarrow} \quad \eta^+ = \sum_{j=1}^L c_{j\downarrow}^\dagger c_{j\uparrow}^\dagger \quad \eta^z = \frac{L}{2} - \sum_{j=1}^L n_j \quad (28)$$

which form the  $su(2)$  algebra and satisfies  $[\eta, \eta^\dagger] = 2\eta^z$ ,  $[\eta^\pm, \eta^z] = \pm\eta^\pm$ . Here the fermions have spins and the operator  $n_j = c_{j\downarrow}^\dagger c_{j\downarrow} + c_{j\uparrow}^\dagger c_{j\uparrow}$ . The operators  $\eta^\pm$  also satisfy the relations

<sup>4</sup> This is immediately seen from the equation  $\text{Tr}[\rho_k(n_k + n_{-k})] = 1 - 2 \cot \theta_k |\Delta_k|$ .

$(\eta^\pm)^{L+1} = 0$ , which reflect the Pauli principle, i.e. the impossibility of occupying a given site by more than one pair  $c_{j\downarrow}^\dagger c_{j\uparrow}^\dagger$ .

In this context the relevant state-space is the one spanned by the  $2^L$  basis vectors

$$|n_1, \dots, n_L\rangle = \prod_{l=1}^L (c_{l\downarrow}^\dagger c_{l\uparrow}^\dagger)^{n_l} |\text{vac}\rangle \quad (n_l = 0, 1 \forall l). \quad (29)$$

From the above basis it is evident that the space  $\text{span}\{|n_1, \dots, n_L\rangle\}$  is isomorphic to the  $L$ -qubit space. This is easily seen by defining the mapping

$$\Lambda' := |n_1, \dots, n_L\rangle \mapsto \bigotimes_{l=1}^L |n_l\rangle = \bigotimes_{l=1}^L (\sigma_l^+)^{n_l} |0\rangle. \quad (30)$$

Then we can produce  $L$  ‘number’ states  $|N\rangle$  by applying successive powers of  $\eta^+$  on the vacuum state defined by  $\eta|0\rangle = 0$ . So

$$|N\rangle = \mathcal{N}^{-1/2} \eta^{+N} |0\rangle \quad N = 0, \dots, L \quad (31)$$

where  $\mathcal{N} = L!N!/(L-N)!$ . The span of the  $|N\rangle$  ( $N = 0, \dots, L$ ), known as  $\eta$ -paired states, forms an irreducible spin- $L/2$  representation space. As mentioned above, what makes the number states interesting is the fact that they have been shown to have ODLRO. Indeed, from equation (31) the following distance-independent correlation function is obtained

$$\mathcal{O}_{N,L} = \langle N | c_{j\downarrow}^\dagger c_{j\uparrow}^\dagger c_{l\uparrow} c_{l\downarrow} | N \rangle = \frac{N(L-N)}{L(L-1)}. \quad (32)$$

In the thermodynamical limit ( $N, L \rightarrow \infty$  with  $N/L = n$ )  $\mathcal{O}_{N,L}$  goes to  $n(1-n)$ , which is nonvanishing as  $|j-l| \rightarrow \infty$ . In other words, the number state exhibits ODLRO, and thus is superconducting.

The two-site reduced density matrix has the form (10) in which

$$u = \frac{(L-N)(L-N-1)}{L(L-1)} \quad z = \mathcal{O}_{N,L} \quad v = \frac{N(N-1)}{L(L-1)}. \quad (33)$$

From these relations and equation (12), one finds

$$C = 2 \left\{ \mathcal{O}_{N,L} - \left[ \mathcal{O}_{N,L} \frac{(N-1)(L-N-1)}{L(L-1)} \right]^{1/2} \right\}. \quad (34)$$

Note that the above formula could have been directly obtained from [17] where the entanglement between any pair of qubits in a Dicke state has been computed. Indeed by means of the mapping (30), one can identify the number state with the usual Dicke state.

In the thermodynamical limit one has  $u \mapsto (1-n)^2$ ,  $v \mapsto n^2$ ,  $z = \mathcal{O}_{N,L} \mapsto n(1-n)$ ; thus, from equation (12) the entanglement becomes zero. So we see that pairwise quantum entanglement does not exist although we have  $\eta$ -pairing superconductivity in the number state. We finally note that in the  $\eta$ -pair coherent states discussed in [34], there is ODLRO, but being a product there is obviously no entanglement.

## 5. Conclusions

The Fock space of many local fermionic modes can be mapped isomorphically onto a many-qubit space. Using such a mapping we studied entanglement between pairs of (spinless) fermionic modes. This has been done both for the eigenstates and for the thermal state for a model of free fermions hopping in a lattice (entanglement between local modes as a function of temperature and filling). In the free fermionic model we analysed entanglement between

local modes as a function of temperature and filling. In particular, we found that above a threshold temperature the thermal state becomes separable.

We studied the relations between pairwise entanglement and the superconducting correlation in both the BCS-like model and  $\eta$ -pair superconductivity. For the BCS-model, a finite value of the superconducting-order parameter is required to obtain entanglement in the thermal state. Note that this last statement establishes a direct connection between quantum entanglement and a real phase transition [35]. For  $\eta$ -pair superconductivity we found that pairwise entanglement is not a necessary condition for the superconductivity.

Despite their simplicity, our results seem to suggest that the quantum information-theoretic relevant notion of quantum entanglement can provide useful physical insights into the physics of many-body systems of indistinguishable particles.

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