Possible condensation of Cooper triples

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We theoretically discuss the possible condensation of Cooper triples, which correspond to a three-body version of Cooper pairs, in three-component Fermi systems with three-body attractive interactions. A macroscopic number of Cooper triples can occupy a zero center-of-mass momentum state in the presence of a Fermi surface of constituent particles, even though the three-body operator exhibits anti-commutation relation associated with the Fermi–Dirac statistics. Such a condensation with internal degrees of freedom is similar to bosonization in a system of infinite-component fermions. We propose a variational wave function for condensed Cooper triples and show that in the ground state, the condensed state is energetically favored compared to the normal state. Also, we discuss effects of the Fermi-surface distortion in a lattice system described by a three-component Hubbard model.

KEYWORDS: Cooper triple, fermionic condensates, Variational approach

1. Introduction

The Bardeen Cooper-Schrieffer (BCS) theory [1], which explains the microscopic mechanism of Cooper-pair formation and its condensation due to attractive two-body interactions between two different species, has had a major impact not only in condensed matter physics but also nuclear and particle physics. The Cooper-pair condensation has been understood as a bosonic-like condensation in which many Cooper pairs occupy a zero center-of-mass (COM) momentum state.

In recent years, the concept of Cooper pairs has been generalized to cluster states consisting of three or more particles, such as Cooper triples [2, 3] and Cooper quartets [4–6]. While these kinds of states have been widely discussed in nuclear and condensed matter systems, ultracold atomic gases may provide a promising platform to investigate the existence of nontrivial Cooper multiplets. In fact, the momentum distribution of fermions forming Cooper pairs has been directly observed in a recent state-of-the-art experiment [8]. Moreover, multi-component Fermi gases can be realized by using different hyperfine states of ultracold atoms (e.g., ⁶Li [10], ¹⁷³Yb [11]). The long-range order in a multi-component attractive Hubbard model has also been discussed theoretically [12, 13]. The realization of a three-body interaction, which is deeply related to the formation of Cooper triples, has also been proposed in cold atomic systems [3, 7, 14, 15]. The three-body condensation has also been predicted in non-equilibrium bosonic systems [17].

In this paper, as a consequence of the formation of a macroscopic number of Cooper triples, we show that Cooper triples may condense at zero COM momentum in a three-component Fermi system by utilizing internal degrees of freedom such as relative momenta among constituent particles (see Fig. 1). For convenience, we schematically compare this nontrivial condensation with the conventional quantum degenerate states of point-like fermions/bosons and Cooper pairs. As in the case of Cooper pairs with nonzero relative momentum between two fermions (in contrast to tightly bound dimers), Cooper triples are regarded as loosely bound three-body states where constituent fermions possess nonzero momenta being close to the Fermi momentum. In the following, we call the con-
Einstein condensation (a), the Fermi degeneracy (b), the Cooper pairs’ condensation (c), and the Cooper triples’ condensation (d). Diff Fig. 1. Schematic diagrams of the occupation of particles and bound states at zero temperature for the Bose–Einstein condensation (a), the Fermi degeneracy (b), the Cooper pairs’ condensation (c), and the Cooper triples’ condensation (d). Different colors represent different components. (e) The in-plane configuration of the three fermions near the Fermi surface (FS) with zero COM momentum as the three-body scattering occurs only in the vicinity of the FS at sufficiently low temperatures and weak interactions, as described by the Hamiltonian

\[
\hat{H} = \sum_{\gamma=r,g,b} \sum_{k} \xi_{k} \hat{n}_{k,\gamma} + \sum_{k,\hat{R}} \sum_{k',\hat{R}'} U_{k,k'} \hat{F}_{k',\hat{R}'}^{\dagger} \hat{F}_{k,\hat{R}}
\]

Here, \(\xi_{k}\) is the kinetic energy of a fermion with the lattice momentum \(k = (k_x, k_y)\). While the kinetic energy in a gas system is given by the parabolic dispersion \(\xi_{k}^{\text{gas}} = k^2/(2m) - \mu\) (where \(\mu\) is the chemical potential), it is given by \(\xi_{k} = -2t \cos k_x - 2t \cos k_y - \mu\) in the two-dimensional square lattice where \(t\) is the hopping parameter and the lattice constant is taken to be unity. However, the low-momentum expansion of \(\xi_{k}\) reproduces the parabolic dispersion as \(\xi_{k} = tk^2 - \mu + O(k^4)\) where the constant energy shift is omitted. First, for simplicity, we consider the low-filling case where the FS can be assumed to be isotropic in the following (effects of FS anisotropy will be discussed in the next section). \(\hat{n}_{k,\gamma} = \hat{c}_{k,\gamma}^{\dagger} \hat{c}_{k,\gamma}\) is the single-particle number operator with the annihilation (creation) operator \(\hat{c}_{k,\gamma}^{(\dagger)}\) for fermions of hyperfine state \(\gamma = r, g, b\). In this paper, we consider the equally-populated three-component mixture in the thermodynamic limit.

The second term in Eq. (1) denotes the three-body interaction with a contact-type coupling constant \(U_{k,k'} (< 0)\). \(\hat{F}_{k,\hat{R}}^{(\dagger)}\) is the three-body annihilation (creation) operator defined in terms of \(\hat{c}_{k,\gamma}\) as

\[
\hat{F}_{k,\hat{R}}^{\dagger} = \hat{c}_{k,r}^{\dagger} \hat{c}_{k,g}^{\dagger} \hat{c}_{k,b}^{\dagger}, \quad \hat{F}_{k,\hat{R}} = \hat{c}_{k,r} \hat{c}_{k,g} \hat{c}_{k,b}.
\]
\( \hat{R} \) is the 2\( \pi/3 \)-rotation operator acting on the lattice momentum in the COM frame. For each of the three fermions near the FS, the absolute value of the momentum \(|k|, |\hat{R}k|, \) and \( |\hat{R}^2 k| \) are close to the Fermi momentum \( k_F \), while the COM momentum remains zero (i.e., \( k + \hat{R}k + \hat{R}^2 k = 0 \)). \( k, \hat{R}k, \) and \( \hat{R}^2 k \) are on the same plane with \( 2\pi/3 \) and \( 4\pi/3 \) rotations in the momentum space as shown in Fig. 1. Therefore, by fixing \( k \) and the rotational axis, the remaining two momenta, \( \hat{R}k \) and \( \hat{R}^2 k \), are automatically determined. \( \hat{F}^{(r)}_{k,\hat{R}} \) satisfies the following anti-commutation relations

\[
\begin{align*}
\{ \hat{F}_{k,\hat{R}}, \hat{F}_{k',\hat{R}} \} &= \{ \hat{F}^\dagger_{k,\hat{R}}, \hat{F}^\dagger_{k',\hat{R}} \} = 0, \\
\{ \hat{F}_{k,\hat{R}}, \hat{F}^\dagger_{k',\hat{R}} \} &= \delta_{k,k'} \delta_{\hat{R}k,\hat{R}k'} \delta_{\hat{R}^2 k,\hat{R}^2 k'} \left[ (\hat{\imath} - \hat{n}_{k,\hat{R}})(\hat{\imath} - \hat{n}_{\hat{R}k,\hat{R}}) + \hat{n}_{k,\hat{R}} \hat{n}_{\hat{R}k,\hat{R}}, \hat{n}_{\hat{R}^2 k,\hat{R}} \right].
\end{align*}
\]

In particular, from the anti-commutation relation associated with \( \hat{c}^\dagger_{k,\gamma} \), one finds

\[
\hat{F}^\dagger_{k,\hat{R}} \hat{F}_{k',\hat{R}} |0\rangle \neq 0 \quad (k \neq k', \hat{R}k \neq \hat{R}'k', \hat{R}^2 k \neq \hat{R}^2 k'),
\]

where \(|0\rangle\) is the normalized vacuum state. Eq. (5) indicates that two-body states with zero COM momentum can coexist as long as the momenta of a certain component are different. Since there are an infinite number of ways to take \( k \), one can find a macroscopic number of TPTC in the presence of FS. Thus, even though the Cooper triples obey the Fermi–Dirac statistics, these three-body states can macroscopically occupy a zero COM momentum state and form the condensate. We recall that the relative momenta of constituent fermions plays a key role in the condensation of Cooper triples as shown in Fig. 1. Such internal degrees of freedom also exist in usual Cooper pairs and makes a difference between Cooper pairs and tightly bound dimers in terms of the spatial structure of wave functions [18].

Using the variational wave function inspired by the BCS theory [7], we show that the condensed state of Cooper triples are favored over the normal phase. We consider the variational wave function

\[
|\Psi_T\rangle = \prod_k (u_k + v_k \hat{F}_{k,\hat{R}_0}^\dagger) |0\rangle,
\]

where \( u_k \) and \( v_k \) are variational parameters satisfying the normalization condition \( |u_k|^2 + |v_k|^2 = 1 \) (associated with \( \langle \Psi_T|\Psi_T \rangle = 1 \)). We note that the state (6) breaks the \( U(1) \) gauge symmetry via the superposition of the Cooper triples. Here, we set \( \hat{R}_0 \) such that if the momentum \( k \) of a fermion with \( \gamma = r \) is in the direction of \( e_1 = (0,0)^T \), then the momentum \( \hat{R}_0 k \) (\( \gamma = g \)) parallels \( e_2 = (-\sqrt{3}/2, -1/2)^T \) and the remaining one \( \hat{R}_0^2 k \) (\( \gamma = b \)) parallels \( e_3 = (\sqrt{3}/2, -1/2)^T \). For other \( k \)'s, \( k, \hat{R}_0 k, \) and \( \hat{R}_0^2 k \) are oriented in the direction of \( \{Ve_1, Ve_2, Ve_3\} \), respectively, with an appropriate rotation matrix \( V \). In this sense, although this choice of \( \hat{R}_0 \) leads to a specific orientation in momentum space, Eq. (6) can have any momenta of each component picked up once in the infinite product of \( k \). This fact is also important for reproducing the normal Fermi degenerate state \( |FS\rangle = \prod_{|k| \leq k_F} \hat{c}^\dagger_{k,\gamma} |0\rangle \) within the variational space of Eq. (6). Note that one can consider a different \( \hat{R}_0 \) by considering different momentum plane. The resultant state is degenerate with the original state. Such degeneracy is similar to the case of different gauge orientations, and the variational parameters can be regarded as independent of the choice of \( \hat{R}_0 \) as well as the gauge. In the BCS state, only \( k \) determines the relative momentum of a Cooper pair, but in the present state, not only \( k \) but also \( \hat{R}_0 \) characterizes the relative momentum between two of three fermions forming a Cooper triple.

Using Eq. (6), we evaluate the ground-state energy \( E_0 = \langle \Psi_T | \hat{H} | \Psi_T \rangle \) as

\[
E_0 = \sum_k 3\xi_k |v_k|^2 + \sum_k \sum_{k'} U_{k,k'} v_k^* v_{k'} u_{k'} u_k.
\]
The minimization of $E_0$ with respect to the variational parameters leads to $u_k = \frac{1}{\sqrt{2}} \left(1 + \frac{\xi_k}{\sqrt{\xi_k + \Delta}}\right)^{1/2}$, $v_k = \frac{1}{\sqrt{2}} \left(1 - \frac{\xi_k}{\sqrt{\xi_k + \Delta}}\right)^{1/2}$, where $\Delta_k \equiv -\frac{2}{3} \sum_{k'} U_{k,k'} u_k v_{k'}$ is the order parameter characterizing the Cooper triple condensation. $\Delta_k$ can also be expressed as

$$\Delta_k = -\frac{2}{3} \sum_{k'} U_{k,k'} \langle \hat{c}_{k',\sigma}^\dagger \hat{c}_{k,\sigma}^\dagger \hat{c}_{k,\bar{\sigma}}^\dagger \hat{c}_{k',\bar{\sigma}} \rangle,$$

which breaks the global U(1) symmetry. $\Delta_k$ is the expectation value of fermionic (Grassmann odd) operators, which is in contrast to the BCS ground state. We note that the nonzero expectation value of the Grassmann-odd operators $\langle \hat{c}_{k',\sigma}^\dagger \hat{c}_{k,\sigma}^\dagger \hat{c}_{k,\bar{\sigma}}^\dagger \hat{c}_{k',\bar{\sigma}} \rangle \equiv \langle \Psi_T | \hat{c}_{k',\sigma}^\dagger \hat{c}_{k,\sigma}^\dagger \hat{c}_{k,\bar{\sigma}}^\dagger \hat{c}_{k',\bar{\sigma}} | \Psi_T \rangle$ can be realized due to the Grassmann-odd feature of $|\Psi_T\rangle$ as well as the anti-commutation relation of $\hat{F}_{k,\tilde{k}}$ with additional internal degrees of freedom given by Eq. (4). From Eq. (7), we obtain

$$E_0 = \frac{3}{2} \sum_k \xi_k \left(1 - \frac{\xi_k}{\sqrt{\xi_k + \Delta}}\right) + \frac{1}{4} \sum_k \sum_{k'} U_{k,k'} \frac{\Delta_k}{\sqrt{\xi_k + \Delta}} - \frac{\Delta_{k'}}{\sqrt{\xi_k + \Delta}}.$$

To proceed further, we consider the simplified coupling

$$U_{k,k'} = -U_0 \theta(\Lambda - |\xi_k|) \theta(\Lambda - |\xi_{k'}|),$$

where $U_0$ is the positive constant and $\Lambda$ is an energy cutoff so that the interaction acts only on the three fermions with momentum close to the FS. $\Lambda$ corresponds to the Debye frequency of conventional BCS superconductors with phonon-mediated interactions. Note that $U_0$ and $\Lambda$ in the case of fermion-mediated interaction associated with an additional fermionic bath is discussed in Ref. [7]. Substituting Eq. (10) to Eq. (8), we obtain $\Delta_k = \Delta \theta(\Lambda - |\xi_k|)$, where $\Delta$ is the amplitude of the order parameter. In the weak coupling limit ($\Delta \ll \Lambda$ and $\mu = E_F$), as in BCS theory, $\Delta$ can be obtained analytically as

$$\Delta \approx 2 \Lambda \exp \left(-\frac{3}{2 \rho(0) U_0}\right),$$

where $\rho(\omega) = \sum_k \delta(\omega - \xi_k)$ is the density of states as a function of the single-particle energy $\omega$. We used

$$\Delta = \frac{2}{3} U_0 \sum_{|\xi_k| < \Lambda} \frac{\Delta}{2 \sqrt{\xi_k + \Delta^2}} \rightarrow 1 = \frac{2}{3} U_0 \rho(0) \int_{-\Lambda}^{\Lambda} \frac{d\xi_k}{2 \sqrt{\xi_k + \Delta^2}} \approx \frac{2}{3} U_0 \rho(0) \ln \left(\frac{2\Lambda}{\Delta}\right).$$

From Eqs. (9) and (10), the ground-state energy can be expressed as

$$E_0 \approx E_0^{FS} + \frac{3}{2} \sum_{|\xi_k| < \Lambda} \frac{\xi_k}{\sqrt{\xi_k + \Delta^2}} - \frac{9 \Delta^2}{4 U_0},$$

where we divide the summation in Eq. (9) as $\sum_k = \sum_{|\xi_k| > \Lambda} + \sum_{|\xi_k| < \Lambda}$. The summation $\sum_{|\xi_k| > \Lambda}$ contributes only to the noninteracting Fermi-gas energy $E_0^{FS}$ because of $U_{k,k'} = 0$ there. On the other hand, the summation $\sum_{|\xi_k| < \Lambda}$ is responsible for the effect of interaction near the FS. The difference between the ground-state energies of the Cooper triple condensed state and the normal Fermi degenerate state is given by

$$E_0 - E_0^{FS} \approx -3 \rho(0) \Lambda^2 \exp \left(-\frac{3}{\rho(0) U_0}\right) < 0$$

Thus, whenever $U_0$ is nonzero, the ground-state energy of the Cooper triple condensed state is lower than the ground-state energy of the normal Fermi gas. Eq. (14) can also be regarded as the condensation energy of the Cooper triple, as in the BCS ground-state with the condensation of Cooper pairs [1].
Fig. 2. Probability $P$ for the realization of TPTC as a function of $E_F/t$. In this plot, $\Lambda/t = 0.04$ is used. In the right side, the flow chart for the evaluation of $P$ is presented (see also Eq. (16)).

We briefly note that our variational method does not necessarily describe an exact ground state as is the case with the usual BCS variational method for superconductors. Indeed, there would be a way to improve the ansatz by enlarging the variational-parameter space. Nevertheless, our result suggests the macroscopic occupation of Cooper triples at zero center-of-mass momentum (i.e., $F^+_{k\hat{R}}, F^+_{k'\hat{R}}, F^+_{k''\hat{R}}, \cdots |0\rangle$) can be possible in the present system. A similar discussion associated with the validity of the quartet BCS theory by comparison with the quartet condensation model in finite nuclei has been made in Ref. [5].

3. Discussion: Effects of the Fermi-surface anisotropy in the lattice model

While we have examined the possibility of Cooper-triple condensation in the low-filling case where the FS anisotropy is negligible, such a deformation would be important for TPTC in the high-density regime. The FS anisotropy originates from higher-order derivative terms of $\xi_k$ as

$$\xi_k = tk^2 - \frac{t}{12}(k_x^4 + k_y^4) - \mu + O(k^6),$$

for the two-dimensional square lattice. For convenience, we define the isotropic Fermi energy as $E_F \equiv \mu = tk_F^2$ (note that this is correct only in the low-filling limit) as in the previous section and discuss effects of the second term in Eq. (15). To see how TPTC ansatz can be justified even in the presence of the FS anisotropy, we evaluate the momentum configuration of three particles by defining

$$P = \frac{C}{N} \equiv \frac{\sum_k \theta(\Lambda - |\xi_k|)\theta(\Lambda - |\xi_{k\hat{R}}|)\theta(\Lambda - |\xi_{k\hat{R}^2}|)}{\sum_k \theta(\Lambda - |\xi_k|)},$$

where $C$ (numerator) corresponds to the momentum space of TPTC within the Debye-frequency-like energy shell (i.e., $E_F \pm \Lambda$) for the three-body interaction and $N = \sum_k \theta(\Lambda - |\xi_k|)$ (denominator) is the configuration number where at least one fermion with $\gamma = r$ is inside of that energy shell. In this regard, a large $P$ indicates that TPTC frequently appears in the momentum space. We have summarized the flow chart for evaluating $P$ by using the Monte Carlo sampling with respect to the momentum integration in Fig. 2. The left panel of Fig. 2 shows $P$ as a function of $E_F/t$ ($\equiv \mu/t$) in Eq. (15), where $\Lambda/t = 0.04$ is employed. We find that TPTC are formed frequently in the region where $E_F/t$ is sufficiently small, namely, in the low-filling regime. With increasing $E_F/t$, $P$ decreases exponentially, but fluctuation effects will take over. One may expect the formation of Cooper triples or in-medium trimer states due to the interactions or cluster hopping even in the higher-filling case [19, 20]. While the reduction of $P$ in the higher-filling region does not immediately suppress the possibility
of condensed Cooper triples, one should seriously examine such a fluctuation effect beyond the BCS-like state discussed in the previous section.

4. Conclusion

We have discussed the condensation of Cooper triples in three-component fermionic systems by using a variational method based on the analogue of the BCS theory. We have found that Cooper triples can macroscopically occupy the zero COM momentum state and form the condensate. In such a nontrivial condensation, the internal degrees of freedom associated with constituent fermions in Cooper triples (i.e., relative momenta) play a crucial role in forming the condensate without conflicting with Pauli-exclusion principle. We have also discussed effects of the FS anisotropy in the two-dimensional Hubbard model. While TPTC (characterizing the configuration of condensed Cooper triples) within the interaction energy shell can frequently appear in the low-filling regime, other kinds of configurations accompanied by fluctuations are expected to be dominant in the higher-filling case.

While we consider the two-dimensional system, it is an interesting topic to see whether the Mermin–Wagner–Hohenberg theorem [21, 22] holds or not in such an exotic Fermi condensation. Also, it is worth considering the nature of excited Cooper triples, the formation of Cooper triples when two- and three-body interactions coexist, to consider other lattices, such as honeycomb lattices [23], and application of our approach to dense quark matter [24, 25].

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