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Quantum entanglement in second-quantized condensed matter systems

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Abstract

The entanglement between occupation numbers of different single particle basis states depends on coupling between different single particle basis states in the second-quantized Hamiltonian. Thus, in principle, interaction is not necessary for occupation-number entanglement to appear. However, in order to characterize *quantum correlation caused by interaction*, we use the eigenstates of the single-particle Hamiltonian as the single particle basis upon which the occupation-number entanglement is defined. Using this so-called proper single particle basis, if there is no interaction, the many-particle second-quantized Hamiltonian is diagonalized and thus cannot generate entanglement, while its eigenstates can always be chosen to be non-entangled. If there is interaction, entanglement in the proper single particle basis arises in energy eigenstates and can be dynamically generated. Using the proper single particle basis, we discuss occupation-number entanglement in important eigenstates, especially ground states, of systems of many identical particles, in exploring insights the notion of entanglement sheds on many-particle physics. The discussions on Fermi systems start with Fermi gas, the Hartree–Fock approximation and the electron–hole entanglement in excitations. In the ground state of a Fermi liquid, in terms of the Landau quasiparticles, entanglement becomes negligible. The entanglement in a quantum Hall state is quantified as $-f \ln f - (1-f)\ln(1-f)$, where f is the proper fractional part of the filling factor. For BCS superconductivity, the entanglement is a function of the relative momentum wavefunction of the Cooper pair $g_{\mathbf{k}}$, and is thus directly related to the superconducting energy gap, and vanishes if and only if superconductivity vanishes. For a spinless Bose system, entanglement does not appear in the Hartree–Gross–Pitaevskii approximation, but becomes important in the Bogoliubov theory, as a characterization of two-particle correlation caused by the weak interaction. In these examples, the interaction-induced entanglement as calculated is directly related to the macroscopic physical properties.

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1. Introduction

Quantum entanglement is a situation where a quantum state of a composite system is not a direct product of the states of the subsystems [1]. It is an essential quantum feature without classical analogy [2, 3]. For many decades, the notion of entanglement has been mostly used in the foundations of quantum mechanics. Recently it was found to be crucial in quantum information processing. For a bipartite pure state $|\psi_{AB}\rangle$, the entanglement can be quantified as the von Neumann entropy of the reduced density matrix of either party, $S = -\mathrm{tr}_A\, \rho_A \ln \rho_A = -\mathrm{tr}_B\, \rho_B \ln \rho_B$, where $\rho_A = \mathrm{tr}_B(|\psi_{AB}\rangle\langle\psi_{AB}|)$, $\rho_B = \mathrm{tr}_A(|\psi_{AB}\rangle\langle\psi_{AB}|)$ [4]. Thus $0 \leqslant S \leqslant \ln D$, where D is the smaller of the dimensions of the Hilbert spaces of A and B. The larger the S the stronger the entanglement. Recall that the von Neumann entropy of a density matrix is a measure of the distribution of its eigenvalues; the more homogeneous this distribution the larger the von Neumann entropy.

Since quantum entanglement is an essential quantum correlation, it is natural and interesting to consider useful or even fundamental insights that the notion of entanglement may provide on quantum many-body physics and quantum field theory. Historically, a similar consideration was made in Yang's study of off-diagonal long-range order [5] and in Leggett's study of disconnectivity [6]. The recent development of quantum information theory may be useful to some important issues in the frontiers of physics [7]. Some investigations have been made on entanglement between spins at different sites in some spin lattice models [8–14]. Nevertheless, the bulk of quantum many-body physics concerns identical particles, with the localized spin models as special cases. Hence in this regard, it is inevitable to address the issue of entanglement in systems of identical particles. This topic, related to both quantum information and condensed matter physics, is pursued in various approaches [15–30].

As the quantum correlation beyond the symmetrization or anti-symmetrization of identical particles, entanglement between occupation numbers of different single particle basis states (modes) is an appropriate characterization. Lloyd and co-workers recognized the occupation number basis as a suitable basis for quantum simulation of second quantized many-particle systems, exemplified by using the Hubbard model [15]. Furthermore, occupation was also proposed as the degree of freedom to implement a qubit [16–20]. Zanardi noted the isomorphism between the full Fock space and qubit space and investigated the entanglement in grand canonical ensembles [21]. Afterwards, from a physical standpoint and the relation between occupation number state and the (anti)symmetrized particle state, the present author carefully justified the use of Fock space in investigating the entanglement issue, even in the case of particle number conservation, and thus helped establish the applicability of this approach to many-particle pure states [23, 24]. It is also noted that the magnetic spin entanglement is a special case of occupation-number entanglement of identical particles [23]. Some related papers appeared after the present work was actually done [24]. Vedral made some very interesting investigations, where the application of two-mode squeezing to Bose condensates and related systems was analysed, and two-particle fermionic entanglement due to symmetrization was computed [27].

In this approach, clearly the entanglement in the many-particle system depends on which single particle basis is chosen. This point might seem uncomfortable to some researchers, according to whom entanglement should not be affected by local operations. Let us emphasize that the subsystems are defined by modes, not by particles. The choice of single particle basis defines how to partition the system into subsystems, and actually defines the single particles[1]. Once the single particle basis is chosen, i.e. the partition into subsystems is defined, the

[1] A particle in a classical sense can emerge as a consequence of decoherence [31].

entanglement is invariant under unitary operations on individual subsystems, i.e. the modes, which is fully consistent with the general notion about entanglement. Naturally a question arises: which single particle basis does one choose? The answer is that it depends on the relevance to the question one is concerned with, or which single particle basis corresponds to the particles that are detected in the circumstance.

Given that in this approach, the entanglement is between the occupation numbers of different single particle basis states, whether it can be generated by, or whether it exists in an eigenstate of, a many-particle second-quantized Hamiltonian $\mathcal{H}$ depends on whether there is a coupling between different single particle basis states in $\mathcal{H}$, in contrast with the case of distinguishable particles, for which the entanglement depends on interaction of particles. Hence generically speaking, interaction is *not* necessary for the generation or existence of occupation-number entanglement. For example, in a single particle basis in which $\mathcal{H}$ is not diagonal, the occupation-number entanglement exists in eigenstates of $\mathcal{H}$, and can be dynamically generated.

Here we note, however, that there is a special single particle basis in which, if there is no interaction, entanglement cannot be generated from a non-entangled state, while each *energy eigenstate* must be non-entangled (except the insignificant case of a superposition of two degenerate non-entangled eigenstates with different occupation numbers in at least two single particle basis states). In this single particle basis, entanglement in a non-degenerate energy eigenstate is only caused by interaction. Hence this single particle basis is very suitable in characterizing the *quantum correlation due to interaction*, rather than the entanglement that appears merely as a consequence of Bogoliubov mode transformation. For convenience, let us call this special single particle basis *the proper single particle basis*.

The so-called proper single particle basis is just the set of eigenstates of the single particle Hamiltonian. It is indexed by the (continuous or discrete) momentum in the case of free particles, the Bloch wave vector plus the band index in the case of particles in a periodic potential, the degree of the Hermite polynomial and the perpendicular momentum in the case of electrons in a magnetic field, etc. The inclusion of spin as an additional index is straightforward.

It is instructive and amusing to consider our method of characterizing interaction-induced entanglement as an extension of the novel way of counting states of a system of identical particles invented by Bose, Einstein and Dirac [32]. They considered an ideal gas, hence the underlying many-particle states are just all the possible occupation-number basis states in the momentum basis, which is the proper single particle basis in this question. Each of these occupation-number basis states is a direct product of the occupation states of single particle basis states (modes). There is no superposition of these occupation-number basis states and no entanglement between the proper single particle basis states. Hence the classical Boltzmann counting is applicable when one considers the occupations of the single particle states, rather than the particles themselves. The entanglement between these different single particle states emerges when there is interaction, as discussed in this paper.

In this paper, using the proper single particle basis, we shall explore the *interaction-induced* entanglement in representative many-particle states, which are of fundamental importance in condensed matter physics and the like. In particular, we emphasize the role of the Hamiltonian and the relation between entanglement with macroscopic physical properties.

Energy eigenstates, especially the ground states, are of utmost importance in many-body and statistical physics. Besides, adiabatically controlled ground states are also used in some quantum computing schemes [33–35]. Hence it is important to address the issue of entanglement in the energy eigenstates, especially the ground state. These aspects further motivate our work.

The organization of this paper is the following. First an introduction and a clarification are made on occupation-number entanglement in a system of many identical particles, and especially on the so-called proper single particle basis. Then we discuss the ground state and excitations of normal Fermi systems, especially the electron–hole entanglement in the Hartree–Fock approach. In the next two sections, we carry out detailed investigations into entanglement in the quantum Hall effect and Bardeen–Cooper–Schrieffer (BCS) superconductivity, respectively. Afterwards there is a section devoted to bosonic entanglement, in which entanglement in the Bogoliubov theory is calculated. We summarize after making some additional remarks.

2. The proper single particle basis

In the standard formalism of second quantization, one can write a state of many identical particles in terms of an arbitrarily chosen single particle basis as

$$|\psi\rangle = \sum_{n_1,\ldots,n_\infty} f(n_1,\ldots,n_\infty)|n_1,\ldots,n_\infty\rangle \tag{1}$$

where n_i is the occupation number of single particle state i in the chosen single particle basis, $|n_i\rangle \equiv (1/\sqrt{n_i})a_i^{\dagger n_i}|0\rangle|n_1,\ldots,n_\infty\rangle$ corresponds to a Slater determinant or permanent wavefunction in the configuration space. For a fixed number of particles, whether a many-particle state is entangled depends on whether the wavefunction is a single Slater determinant or permanent. In principle, entanglement in a system of identical particles is a property dependent on which single particles and which single particle basis are chosen in representing the many-particle system, and can be quantified as that among occupation numbers of different single particle states.

Choosing a different single particle basis means partitioning the system into a different set of subsystems, based on which the entanglement is then defined. But once a single particle basis is chosen, the entanglement in invariant under any unitary operation on individual single particle basis states, i.e. when there is no coupling between different single particle basis states. In other words, in the present case, the meaning of 'local operations' as previously used in quantum information theory is generalized to operations on the corresponding single particle basis states, as indexed by the subscript i above. Of course, it is constrained that some kinds of generalized 'local' unitary operations do not exist physically. Once this generalization of the meaning of subsystems and local operations is made, the usual method of calculating the amount of entanglement, as developed in quantum information theory, can be applied.

Quantitatively, one considers the Fock-state reduced density matrix of a set of single particle basis states $1,\ldots,l$,

$$\langle n_1',\ldots,n_l'|\rho_l(1\cdots l)|n_1,\ldots,n_l\rangle \equiv \sum_{n_{l+1},\ldots,n_\infty} \langle n_1',\ldots,n_l',n_{l+1},n_\infty|\rho|n_1,\ldots,n_l,n_{l+1},n_\infty\rangle. \tag{2}$$

Its von Neumann entropy measures the entanglement of this set of single particle basis states and the rest of the system, relative to the empty state. If the total number of particles is conserved, then it is constrained that the only matrix elements which may be nonzero are those with $\sum_{i=1}^{l} n_i' = \sum_{i=1}^{l} n_i$. In particular, the reduced density matrix of one single particle basis state is always diagonal, indicating entanglement whenever there is more than one nonzero diagonal element.

In this approach, the statistics determines the dimensions of the Hilbert space of each mode. For fermions, $n_i = 0, 1$, $D = 2$, hence the entanglement between one single particle basis state and the rest of the system is $0 \leqslant S \leqslant \ln 2$. For bosons, n_i is arbitrary, hence D is infinity. This point does not pose real difficulties; however, further investigation is interesting.

One can also define the entanglement relative to the ground state, by considering only the effect of creation and annihilation operators acting on the ground state. Then n_i in (2) is understood as the number of excited particles, which are absent in the ground state $|G\rangle$, i.e. $|n_1, \ldots, n_\infty\rangle \equiv (1/\sqrt{n_1! \cdots n_\infty!}) {a_1^\dagger}^{n_1} \cdots {a_\infty^\dagger}^{n_\infty} |G\rangle$.

The non-relativistic field theoretic or second-quantized Hamiltonian is

$$\mathcal{H} = \int \mathrm{d}^3 r\, \hat{\psi}^\dagger(\mathbf{r}) h(\mathbf{r}) \hat{\psi}(\mathbf{r}) + \int \mathrm{d}^3 r\, \hat{\psi}^\dagger(\mathbf{r}) h'(\mathbf{r}) \hat{\psi}(\mathbf{r}) + \frac{1}{2} \int \mathrm{d}^3 r \int \mathrm{d}^3 r'\, \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}^\dagger(\mathbf{r}') V(\mathbf{r}, \mathbf{r}') \hat{\psi}(\mathbf{r}') \hat{\psi}(\mathbf{r}) \tag{3}$$

where $h(\mathbf{r})$ is the single particle Hamiltonian including the kinetic energy, $V(\mathbf{r}, \mathbf{r}')$ is the particle–particle interaction, $h'(\mathbf{r})$ is some external potential which is not included in $h(\mathbf{r})$ for convenience. In the examples in this paper, $h' \neq 0$ only in the case of generation of electron–hole excitations by electron–light interaction; $h' = 0$ in all discussions on entanglement in many-particle energy eigenstates. The field operator $\hat{\psi}(\mathbf{r})$ can be expanded in an arbitrarily chosen single particle basis as $\hat{\psi}(\mathbf{r}) = \sum_i \phi_i(\mathbf{r}) a_i$, where i is the collective index of the single particle state, which may include spin if needed, a_i is the annihilation operator and $\phi_i(\mathbf{r})$ is the single particle wavefunction in position space. We use the same notation for fermions and bosons. Thus $\mathcal{H}$ can also be written as

$$\mathcal{H} = \sum_{ij} \langle i|h|j\rangle a_i^\dagger a_j + \sum_{ij} \langle i|h'|j\rangle a_i^\dagger a_j + \frac{1}{2} \sum_{ijlm} \langle ij|V|lm\rangle a_i^\dagger a_j^\dagger a_m a_l. \tag{4}$$

The generalization to the existence of more species of identical particles is straightforward. Single particle basis transformation leads to a unitary transformation in the creation and annihilation operators. There may be more general transformations of the creation and annihilation operators, and some even involve combination of operators of different species. Such a transformation means describing the system in terms of a different set of single particles or quasiparticles.

Even if $V = 0$ and $h' = 0$, as long as $\langle i|h|j\rangle \neq 0, \mathcal{H}$ can generate occupation-number entanglement between single particle basis states i and j.

An eigenstate of a second-quantized interacting Hamiltonian is often entangled. In the chosen single particle basis, if an eigenstate of (4) is non-entangled, it must be of the form $|\psi\rangle = \otimes_i |n_i\rangle$. Consequently for each $i, \mathcal{H}\hat{n}_i|\psi\rangle = \hat{n}_i \mathcal{H}|\psi\rangle$, where $\hat{n}_i = a_i^\dagger a_i$. It can be seen that this is often not satisfied by $\mathcal{H}$ in (4).

However, when we use entanglement to characterize the *quantum correlation caused by interaction*, it is suitable to use the set of eigenstates of the single particle Hamiltonian h, which we call proper single particle basis. In this single particle basis, with $h\phi_\mu = \epsilon_\mu \phi_\mu$, $\int \mathrm{d}^3 r\, \hat{\psi}^\dagger(\mathbf{r}) h(\mathbf{r}) \hat{\psi}(\mathbf{r}) = \sum_\mu \epsilon_\mu a_\mu^\dagger a_\mu$, whose eigenstates are of the form $\otimes_\mu |n_\mu\rangle$, where μ is the collective index of the proper single particle basis.

Therefore in the proper single particle basis, entanglement can be used to characterize the effect of interaction. In the case $h' = 0$, it characterizes the effect of the particle–particle interaction. Each non-degenerate energy eigenstate of the non-interacting system must be non-entangled. When there is degeneracy, an entangled energy eigenstate of a free system may be constructed as a superposition of degenerate non-entangled states that differ in the occupation numbers of at least two single particle basis states (on the other hand, particle number conservation constrains that it is impossible for two states to be different only in one single particle basis state). But one can always use a set of non-entangled eigenstates. If in the proper single particle basis, entangled energy eigenstates inevitably arise, there must be interaction.

Besides, the proper single particle basis directly corresponds to the energy spectrum of single particle excitations, and is experimentally more accessible.

For the so-called strongly correlated systems, e.g., Luttinger liquid and fractional quantum Hall state discussed below, peculiar physical properties are caused by the strong (Coulomb) interaction, hence it is particularly interesting to consider occupation-number entanglement in the proper single particle basis. By generalizing the method to relativistic field theory, it may be useful for quantum chromodynamics.

On the other hand, when an improper single particle basis is used, even the one-body term in $\mathcal{H}$ is not diagonal, and the eigenstates are entangled even when there is no interaction, as seen by transforming $a_\mu^\dagger$ in $\otimes_\mu|n_\mu\rangle \equiv \otimes_\mu(1/\sqrt{n_\mu})a_\mu^{\dagger\,n_\mu}|0\rangle$. Nevertheless, entanglement in an improper basis may be interesting in problems such as hopping, tunnelling, Mott transition, etc. For example, in a two-state problem, of which the double well potential problem is an example, the proper basis states are linear superpositions of the two states, but in many cases it is these two states that are observed. As occupation-number entanglement in an improper single particle basis is present even when there is no interaction, it may be valuable for quantum information processing.

When there is more than one index in the single particle basis, one of them can be used as the tag effectively distinguishing the particles, and the other indices determine whether they are entangled in these degrees of freedom. With this effective distinguishability, the state in the configuration space of the remaining degrees of freedom can be directly obtained from the second-quantized state. For example, in $\frac{1}{\sqrt{2}}\left(a_{\mathbf{k}'\uparrow}^\dagger a_{\mathbf{k}\downarrow}^\dagger + a_{\mathbf{k}'\downarrow}^\dagger a_{\mathbf{k}\uparrow}^\dagger\right)|0\rangle$, where $\mathbf{k}'$ and $\mathbf{k}$ represent momenta, one can say that the particle in $|\mathbf{k}'\rangle$ and the particle in $|\mathbf{k}\rangle$ are spin-entangled. One can also say that the particle in $|\uparrow\rangle$ and the particle in $|\downarrow\rangle$ are momentum-entangled. With the momentum as the distinguishing tag, the spin state is $\frac{1}{\sqrt{2}}(|\uparrow\rangle_{\mathbf{k}'}|\downarrow\rangle_{\mathbf{k}} + |\uparrow\rangle_{\mathbf{k}'}|\downarrow\rangle_{\mathbf{k}})$. Alternatively, with the spin as the distinguishing tag, the momentum state is $\frac{1}{\sqrt{2}}(|\mathbf{k}'\rangle_\uparrow|\mathbf{k}\rangle_\downarrow + |\mathbf{k}\rangle_\uparrow|\mathbf{k}'\rangle_\downarrow)$.

The ideas about the occupation-number entanglement can be consistently applied even to a one-particle state $|\phi\rangle = \sum_i c_i|i\rangle$, where $|i\rangle$ are a set of basis states. In terms of occupation numbers of different basis states, the state can be written as $|\phi\rangle = \sum_i c_i|1\rangle_i \prod_{j\neq i}|0\rangle_j$. Thus the occupation number of basis state $|i\rangle$ is entangled with other basis states, with the amount of entanglement $-|c_i|^2\ln|c_i|^2 - (1-|c_i|^2)\ln(1-|c_i|^2)$. When $|\phi\rangle$ and $|i\rangle$ are eigenstates of the Hamiltonian, $|\phi\rangle = |I\rangle$, thus $c_I = 1$ while $c_j = 0$ for $j \neq I$; consequently in $|\phi\rangle$, each basis state is non-entangled with other basis states. In the example of an electron in a superposition of a state $|-\mathbf{k}'\rangle_e$ in a Fermi sea and a state $|\mathbf{k}\rangle_e$ out of the Fermi sea, written in terms of the occupation numbers of these two electronic states, $a|0\rangle_{e\mathbf{k}}|0\rangle_{e-\mathbf{k}'} + b|1\rangle_{e\mathbf{k}}|1\rangle_{e-\mathbf{k}'}$ can also be written in terms of occupation numbers of the electron state $|\mathbf{k}\rangle_e$ and the hole state $|\mathbf{k}'\rangle_h$ as $a|0\rangle_{e\mathbf{k}}|0\rangle_{h\mathbf{k}'} + b|1\rangle_{e\mathbf{k}}|1\rangle_{h\mathbf{k}'}$. This becomes a superposition of the absence and presence of an electron–hole pair. But this kind of electron–hole entanglement is different from the entanglement between an existing electron and an existing hole.

Now we start our discussions on occupation-number entanglement in important energy eigenstates in many-particle physics, using the so-called proper single particle basis. These systems play fundamental roles in condensed matter physics.

3. Fermi systems

First let us consider a Fermi gas, which plays a fundamental role in understanding condensed matter physics. The proper single particle basis here is the tensor product of single-particle momentum and spin states.

The ground state of a free Fermi gas is $|G\rangle = \prod_{\mathbf{k}}^{|\mathbf{k}|<k_F} a^\dagger_{\mathbf{k}\uparrow} a^\dagger_{\mathbf{k}\downarrow}|0\rangle$, where k_F is the Fermi momentum. It is clearly non-entangled. An excited state such as $a^\dagger_{\mathbf{k}s} b^\dagger_{\mathbf{k}'s'}|G\rangle$ is still separable, where $|\mathbf{k}| > k_F > |\mathbf{k}'|$, $b^\dagger_{\mathbf{k}s} = a_{-\mathbf{k}-s}$ is the hole operator. It is simple to check that for each of these non-entangled states, a Fock-space reduced density matrix, as in (2), always has only one nonzero element, hence the entanglement between the occupation numbers of any set of single particle basis states and the rest of the system indeed vanishes.

There may be entanglement in an excited state of a Fermi gas, because of degeneracy due to spin degree of freedom. For example, there is maximal entanglement in the electron–hole pair $\frac{1}{\sqrt{2}}\left(a^\dagger_{\mathbf{k}\uparrow} b^\dagger_{\mathbf{k}'\downarrow} + a^\dagger_{\mathbf{k}\downarrow} b^\dagger_{\mathbf{k}'\uparrow}\right)|G\rangle$. For a free gas, it is a superposition of the degenerate non-entangled states $a^\dagger_{\mathbf{k}\uparrow} b^\dagger_{\mathbf{k}'\downarrow}|G\rangle$ and $a^\dagger_{\mathbf{k}\downarrow} b^\dagger_{\mathbf{k}'\uparrow}|G\rangle$. With respect to the empty state, it is an entanglement between the occupation numbers of the excited electron state and others. Since $|G\rangle$ is non-entangled, entanglement in an excited state relative to the empty state is equal to the entanglement relative to $|G\rangle$. The entanglement in $\frac{1}{\sqrt{2}}\left(a^\dagger_{\mathbf{k}\uparrow} b^\dagger_{\mathbf{k}'\downarrow} + a^\dagger_{\mathbf{k}\downarrow} b^\dagger_{\mathbf{k}'\uparrow}\right)|G\rangle$ is simply electron–hole entanglement with respect to the ground state. Moreover, an electron and a hole, by definition, correspond to different single particle states, and can be regarded as distinguishable particles, as tagged by the fact that a creation operator of a hole corresponds to annihilation of an electron. In the absence of interaction, however, one can always use a set of non-entangled energy eigenstates as the orthonormal set.

More realistic treatment, in the context of solid state physics, takes into account the Coulomb interaction between the electrons, as well as the crystal structure, which provides a single particle (periodic) potential. A basic method is the Hartree–Fock approach [36]. The ground state is still non-entangled, since the Hartree–Fock treatment only modifies the single particle states and ground state energy. But entanglement inevitably arises in excited states. To illustrate the idea, the simplest model of electronic excitations in solids is considered in the following.

Consider that one electron is excited from a valence band to a conduction band. An eigenstate of this excitation, an exciton, is $\sum_{\mathbf{k},\mathbf{k}'} A_{\mathbf{k},\mathbf{k}'} a^\dagger_{\mathbf{k}} b^\dagger_{\mathbf{k}'}|G\rangle$ in the spinless case. For brevity, the band indices are omitted, as one corresponds to the electron operator while the other corresponds to the hole operator. The occupation numbers of the basis states $|\mathbf{k}\rangle_e$ and $|\mathbf{k}'\rangle_h$ respectively occupied by the excited electron and the hole are the same as those relative to the ground state, since they are zero in the ground state. The Fock-space reduced density matrix elements of $\mathbf{k}$ can be obtained as $\langle 1|\rho_1(\mathbf{k})|1\rangle = \alpha_{\mathbf{k}} \equiv \sum_{\mathbf{k}'} |A_{\mathbf{k},\mathbf{k}'}|^2$, $\langle 0|\rho_1(\mathbf{k})|0\rangle = 1-\alpha_{\mathbf{k}}$. Therefore the occupation-number entanglement between the electron basis state $|\mathbf{k}\rangle_e$ and the rest of the system is $-\alpha_{\mathbf{k}}\ln\alpha_{\mathbf{k}} - (1-\alpha_{\mathbf{k}})\ln(1-\alpha_{\mathbf{k}})$. The occupation-number entanglement between the hole basis state $|\mathbf{k}'\rangle_h$ and the rest of the system is $-\alpha_{\mathbf{k}'}\ln\alpha_{\mathbf{k}'} - (1-\alpha_{\mathbf{k}'})\ln(1-\alpha_{\mathbf{k}'})$, where $\alpha_{\mathbf{k}'} = \sum_{\mathbf{k}} |A_{\mathbf{k},\mathbf{k}'}|^2$. The Fock-space reduced density matrix $\rho_{1,1}$ of the electron basis state $|\mathbf{k}\rangle_e$ plus the hole basis state $|\mathbf{k}'\rangle_h$ as a subsystem is calculated by considering that this electron and the hole belong to different species of identical particles. $\langle 1,1|\rho_{1,1}(\mathbf{k},\mathbf{k}')|1,1\rangle = |A_{\mathbf{k},\mathbf{q}'}|^2$, $\langle 1,0|\rho_{1,1}(\mathbf{k},\mathbf{k}')|1,0\rangle = \gamma_{\mathbf{k}} \equiv \sum_{\mathbf{q}'\neq\mathbf{k}'} |A_{\mathbf{k},\mathbf{q}'}|^2$, $\langle 0,1|\rho_{1,1}(\mathbf{k},\mathbf{k}')|0,1\rangle = \gamma_{\mathbf{k}'} \equiv \sum_{\mathbf{q}\neq\mathbf{k}} |A_{\mathbf{q},\mathbf{k}'}|^2$. Furthermore, $\rho_{1,1}(\mathbf{k},\mathbf{k}')$ must be diagonal. Hence their occupation-number entanglement with the rest of the system is $-|A_{\mathbf{k},\mathbf{k}'}|^2\ln|A_{\mathbf{k},\mathbf{k}'}|^2 - \gamma_{\mathbf{k}}\ln\gamma_{\mathbf{k}} - \gamma_{\mathbf{k}'}\ln\gamma_{\mathbf{k}'} - (1-|A_{\mathbf{k},\mathbf{k}'}|^2-\gamma_{\mathbf{k}}-\gamma_{\mathbf{k}'})\ln(1-|A_{\mathbf{k},\mathbf{k}'}|^2-\gamma_{\mathbf{k}}-\gamma_{\mathbf{k}'})$.

With the electron and the hole effectively distinguishable, the state can be written, in the configuration space, as $\sum_{\mathbf{k},\mathbf{k}'} A_{\mathbf{k},\mathbf{k}'}|\mathbf{k}\rangle_e|\mathbf{k}'\rangle_h$. The entanglement between these two distinguishable particles is obtained by finding the eigenvalues of the reduced density matrix for either particle.

With spin degeneracy, the excitonic states are $\sum_{\mathbf{k},\mathbf{k}'} A_{\mathbf{k},\mathbf{k}'}|S,S_z\rangle_{\mathbf{k},\mathbf{k}'}$, where $|S,S_z\rangle_{\mathbf{k},\mathbf{k}'}$ represents three triplet states as the ground states, $|1,1\rangle_{\mathbf{k},\mathbf{k}'} = a^\dagger_{\mathbf{k}\uparrow} b^\dagger_{\mathbf{k}'\uparrow}|G\rangle$, $|1,0\rangle_{\mathbf{k}\mathbf{k}'} =$

$\frac{1}{\sqrt{2}}(a^\dagger_{\mathbf{k}\uparrow}b^\dagger_{\mathbf{k}'\downarrow} - a^\dagger_{\mathbf{k}\downarrow}b^\dagger_{\mathbf{k}'\uparrow})|G\rangle$ and $|1,-1\rangle_{\mathbf{k},\mathbf{k}'} = a^\dagger_{\mathbf{k}\downarrow}b^\dagger_{\mathbf{k}'\downarrow}|G\rangle$, and one singlet state $|0,0\rangle_{\mathbf{k},\mathbf{k}'} = \frac{1}{\sqrt{2}}(a^\dagger_{\mathbf{k}\uparrow}b^\dagger_{\mathbf{k}'\downarrow} + a^\dagger_{\mathbf{k}\downarrow}b^\dagger_{\mathbf{k}'\uparrow})|G\rangle$.

The occupation-number entanglement, with the full collective index including Bloch wavevector and spin, can be calculated in a way similar to the spinless case. The above discussions on the spinless case apply similarly to $\sum_{\mathbf{k},\mathbf{k}'} A_{\mathbf{k},\mathbf{k}'}|1,\pm1\rangle_{\mathbf{k},\mathbf{k}'}$. For $\sum_{\mathbf{k},\mathbf{k}'} A_{\mathbf{k},\mathbf{k}'}\frac{1}{\sqrt{2}}(a^\dagger_{\mathbf{k}\uparrow}b^\dagger_{\mathbf{k}'\downarrow} \pm a^\dagger_{\mathbf{k}\downarrow}b^\dagger_{\mathbf{k}'\uparrow})|G\rangle$, one can find, for example, that the occupation-number entanglement between the electron basis state $|\mathbf{k},\uparrow\rangle_e$ plus the hole basis state $|\mathbf{k}',\downarrow\rangle_h$ as a subsystem and the rest of the system is $-(|A_{\mathbf{k},\mathbf{k}'}|^2/2)\ln(|A_{\mathbf{k},\mathbf{k}'}|^2/2) - (\gamma_{\mathbf{k}}/2)\ln(\gamma_{\mathbf{k}}/2) - (\gamma_{\mathbf{k}'}/2)\ln(\gamma_{\mathbf{k}'}/2) - (1-\gamma_{\mathbf{k}}/2-\gamma_{\mathbf{k}'}/2-|A_{\mathbf{k},\mathbf{k}'}|^2/2)\ln(1-\gamma_{\mathbf{k}}/2-\gamma_{\mathbf{k}'}/2-|A_{\mathbf{k},\mathbf{k}'}|^2/2)$, and that the occupation-number entanglement between the electron basis state $|\mathbf{k},\uparrow\rangle_e$ plus the hole basis state $|\mathbf{k}',\uparrow\rangle_h$ as a subsystem and the rest of the system is $-(\alpha_{\mathbf{k}}/2)\ln(\alpha_{\mathbf{k}}/2) - (\alpha_{\mathbf{k}'}/2)\ln(\alpha_{\mathbf{k}'}/2) - (1-\alpha_{\mathbf{k}}/2-\alpha_{\mathbf{k}'}/2)\ln(1-\alpha_{\mathbf{k}}/2-\alpha_{\mathbf{k}'}/2)$.

The entanglement considered above is determined by the Coulomb interaction, as $A_{\mathbf{k},\mathbf{k}'}$ is determined by the Schrödinger equation in momentum representation. When Coulomb interaction is negligible, $A_{\mathbf{k},\mathbf{k}'} = 1$ for a specific pair of values of $\mathbf{k}$ and $\mathbf{k}'$, and consequently various entanglements concerning $\mathbf{k}$ and $\mathbf{k}'$ as discussed above consistently vanish. The spin part of the eigenstates can be chosen to be non-entangled. Interaction causes spread of $A_{\mathbf{k},\mathbf{k}'}$ and thus non-vanishing entanglement in the Bloch wavevectors, as well as the spin-entanglement. It is noteworthy that the detail of the interaction only affects $A_{\mathbf{k},\mathbf{k}'}$, but does not affect the structure of the spin states.

With the electron and the hole effectively distinguishable, the state can be written, in the configuration space, as $\sum_{\mathbf{k},\mathbf{k}'} A_{\mathbf{k},\mathbf{k}'}|\mathbf{k}\rangle_e|\mathbf{k}'\rangle_h|S,S_z\rangle$. So the orbital and spin degrees of freedom are actually separated, as consistent with the fact that the spin–orbit coupling has been neglected here.

An excited state is often generated by electron–light interaction switched on for a period. Light is treated as classical. The electron–light interaction corresponds to h' in section 2. With coupling between different single electron and hole basis states, it can generate electron–hole entanglement. This underlies a recent experimental result [37], a theoretical analysis of which, with spin–orbit coupling taken into account, will be given elsewhere [38].

If an interacting Fermi system can be described as a Fermi liquid, then there is a one-to-one correspondence between the particles in the non-interacting system and the quasi-particles of the interacting system, obtained by adiabatically turning on the interaction [39]. Therefore in terms of the quasiparticles, the ground state of a Fermi liquid is non-entangled. One may say that the electron entanglement caused by the interaction can be renormalized away. In contrast, the ground state of a Luttinger liquid is a global unitary transformation of a Fermi sea [40] and is entangled. New ground states emerge in phenomena such as the quantum Hall effect and superconductivity, in which entanglement is important, as shown in the next two sections.

4. Quantum Hall effect

Quantum Hall states are obtained by filling the spin polarized electrons in the degenerate (single particle) Landau levels [41]. The single particle Hamiltonian, corresponding to the proper single particle basis, is the Hamiltonian of a two-dimensional electron in a magnetic field. One knows that the degeneracy of each Landau level, i.e. the number of different states of each energy eigenstate, is the same. The key quantity in the quantum Hall effect is the filling factor ν, which is the number of electrons divided by the degeneracy of each Landau level, and manifested in quantized Hall resistivity.

We show that the filling factor ν determines the entanglement. First, the entanglement vanishes in the integer quantum Hall effect, which appears when $\nu = n$ is an integer. The n lowest Landau levels are completely filled while the others are empty. Because of the energy gap, the interaction is not important, and the ground state of the interacting systems can be smoothly connected to that of the non-interacting system. Thus the ground state is just a product state $\prod_\mu a_\mu^\dagger|0\rangle$, where μ runs over the filled states. Hence the occupation number of each single particle state belonging to completely filled Landau levels is 1, while the occupation number of every other single particle state is 0. In the Fock-space reduced density matrix of a single particle basis state, for a state μ belonging to a completely filled Landau level, only $\langle 1|\rho_1(\mu)|1\rangle = 1$ is nonzero, while for a state μ belonging to an empty Landau level, only $\langle 0|\rho_1(\mu)|0\rangle = 1$ is nonzero. It is like the ground state of a free Fermi gas. All single particle basis states are separable from one another, and there is no entanglement.

In a fractional quantum Hall state of $\nu = n + f$, where f is the proper fractional part, $n \geqslant 0$ lowest Landau levels are completely filled, f of the next Landau level are filled and the higher Landau levels are empty. Because of partial filling, the interaction cannot be treated perturbatively, and in the ground state, electrons are strongly correlated. Each single particle basis state belonging to one of the n completely filled levels or the empty levels is separated, i.e. the occupation number is either 0 or 1 and is just a factor in the many-particle state in the particle number representation.

For each single particle basis state in the partially filled Landau level, the entanglement with the rest of the system is obtained as follows. Consider the identity

$$\langle 1|\rho_1(\mu)|1\rangle = \sum_{n_1,\ldots,n_\infty} n_\mu \langle n_1,\ldots,n_\infty|\rho|n_1,\ldots,n_\infty\rangle = \langle \hat{n}_\mu\rangle \tag{5}$$

where $n_\mu = 0, 1$ $(\mu = 1,\ldots,\infty)$, $\langle \hat{n}_\mu\rangle \equiv \mathrm{tr}(\rho\hat{n}_\mu)$ is the expectation value of the particle number at state μ. The first equality is valid only for fermions while the second is valid for both fermions and bosons. On the other hand, in an isotropic uniform state, for each single particle basis state belonging to the partially filled Landau level,

$$\langle \hat{n}_\mu\rangle = f. \tag{6}$$

Therefore the entanglement between a single particle basis state belonging to the partially filled Landau level and the rest of the system is

$$S = -f\ln f - (1-f)\ln(1-f). \tag{7}$$

This simple expression of entanglement, in terms of the proper fractional part of the filling factor, gives a useful measure of the quantum correlation in a quantum Hall state. The entanglement increases from 0 at $f = 0$, corresponding to the integer quantum Hall effect, to the maximum $\ln 2$, after which it decreases to 0 at $f = 1$, corresponding to the integer quantum Hall effect again. Note that the filling factor, and hence the entanglement, is extremely precisely measured, with topological stability. Anyons have been proposed as a candidate to implement fault-tolerant quantum computing [17, 44]. The present result confirms the intrinsic entanglement, which is needed for quantum computing.

The amount of entanglement obtained above is consistent with the fact that for an integer quantum Hall effect, the many-particle wavefunction is a single Slater determinant, indicating separability, while for the fractional quantum effect, it is not [42], indicating the existence of entanglement. The Laughlin state is indeed isotropic uniform.

The fractional quantum Hall effect can be understood in terms of the composite fermions or composite bosons [41], which are non-entangled. For example, the state at $\nu = 1/(2p+1)$ can be viewed as the $\nu_{\text{eff}} = 1$ integer quantum Hall state of composite fermions, or equivalently as Bose condensation of composite bosons, while the $\nu = 1/2p$ state is a free Fermi gas with a

Fermi surface. In each of these descriptions, the system of the composite particles is separable. This separability can also be inferred from the off-diagonal long-range order (ODLRO) exhibited by these composite particles [43], because disentanglement of the condensate mode from other modes underlies ODLRO [25]. ODLRO is an important notion in many-particle physics, and is the hallmark of Bose condensation and superconductivity [5].

5. BCS superconductivity

As another example of using the concept of entanglement to further our understanding of many-particle physics, we now consider BCS superconductivity [45, 46]. The Hamiltonian is $\mathcal{H} = \sum_{\mathbf{k},s} \epsilon_{\mathbf{k}} n_{\mathbf{k},s} + \sum_{\mathbf{k},\mathbf{k}'} \langle \mathbf{k}', -\mathbf{k}'|V|\mathbf{k}, -\mathbf{k}\rangle a^\dagger_{\mathbf{k}'\uparrow} a^\dagger_{-\mathbf{k}'\downarrow} a_{-\mathbf{k}\downarrow} a_{\mathbf{k}\uparrow}$. The proper single particle basis is $(\mathbf{k}, s)$, in which the one-body term in $\mathcal{H}$ is diagonalized. The BCS superconducting ground state is

$$|\psi_0\rangle = \mathcal{N}_0 \prod_{\mathbf{k}} \left(1 + g_{\mathbf{k}} a^\dagger_{\mathbf{k}\uparrow} a^\dagger_{-\mathbf{k}\downarrow}\right)|0\rangle \tag{8}$$

where $\mathcal{N}_0 = \prod_{\mathbf{k}} (1 + |g_{\mathbf{k}}|^2)^{-1/2}$ is the normalization factor. For $|\psi_0\rangle$, in which the particle number is not conserved, the entanglement is only between each pair $(\mathbf{k}, s)$ and $(-\mathbf{k}, -s)$ given by

$$S_0 = -z_{\mathbf{k}} \ln z_{\mathbf{k}} - (1 - z_{\mathbf{k}}) \ln(1 - z_{\mathbf{k}}) \tag{9}$$

where $z_{\mathbf{k}} = 1/(1 + |g_{\mathbf{k}}|^2)$. There is no entanglement between different pairs.

However, for a system of N electrons, with N fixed, the exact state is the projection of $|\psi_0\rangle$ onto the N-particle space, which is [46][2]

$$|\psi(N)\rangle = \mathcal{N}_N \sum g_{\mathbf{k}_1} a^\dagger_{\mathbf{k}_1\uparrow} a^\dagger_{-\mathbf{k}_1\downarrow} \cdots g_{\mathbf{k}_{N/2}} a^\dagger_{\mathbf{k}_{N/2}\uparrow} a^\dagger_{-\mathbf{k}_{N/2}\downarrow}|0\rangle \tag{10}$$

where $\mathcal{N}_N = \left(\sum |g_{\mathbf{k}_1}|^2 \cdots |g_{\mathbf{k}_{N/2}}|^2\right)^{-1/2}$, $\sum$ represents summations over $\mathbf{k}_1, \ldots, \mathbf{k}_{N/2}$, with the constraint $\mathbf{k}_i \neq \mathbf{k}_j$. One can observe that this state is given by the superposition of all kinds of products of $N/2$ different $g_{\mathbf{k}} a^\dagger_{\mathbf{k}\uparrow} a^\dagger_{-\mathbf{k}\downarrow}$. This feature leads to entanglement between different Cooper paired modes.

Let us investigate the entanglement in $|\psi(N)\rangle$. First we evaluate the elements of the Fock-space reduced density matrix of mode $(\mathbf{k}, s)$, denoted as $\langle n_{\mathbf{k},s}|\rho_1(\mathbf{k}, s)|n_{\mathbf{k},s}\rangle$. One can obtain

$$\langle 1_{\mathbf{k},s}|\rho_1(\mathbf{k}, s)|1_{\mathbf{k},s}\rangle = x_{\mathbf{k}} = \frac{|g_{\mathbf{k}}|^2 \sum' |g_{\mathbf{k}'_2}|^2 \cdots |g_{\mathbf{k}'_{N/2}}|^2}{\sum |g_{\mathbf{k}_1}|^2 \cdots |g_{\mathbf{k}_{N/2}}|^2}$$

where $\sum'$ represents the summations over $\mathbf{k}'_2, \ldots, \mathbf{k}'_{N/2}$, with the constraint $\mathbf{k}'_i \neq \mathbf{k}'_j$ and $\mathbf{k}'_i \neq \mathbf{k}$, where $i, j = 2, \ldots, N/2$. One can obtain $\langle 0_{\mathbf{k},s}|\rho_1(\mathbf{k}, s)|0_{\mathbf{k},s}\rangle = 1 - x_{\mathbf{k}}$. Hence in the basis $(|0_{\mathbf{k},s}\rangle, |1_{\mathbf{k},s}\rangle)$,

$$\rho_1(\mathbf{k}, s) = \mathrm{diag}(1 - x_{\mathbf{k}}, x_{\mathbf{k}}). \tag{11}$$

One can also obtain that the element of the reduced density matrix for one pair of modes with opposite $\mathbf{k}$ and s, denoted as $\langle n_{\mathbf{k},s}, n_{-\mathbf{k},-s}|\rho_2(\mathbf{k}, s; -\mathbf{k}, -s)|n_{\mathbf{k},s}, n_{-\mathbf{k},-s}\rangle$, is $x_{\mathbf{k}}$ when $n_{\mathbf{k},s} = n_{-\mathbf{k},-s} = 1$, is $1 - x_{\mathbf{k}}$ when $n_{\mathbf{k},s} = n_{-\mathbf{k},-s} = 0$ and is 0 otherwise. Hence in the basis $(|0_{\mathbf{k},s} 0_{-\mathbf{k},-s}\rangle, |0_{\mathbf{k},s} 1_{-\mathbf{k},-s}\rangle, |1_{\mathbf{k},s} 0_{-\mathbf{k},-s}\rangle, |1_{\mathbf{k},s} 1_{-\mathbf{k},-s}\rangle)$,

$$\rho_2(\mathbf{k}, s; -\mathbf{k}, -s) = \mathrm{diag}(1 - x_{\mathbf{k}}, 0, 0, x_{\mathbf{k}}). \tag{12}$$

[2] Without loss of essence, suppose N to be even here. It is straightforward to extend to the case in which the number of particles is odd or the system is in an excited state. For example, if one particle at $(\mathbf{p}, \uparrow)$ has no mate $(-\mathbf{p}, \downarrow)$, $|\psi_0\rangle$ is replaced as $\prod_{\mathbf{k}\neq\mathbf{p}} (1 + g_{\mathbf{k}} a^\dagger_{\mathbf{k}\uparrow} a^\dagger_{-\mathbf{k}\downarrow}) a_{\mathbf{p},\uparrow}|0\rangle$.

Therefore the entanglement between the occupation number at mode $(\mathbf{k}, s)$ and others is

$$S = -x_{\mathbf{k}} \ln x_{\mathbf{k}} - (1 - x_{\mathbf{k}}) \ln(1 - x_{\mathbf{k}}) \tag{13}$$

so also is the entanglement between the occupation numbers of the pair $(\mathbf{k}, s)$ and $(-\mathbf{k}, -s)$ on one hand, and the rest of the system on the other. Note that in $|\psi(N)\rangle$, there is no entanglement between each pair $(\mathbf{k}, s)$ and $(-\mathbf{k}, -s)$, as can be simply confirmed by the fact that (12) is diagonal.

If $g_{\mathbf{k}}$ is 1 for $|\mathbf{k}| < k_f$ and is 0 for $|\mathbf{k}| > k_f$, then $x_{\mathbf{k}}$ is 1 for $|\mathbf{k}| < k_f$ and is 0 for $|\mathbf{k}| > k_f$. Consequently for any $\mathbf{k}$, each of those Fock-space reduced density matrices has only one non-vanishing element. Therefore the entanglement S reduces to zero, consistent with the fact that under this limit, the state (10) reduces to the ground state of a free Fermi gas [46].

In the superconducting state, $g_{\mathbf{k}}$ differs from that of the free Fermi gas in the vicinity of the Fermi surface, consequently the amount of entanglement becomes nonzero. $g_{\mathbf{k}}$ is just the relative momentum wavefunction of each Cooper-paired electron, and is directly related to the superconducting energy gap $\Delta_{\mathbf{k}}$ as $g_{\mathbf{k}}\big/\big(1 + g_{\mathbf{k}}^2\big) = \Delta_{\mathbf{k}}/2E_{\mathbf{k}}$, where $E_{\mathbf{k}} = \sqrt{\mathbf{k}^2/2m + \Delta_{\mathbf{k}}^2}$. As the order parameter, the superconducting energy gap is a key physical property of superconductivity.

Therefore we have obtained a direct relation between entanglement and the superconducting energy gap and thus various physical properties of superconductivity. The entanglement vanishes if and only if the superconductivity vanishes.

Although superconductivity may be loosely described as Bose condensation of Cooper pairs, it is understood that a Cooper pair is still different from a boson, and the strong overlap and correlations between Cooper pairs give rise to the gap which is absent in the case of a Bose gas [46]. The crossover between Bose condensation and BCS superconductivity has been an interesting topic for a long time. Here we have found that entanglement in $|\psi(N)\rangle$ provides quantitative characterizations of the correlations between Cooper pairs and thus may be useful in studying the crossover between Bose condensation and superconductivity.

After this work was completed, there appeared a preprint on entanglement in the BCS state involving strong interaction [48].

6. Bose systems

Consider a system of spinless bosons. The proper single particle basis is the momentum state. An eigenstate of a free spinless boson system is simply $\left|n_{\mathbf{q}_1}, n_{\mathbf{q}_2}, \ldots\right\rangle = \left(a_{\mathbf{q}_1}^{\dagger}\right)^{n_{\mathbf{k}_1}} \left(a_{\mathbf{q}_2}^{\dagger}\right)^{n_{\mathbf{q}_2}} \cdots |0\rangle$. In the ground state $\left(a_0^{\dagger}\right)^N |0\rangle$, all particles occupy the zero momentum state. This is Bose–Einstein condensation. The system is obviously non-entangled, in the proper single particle basis, in all the eigenstates. Thus there is entanglement in the position basis, consistent with a related work [47].

For a weakly interacting spinless boson gas, entanglement between occupation numbers of different momentum states is still absent under the Hartree–Gross–Pitaevskii approximation. In this approach, an energy eigenstate is approximated as a product of single particle states, with symmetrization, hence there is no occupation-number entanglement. The ground state is a product of the same single particle state. The weak interaction only affects the single particle state. Nevertheless, there may be entanglement when there is spin degree of freedom or in other complex situations [49, 50]. These features are like those of the Hartree–Fock approach to a Fermi gas.

The next level of treatment is the Bogoliubov theory [51], nonzero entanglement appears, even in the ground state. It is first hinted by the Bogoliubov transformation in the original, particle non-conserving, formulation, which defines a new annihilation operator which is a superposition of an annihilation operator $a_{\mathbf{q}}$ and the creation operator for the opposite momentum $a^{\dagger}_{-\mathbf{q}}$, namely, $b_{\mathbf{q}} = u_{\mathbf{q}} a_{\mathbf{q}} + v_{\mathbf{q}} a^{\dagger}_{-\mathbf{q}}$. This transformation diagonalizes the second-quantized Hamiltonian, hence in terms of the newly defined quasiparticles, there is no entanglement, signalling that there exists entanglement in terms of the original particles. Similar to BCS superconductivity, in the particle non-conserving theory, entanglement only exists between each pair of modes $\mathbf{q}$ and $-\mathbf{q}$ ($\mathbf{q} > 0$). The ground state is [52, 53]

$$|\Psi_0\rangle \propto \sum_{n_{\mathbf{q}_1}} \sum_{n_{\mathbf{q}_2}} \cdots \left[\left(-v_{\mathbf{q}_1}/u_{\mathbf{q}_1}\right)^{n_{\mathbf{q}_1}} \left(-v_{\mathbf{q}_2}/u_{\mathbf{q}_2}\right)^{n_{\mathbf{q}_2}} \cdots\right] \left|n_0; n_{\mathbf{q}_1}, n_{\mathbf{q}_1}; n_{\mathbf{q}_2}, n_{\mathbf{q}_2}; \cdots\right\rangle \tag{14}$$

in which there are n_0 particles with zero momentum while there are $n_{\mathbf{q}}$ pairs of particles with $\mathbf{q}$ and $-\mathbf{q}$. Therefore, the entanglement between occupation numbers at $\mathbf{q}$ and $-\mathbf{q}$ is $S = -\sum_i x_i \ln x_i$, where $x_i = y_i / \sum_i y_i, n = 0, 1, \ldots, \infty$, where $y_i = |v_{\mathbf{q}}/u_{\mathbf{q}}|^{2i}$. The condensate mode is indeed disentangled from the rest of the system, consistent with our result obtained from ODLRO.

Vedral studied entanglement in a Bose condensate, using a state similar to equation (14), and calculated a different quantity defined there to measure the amount of entanglement [27].

We now focus on the particle number conserving version of the Bogoliubov theory, which gives the ground state as [54]

$$|\Psi(N)\rangle \propto \left(a_0^{\dagger} a_0^{\dagger} - \sum_{|\mathbf{q}|\neq 0} c_{\mathbf{q}} a^{\dagger}_{\mathbf{q}} a^{\dagger}_{-\mathbf{q}}\right)^{N/2} |0\rangle \tag{15}$$

where $c_{\mathbf{q}}$, with $|c_{\mathbf{q}}| < 1$, is determined by the Hamiltonian and is the effect of the weak interaction. It can be found that

$$\begin{aligned} |\Psi(N)\rangle \propto & \sum_{n_0, n_1, \ldots, n_\infty} p(N/2; n_0, \ldots, n_\infty) \left(-c_{\mathbf{q}_1}\right)^{n_1} \cdots \\ & \times \left(-c_{\mathbf{q}_\infty}\right)^{n_\infty} |2n_0\rangle_0 |n_1\rangle_{\mathbf{q}_1} |n_1\rangle_{-\mathbf{q}_1} \cdots |n_\infty\rangle_{\mathbf{q}_\infty} |n_\infty\rangle_{-\mathbf{q}_\infty} \end{aligned} \tag{16}$$

where $n_0 + n_1 + \cdots + n_\infty = N/2$, $p(N/2; n_0, \ldots, n_\infty) = \frac{(N/2)!}{n_0! n_1! \cdots n_\infty!}$ is the number of partitions of $N/2$ objects into different boxes, with n_0 objects in the box labelled 0, n_1 objects in the box labelled 1, and so on. Then one obtains the Fock-space reduced density matrices of different momentum states. The non-vanishing elements of $\rho_1(0)$ are

$$x_{2n_0}(0) \equiv \langle 2n_0|\rho_1(0)|2n_0\rangle = A \sum_{n_1, \ldots, n_\infty} p^2(N/2 - n_0; n_1, \ldots, n_\infty) \left|c_{\mathbf{q}_1}\right|^{2n_1} \cdots \left|c_{\mathbf{q}_\infty}\right|^{2n_\infty} \tag{17}$$

where $n_1 + \cdots + n_\infty = N/2 - n_0$, the normalization factor $A = \left[\sum_{n_0, \ldots, n_\infty} p^2(N/2; n_0, \ldots, n_\infty) \left|c_{\mathbf{q}_1}\right|^{2n_1} \cdots \left|c_{\mathbf{q}_\infty}\right|^{2n_\infty}\right]^{-1}$, with $n_0 + n_1 + \cdots + n_\infty = N/2$. It can be seen that

$$x_{2n_0}(0) \approx \frac{\left|\sum_{|\mathbf{q}|\neq 0} c_{\mathbf{q}}\right|^{N-2n_0}}{\sum_{n_0=0}^{N/2} \left|\sum_{|\mathbf{q}|\neq 0} c_{\mathbf{q}}\right|^{N-2n_0}} \tag{18}$$

under the assumption that $\sum c^*_{\mathbf{q}_1} c_{\mathbf{q}_2} \approx 0$, where the summation is over all nonzero $\mathbf{q}_1 \neq \mathbf{q}_2$.

The entanglement between the zero momentum state and the rest of the system is

$$S(0) = -\sum_{n_0=0}^{N/2} x_{2n_0}(0) \ln x_{2n_0}(0). \tag{19}$$

For momentum $\mathbf{q}_1 \neq 0$, the non-vanishing elements of $\rho_1(\mathbf{q}_1)$ are

$$x_{n_1}(\mathbf{q}_1) \equiv \langle n_1|\rho_1(\mathbf{q}_1)|n_1\rangle = A\left|c_{\mathbf{q}_1}\right|^{2n_1} \sum_{n_0,n_2,\ldots,n_\infty} p^2(N/2; n_0, \ldots, n_\infty)\left|c_{\mathbf{q}_1}\right|^{2n_2} \cdots \left|c_{\mathbf{q}_\infty}\right|^{2n_\infty} \tag{20}$$

where the summation is subject to $n_0 + n_2 + \cdots + n_\infty = N/2 - n_1$. It can be seen that

$$\begin{aligned} x_{n_1}(\mathbf{q}_1) &\approx \frac{\left|c_{\mathbf{q}_1}\right|^{2n_1} \sum_{n_0=0}^{N/2-n_1} \left|\sum_{|\mathbf{q}|\neq 0,\mathbf{q}_1} c_{\mathbf{q}}\right|^{N-2n_0-2n_1}}{\sum_{n_1=0}^{N/2} \left|c_{\mathbf{q}_1}\right|^{2n_1} \sum_{n_0=0}^{N/2-n_1} \left|\sum_{|\mathbf{q}|\neq 0,\mathbf{q}_1} c_{\mathbf{q}}\right|^{N-2n_0-2n_1}} \\ &= \frac{\left|c_{\mathbf{q}_1}\right|^{2n_1} - \left(\frac{|c_{\mathbf{q}_1}|}{|\sum_{|\mathbf{q}|\neq 0,\mathbf{q}_1} c_{\mathbf{q}}|}\right)^{2n_1} \left|\sum_{|\mathbf{q}|\neq 0,\mathbf{q}_1} c_{\mathbf{q}}\right|^{N+1}}{\sum_{n_1=0}^{N/2} \left[\left|c_{\mathbf{q}_1}\right|^{2n_1} - \left(\frac{|c_{\mathbf{q}_1}|}{|\sum_{|\mathbf{q}|\neq 0,\mathbf{q}_1} c_{\mathbf{q}}|}\right)^{2n_1} \left|\sum_{|\mathbf{q}|\neq 0,\mathbf{q}_1} c_{\mathbf{q}}\right|^{N+1}\right]}. \end{aligned} \tag{21}$$

The entanglement between a nonzero momentum state $\mathbf{q}_1$ and the rest of the system is

$$S(\mathbf{q}_1) = -\sum_{n_1=0}^{N/2} x_{n_1}(\mathbf{q}_1) \ln x_{n_1}(\mathbf{q}_1). \tag{22}$$

Obviously, the entanglement between $-\mathbf{q}_1$ and the rest of the system, and the entanglement between the pair $\mathbf{q}_1$ plus $-\mathbf{q}_1$ and the rest of the system are both also $S(\mathbf{q}_1)$. It can also be seen that there is no entanglement between $\mathbf{q}_1$ and $-\mathbf{q}_1$. On this aspect, there is a similarity with BCS superconductivity.

Consider the identity $\sum_{n_{\mathbf{q}}} n_{\mathbf{q}}\langle n_{\mathbf{q}}|\rho_1(\mathbf{q})|n_{\mathbf{q}}\rangle = \sum'_{\{n_i\}} n_{\mathbf{q}}\langle n_0 \cdots n_\infty|\rho|n_0 \cdots n_\infty\rangle = \langle \hat{n}_{\mathbf{q}}\rangle$, for $n_{\mathbf{q}} = 0, 1, \ldots$, and for different $\mathbf{q}$, where $\sum'_{\{n_i\}}$ represents summations over $n_0, \ldots, n_\infty$, except $n_{\mathbf{q}}$. For the Bogoliubov ground state $|\Psi(N)\rangle$, it is known that $\langle \hat{n}_0\rangle$ is close to N, while $\langle \hat{n}_{\mathbf{q}_1}\rangle \ll N$ for $\mathbf{q}_1 \neq 0$. It is thus constrained that only a small number (compared to N) of the Fock space matrix elements $\langle n_{\mathbf{q}}|\rho_1(\mathbf{q})|n_{\mathbf{q}}\rangle$ is considered for mode $\mathbf{q}$. Thus the entanglement is small. But it is not zero, as in the case of the Hartree approximation.

Furthermore, (18) indicates that $x_{2n_0}(0)$ exponentially decays with n_0, with a rate $1/2 \ln\left|\sum_{|\mathbf{q}|\neq 0} c_{\mathbf{q}}\right|$. Hence indeed a very small number of matrix elements $\langle n_0|\rho_1(0)|n_0\rangle$ is considered, and thus $S(0)$ is small. On the other hand, in (21), the change of $x_{n_1}(\mathbf{q}_1)$ with n_1 is slower since it involves the counteracting of two exponentially increasing terms. Consequently $S(\mathbf{q}_1) > S(0)$.

The small but nonzero entanglement is a characterization of the two-particle correlation caused by the weak interaction, which is the essence of the Bogoliubov theory [54]. This can be seen from equations (18) and (21), which indicate that the entanglement is only dependent on the function $c_{\mathbf{q}}$, which is determined by the weak interaction.

The result in this and the following sections is the entanglement in terms of the original particles. Consistent with the fact that entanglement depends on which single particle is used in representing the many-particle system, it can be shown that in the set of eigenstates of the one-particle reduced density matrix (in the case of Bose condensation) or two-particle reduced density matrix (in the case of superconductivity), the condensate mode is disentangled from the rest of the system [25].

7. Summary and remarks

It is known that quantum correlation in a system of identical particles can be characterized in terms of entanglement between occupation numbers of different single particle basis states, and thus depends on which single particle basis is chosen. Consequently, in general, occupation-number entanglement may be generated, or exists in the energy eigenstates, even in the absence of interaction of particles. Indeed, it is caused by coupling between different single particle basis states (mode–mode coupling) in the many-particle second-quantized Hamiltonian, which may exist even in the one-body term in the Hamiltonian.

However, our purpose in this paper is to use entanglement as a characterization of the effects of interaction. For this purpose, we choose the set of eigenstates of the single particle Hamiltonian as the single particle basis on which the entanglement is defined. For convenience, we call it the proper single particle basis. In this single particle basis, if there is no interaction, the second-quantized Hamiltonian is diagonal in different single particle basis states, and thus the many-particle eigenstates can always be chosen to be non-entangled.

Using the so-called proper single particle basis state, we examined entanglement in eigenstates, especially the ground states, of some important many-particle Hamiltonians. These examples demonstrate that entanglement in the proper single particle basis can indeed characterize the effect of interaction, vanishing as the interaction vanishes. Moreover, the amount of the entanglement calculated is directly related to the macroscopic physical properties. In other words, it is demonstrated that the microscopic entanglement is manifested in the macroscopic physical properties. It appears that entanglement in the proper single particle basis is useful especially for studying the strongly correlated systems, in which interactions are important.

For an interacting Fermi gas, electron–hole entanglement inevitably appears in some excited eigenstates, as described in the Hartree–Fock approach. Electron–hole entanglement can be generated by electron–light interaction, which is not included in the single particle Hamiltonian which defines the proper single particle basis.

When the ground state of a Fermi liquid is expressed in terms of the Landau quasiparticles, i.e. electrons dressed by the interaction, it becomes non-entangled.

We found a nice result that the entanglement in a quantum Hall state is just the entropy of the probability distribution f and $1-f$, where f is the proper fractional part of the filling factor of a Landau level. Hence entanglement here can be extremely precisely measured, with topological stability. This gives support to the well-known proposal to use anyons for fault-tolerant quantum computing.

We also made a detailed calculation of entanglement in the BCS ground state. Both the particle-number non-conserved and the particle-number conserved states are considered. In each case, the amount of entanglement is a function of the relative momentum wavefunction $g_{\mathbf{k}}$ of every two Cooper-paired particles, and thus directly related to the superconducting energy gap. The entanglement vanishes if and only if the superconductivity vanishes.

Finally, we turned to Bose systems. For a spinless system, the entanglement is absent in the eigenstates in the Hartree–Gross–Pitaevskii approximation. However, though small, it is non-vanishing in the Bogoliubov theory, using which we calculate the entanglement in the ground state, where there is a kind of pairing between opposite momenta. Entanglement in the proper single particle basis provides a characterization of the two-particle correlation due to interaction, which is the essence of the Bogoliubov theory.

Many-body entangled states such as those in condensed matter physics may be useful for quantum information processing. One may adiabatically control a time-dependent many-body ground state which encodes the quantum information. If there is a finite energy gap between the ground state and the excited states, as exists in many condensed matter systems, such a quantum information processing should naturally possess some robustness against environmental perturbation.

But more caution is needed in using entanglement in a condensed matter system to demonstrate the Bell theorem and the like. One reason is that in condensed matter physics, many Hamiltonians, usually instantaneous, are effective ones on a certain time scale, with many degrees of freedom renormalized. The formal entangled state and the instantaneous correlations may be meaningful only on a certain coarse-grained time scale.

For identical particles, there is intrinsic built-in non-separability because of the precondition that the spatial wavefunctions overlap, for example, spin magnetism based on exchange interaction originates in antisymmetrizing the spin–orbit states of the electrons interacting with 'instantaneous' Coulomb interaction which is always there. Deeper understanding is still needed on the occupation-number entanglement.

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