Heteronuclear Cooper Pairs in An Ultracold Atomic Gas

Yongle Yu,*

Mathematical Physics, Lund Institute of Technology, SE 221 00 LUND, Sweden
*To whom correspondence should be addressed; E-mail: yongle.yu@matfys.lth.se.

In an ultracold mixture of two different Fermi species of atoms, Cooper pairs can be formed between two different atoms. The masses of one atom and its partner in this kind of Cooper pairs may differ by order of magnitude. In this system, each species of atoms are in the same atomic spin state and two species have the same atomic densities. The pairing gap diminishes if two species have different densities and vanishes when the density imbalance reaches a critical value.

Ultracold atomic gases offer an unprecedented opportunity to study many body physics with short range interaction in the sense that atomic species, density, interaction strength and trapping potential can be altered. Following the achievement of Bose-Einstein Condensation in a Bose gas of atoms, experimenters made rapid progress in manipulating an ultracold degenerate Fermi gas of atoms [7] and observed a superfluid and condensate phase [2, 3, 4, 5, 6, 7, 12] when fermionic atoms interact near Feshbach resonance. Below Feshbach resonance ($a < 0$, $a$ is the $s$-wave scattering length), Cooper pairs are formed due to the many body effect while the two body interaction is strong enough to generate weakly bound molecules (dimers) above Feshbach resonance ($a > 0$). Being of bosonic nature, Cooper pairs and dimers alter
the quantum statistics of the system and modified behaviours of the system fundamentally near zero temperature. By tuning the interaction strength, experiments (8, 9, 10, 11, 13, 12) began to explore BCS-BEC crossover, which is of great theoretical interest for decades (12, 15, 16, 17). Some theoretical treatments of pairing and BCS-BEC crossover in a Fermi gas of atoms can be found in (18, 19, 20, 21, 22, 23, 24, 25, 26).

In all systems, Cooper pairs which have been studied till now are symmetrical pairs in the sense that two partners in a pair are of the same species and may differ only by the projection of spin or pseudospin. In nuclear physics, Cooper pairs composed of a neutron and a proton is considered. However, neutrons and protons can be considered as one species, the nucleons due to well known isospin invariance of nuclear interaction. In this paper, we point out Cooper pairs composed of two different species of atoms can occur in an ultracold gas. The masses of two partners in such unconventional Cooper pairs may differ by order of magnitude (for example, Cooper pairs formed by $^6\text{Li}$ atoms and $^{40}\text{K}$ atoms).

We consider a mixture of two different species of fermionic atoms, denote one species by $A$, the other by $B$ and their atomic masses by $m_A$ and $m_B$, respectively. All atoms of species $A$ are set to be in the same atomic hyperfine state, for example, the lowest Zeeman spin state in a presence of magnetic field, so are the atoms of species $B$. Preparing one species of polarized atoms is not a problem, see (27) for example. The intraspecific interaction in the mixture can be neglected for the following reason. The average interatomic distance is orders of magnitude larger than the interaction range in this dilute system and the interaction is well approximated by a zero-range model. Pauli principle prevents two atoms of the same species and of the same spin state from approaching each other and therefore they hardly interact. Mathematically, it is easy to show that the matrix elements of a zero-range interaction vanish in a basis of many body states with polarized spins, $\langle \psi_j (r_1, r_2, ...) \mid g \delta(r_1 - r_2) \mid \psi_j (r_1, r_2, ...) \rangle = 0$ ( $g$ is the interaction strength). The wavefunctions are antisymmetric under exchange of $r_1$ and $r_2$, which
leads to $\psi_{j1}(r_1, r_1, ...) = -\psi_{j1}(r_1, r_1, ...) = 0$ and $\psi_{j2}(r_1, r_1, ...) = -\psi_{j2}(r_1, r_1, ...) = 0$.

The dominating interaction in the system is the interspecific scattering $V_{AB}(r) = \frac{2\pi h^2 a_{AB}}{m_{AB}} \delta(r)$, where $a_{AB}$ is the s-wave scattering length between two species of atoms and $m_{AB}$ is the reduced mass, $m_{AB} = \frac{m_A m_B}{m_A + m_B}$. A weak attractive interspecific scattering ($a_{AB} < 0$) can cause Cooper instability of normal phase and lower the energy of the system by forming pair correlations between two species of atoms. Note the interatomic force doesn’t influence the atomic spins at this low energy regime. To illustrate condition for Cooper pairing and to study the equation for the pairing gap, let us consider a BCS wave function of the system. For simplicity we only consider a homogeneous system,

$$
| \psi_{BCS} \rangle = \Pi_k (u_k + v_k a_k^\dagger b_k^\dagger) | \text{vac.} \rangle
$$

Where $a_k^\dagger$ and $b_k^\dagger$ are creation operators for atoms of species A and atoms of species B, respectively. Normalization of this wavefunction requires,

$$
| u_k |^2 + | v_k |^2 = 1
$$

$| v_k |^2$ is the occupation probability of state $k$ by the atoms of species A.

Cooper pairs have zero momentum, which implies $h \mathbf{k} + h \mathbf{k} = 0$ and $\mathbf{k} = -\mathbf{k}$. Two species have the same particle density distribution in the momentum space ($| v_k |^2 = | v_{-k} |^2$, as we will see it later) and thus the same densities ($n_A = n_B$). This density relationship is a condition for Cooper pairing and enables a complete pairing correlation between two species of atoms. It is remarkable that two species share the same Fermi momentum rather than the same Fermi energy, which can be easily derived from the density relationship.

A ’ground state’ in normal phase corresponds to a sharp particle distribution near the Fermi surface,

$$
\begin{align*}
\begin{cases}
| u_k |^2 = 1 & k < k_F \\
| u_k |^2 = 0 & k > k_F
\end{cases}
\end{align*}
$$
With $k_F$ is the Fermi wave number, $k_F = (6\pi^2 n_A)^{1/3}$. A superfluid ground state with a smooth particle distribution near the Fermi surface can further lower the energy of the system.

The equation for the gap at zero temperature can be derived using variational principle, similar to what is done in the case of a system with symmetrical Cooper pairs. The Hamiltonian with pairing interaction is written as,

$$H = \sum_k (\epsilon^A_k a_k^\dagger a_k + \epsilon^B_k b_k^\dagger b_k) + \sum_{kl} V_{kl} a_k^\dagger b_{-k} b_{-l} a_l$$

(3)

Where $\epsilon^A_k$ and $\epsilon^B_k$ are the single particle energies in the normal phase, $\epsilon^A_k = \frac{\hbar^2 k^2}{2m_A}$ and $\epsilon^B_k = \frac{\hbar^2 k^2}{2m_B}$ (precisely, there is a mean field shift in $\epsilon^A_k$ and $\epsilon^B_k$. The shift can be neglected in discussion of the equation for the gap).

Since a BCS state is not an eigenstate of particle number operators, restrictions on the average number of particles are imposed,

$$\bar{N}_A \equiv \langle \psi_{BCS} | \sum_k a_k^\dagger a_k | \psi_{BCS} \rangle = N$$

(4)

$$\bar{N}_B \equiv \langle \psi_{BCS} | \sum_k b_k^\dagger b_k | \psi_{BCS} \rangle = N$$

(5)

where $N$ is the number of atoms of each species ($N = N_A = N_B$).

To minimize the ground state energy $E \equiv \langle \psi_{BCS} | H | \psi_{BCS} \rangle$ subject to Eqs.(4, 5), chemical potentials are introduced as Lagrange parameters in finding the absolute minimum of

$$W \equiv E - \mu_A \bar{N}_A - \mu_B \bar{N}_B = \langle \psi_{BCS} | H - \mu_A \sum_k a_k^\dagger a_k - \mu_B \sum_k b_k^\dagger b_k | \psi_{BCS} \rangle$$

(6)

where $\mu_A$ and $\mu_B$ are chemical potentials for atoms of species A and species B, respectively.

Combining Eqs.(1, 2, 3) and (6), and taking $u_k$, $v_k$ to be real and $u_k$ non negative for simplicity, we have,

$$W = 2\xi_k \sum_k v_k^2 + \sum_{kl} V_{kl} \sqrt{1 - v_k^2} \sqrt{1 - v_l^2} v_k$$

(7)
with $\xi_k = \frac{1}{2} (\epsilon^A_k + \epsilon^B_k - \mu_A - \mu_B) = \frac{\hbar^2 (k^2 - k_F^2)}{2m_{AB}} \left( \mu_A \approx \frac{\hbar^2 k_F^2}{2m_A}, \mu_B \approx \frac{\hbar^2 k_F^2}{2m_B} \right)$. 

$\frac{\delta W}{\delta \nu_k} = 0$, which lead to the following equation for the gap,

$$\Delta_k = -\frac{1}{2} \sum_l V_{kl} \frac{\Delta_l}{E_l}$$

(8)

Where $\Delta_k$ is gap parameter, 

$$\Delta_k = -\sum_l V_{kl} u_l v_l$$

(9)

and 

$$E_k = \sqrt{\xi^2_k + \Delta^2_k}$$

(10)

In terms of $\Delta_k$ and $E_k$, the fractional occupation number $v^2_k$ is given by,

$$v^2_k = \frac{1}{2} (1 - \frac{\xi_k}{E_k})$$

(11)

As the Fourier transfer of $V_{AB}(r)$, the pairing interaction is,

$$V_{kl} = \frac{2\pi \hbar^2 a_{AB}}{m_{AB}}$$

(12)

With Eqs. (8) and (12), Gap parameter then is a constant function of $k$ ($\Delta_k = \Delta$. Physically, for a short range interaction, $V_{kl}$ is approximately a constant function of $k$ and $l$ when $\hbar k, \hbar l$ lie in the pairing space near Fermi surface). Given $V_{kl}$ is a constant for any $k$ and $l$, however, the sum over the spectrum in the right side of Eq.(8) formally diverges. This issue can be handled either by imposing a cutoff on the spectrum or by taking a renormalization approach. Since there is no physical reason for introducing an energy cutoff for this system, we take a natural regularization scheme (29,30) to remove the divergence. Using a formula derived in (29) with some replacements, we have the following equation for the gap,

$$\frac{1}{k_F} \int_0^{k_c} dk \frac{\hbar^2 k^2}{\sqrt{\hbar^4 (k^2 - k_F^2)^2 + 4m^2 \Delta^2}}$$

$$= \frac{\pi}{2k_F |a_{AB}|} \left[ 1 + \frac{2k_c |a_{AB}|}{\pi} - \frac{k_F |a_{AB}|}{\pi} \ln \frac{k_c + k_F}{k_c - k_F} \right],$$

(13)
Where \( k_c \) is the cutoff on wave number. \( \Delta \) is essentially independent of \( k_c \) when \( k_c \) is big enough. We numerically computed \( \Delta \) as a function of \( k_F|a_{AB}| \) and plotted it in the Fig. (1).

In atomic gas, the interaction can be tuned. Observations of heteronuclear Feshbach resonance in a mixture of bosons and fermions were reported recently in (32,31). For the system we considered above, The phenomenon of BCS-BEC crossover can be explored if Feshbach resonance between two species is found. Dimers composed of an one atom of species \( A \) and one atom of species \( B \) are formed in the BEC regime.

In the BCS regime, a naturally raised question is what is the case if \( n_A \neq n_B \)? Take for example \( N_A > N_B \), some atoms of species \( A \) are not paired. The unpaired atoms occupy some states near the Fermi surface and the availability of the states for pair scattering is reduced, consequently the pairing gap diminishes. As a monotonic decreasing function of density imbalance \( \chi = |\frac{n_A-n_B}{n_A+n_B}| \), the pairing gap vanishes when \( \chi \) reaches a critical value. Such a density imbalance induced phase transition (for at least one species of atoms) can be studied in an atomic gas and shall enhance our understanding of pairing correlations.

**References and Notes**

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Figure 1: The pairing gap as a function of $k_F |a_{AB}|$, $\epsilon_F = \frac{k_F^2}{4m_{AB}}$. 