Pairing between Atoms and Molecules in Boson-Fermion Resonant Mixture

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(Dated: November 5, 2018)

We consider a mixture of fermionic and bosonic atoms nearby interspecies Feshbach resonances, which have been observed recently in $^6$Li-$^{23}$Na mixture by MIT group, and in $^{40}$K-$^{87}$Rb mixture by JILA group. We point out that the fermion-boson bound state, namely the heteronuclear molecules, will coexist with the fermionic atoms in a wide parameter region, and the attraction between fermionic atoms and molecules will lead to the formation of atom-molecule pairs. The pairing structure is studied in detail, and, in particular, we highlight the possible realization of the Fulde-Ferrel-Larkin-Ovchinnikov state in this system.

**Introduction.** In the latest few years ultracold atomic gases nearby Feshbach resonance have attracted considerable attention, since Feshbach resonance can be utilized to achieve strongly interacting quantum gases exhibiting universal properties, to produce Bose-Einstein condensation of molecules from atomic gases, and to study the physics of BEC-BCS crossover\[2, 3\]. While condensation of molecules from atomic gases\[1\], and to realize universal properties, to produce Bose-Einstein condensed gases nearby Feshbach resonance have attracted considerable attention, some materials in the past decades, and until recently some evidences of discovering this state in CeCoIn\[5\] have been reported. In the latest few years ultracold atomic gases nearby Feshbach resonance have attracted considerable attention, since Feshbach resonance can be utilized to achieve strongly interacting quantum gases exhibiting universal properties, to produce Bose-Einstein condensation of molecules from atomic gases, and to study the physics of BEC-BCS crossover\[2, 3\].

From the resonance, the properties of such a mixture has been extensively discussed before\[12\]. By introducing the operator $\hat{\Phi}$ for the b.a., and the operator $\hat{\Psi}_a$ for the f.a., this mixture can be described by

$$\hat{H}_{AM} = \alpha \int d^3r \left( \hat{\Psi}_m \hat{\Phi} \hat{\Psi}_a + \hat{\Psi}_a \hat{\Phi} \hat{\Psi}_m \right),$$

where $g_1$ is the strength of the self-interaction between b.a., $g_2$ is the strength of interaction between b.a. and f.a., and $m_1$ and $m_2$ are the masses of f.a. and b.a. respectively. Nearby the resonance, the process that converts two atoms into a heteronuclear molecule (h.m.) should be incorporated. In the spirit of the two-channel model\[10\], we introduce an independent fermionic operator $\hat{\Psi}_m$ for this molecule, and describe the resonance process as

$$\hat{H}_{AM} = \alpha \int d^3r \left( \hat{\Psi}_m \hat{\Phi} \hat{\Psi}_a + \hat{\Psi}_a \hat{\Phi} \hat{\Psi}_m \right).$$

And finally the molecules are described by

$$\hat{H}_{M} = \int d^3r \left[ \frac{\hbar^2}{2m_m} | \nabla \hat{\Psi}_m |^2 + \mu_0 \hat{\Psi}_m \hat{\Psi}_m + g_2 \hat{\Psi}_m \hat{\Psi}_m \hat{\Phi} \hat{\Phi} \right].$$

Here the mass $m_m$ of h.m., which equals $m_1 + m_2$, will be much larger than $m_1$ provided that $m_2$ is times larger than $m_1$. $g_2$ is the interaction strength between h.m. and b.a., and the molecular binding energy $\mu_0$ can be tuned by an external magnetic field. Therefore the total Hamiltonian is given by $\hat{H} = \hat{H}_A + \hat{H}_M + \hat{H}_{AM}$. Since we are mostly interested in the behavior of the fermions in a bosonic background, we consider the situation that the density of bosons $n_0$ is much larger than the density of fermions $n$, and therefore we can neglect the feedback
on bosons safely. The opposite situation where \( n \) is comparable to \( n_0 \) has been considered recently\([18]\), and the mean-field solution of the equal mixing case has also been provided\([18]\).

The mean-field solution. At nearly zero temperature, the bosonic atoms are condensed. Adopting the standard Bogoliubov approximation, we expand the operator \( \hat{\Phi} \) as \( \sqrt{n_0} + \sum_k \hat{e}^{ikr} \hat{\phi}_k \). Neglecting some constants, the Hamiltonian at the mean-field level turns out to be \( \hat{H}_0 = \sum_k \epsilon_a(k) \hat{\psi}_a^\dagger \hat{\psi}_a + \epsilon_m(k) \hat{\psi}_m^\dagger \hat{\psi}_m + \alpha \sqrt{n_0} (\hat{\psi}_a^\dagger \hat{\psi}_m + \hat{\psi}_m^\dagger \hat{\psi}_a) \), where \( \epsilon_a(k) \) denotes \( \hbar^2 k^2/(2m_a) \), and \( \epsilon_m(k) \) denotes \( \hbar^2 k^2/(2m_m) + E_b \). Here the binding energy \( \mu_0 \) is normalized to \( E_b \) by the mean-field interactions, i.e. \( E_b = \mu_0 - g_1 n_0 + g_2 n_0 \). This quadratic Hamiltonian can be easily solved, which yields

\[
\epsilon_{\pm} = \frac{1}{2} \left[ \epsilon_a(k) + \epsilon_m(k) \pm \sqrt{(\epsilon_a(k) - \epsilon_m(k))^2 + 4\alpha^2 n_0} \right],
\]

and they are shown in the insets of Fig. 1. Owing to the large mass difference, \( |\epsilon_a(k) - \epsilon_m(k)| \) is usually very large unless \( k \) is very close to \( k_c \), where \( \epsilon_a(k) \) crosses \( \epsilon_m(k) \), the dispersion relations \( \epsilon_{\pm}(k) \) thus can well be approximated by \( \epsilon_{a,m}(k) \) when \( |k - k_c| \gg 2\alpha \sqrt{m_0 m_1 m_2 h^2 k_c} \), as can be seen from the Fig. 1. For a narrow resonance, this approximation is valid in the momentum region where the atom-molecule pairs are formed.

It is noticed that the total number of fermionic atoms, including those in the scattering states and in the bound state, is conserved during the resonance process, i.e. \( \hat{\psi}_m^\dagger \hat{\psi}_m = N \), and these fermions fill the Fermi sphere with respect to \( \epsilon_a(k) \) at zero temperature. Thus we obtain the mean-field phase diagram for different \( N \) and \( E_b \), shown in Fig. 1 from which one can see that in a wide range the atoms and molecules coexist in the system. This feature, contrasting with the Feshbach resonance between the atoms of the same species, arises from the fact that both atoms and molecules in this system should obey the Pauli exclusive principle. Moreover, the Fermi surfaces difference \( \Delta k_F \), which is defined as \( k_{Fm} - k_{Fb} \), is given by \( \left( \sqrt{2m_a} (\mu - E_b) - \sqrt{2m_m} \mu \right) / \hbar \) for fixed chemical potential \( \mu \), and increases as the decrease of \( E_b \). This is of crucial importance for the discussion of atom-molecule pairing below.

**Condensate fluctuation and the attractive interactions.** We now incorporate the coupling between fermions and the condensate fluctuations illustrated in Fig. 2, which includes (a) density-density interaction between f.a. and b.a., \( g_1 \sqrt{n_0} \hat{\psi}_{a,k_1} \hat{\psi}_{a,k_2} (\hat{\psi}_{m,k_3} \hat{\psi}_{m,k_4} + \hat{\psi}_{m,k_4} \hat{\psi}_{m,k_3}) \); (b) density-density interaction between h.m. and b.a., \( g_2 \sqrt{n_0} \hat{\psi}_{m,k_1} \hat{\psi}_{m,k_2} (\hat{\psi}_{a,k_3} \hat{\psi}_{a,k_4} + \hat{\psi}_{a,k_4} \hat{\psi}_{a,k_3}) \); and (c) the Feshbach resonance, \( \alpha (\hat{\psi}_{m,k_1} \hat{\psi}_{m,k_2} + \hat{\psi}_{m,k_2} \hat{\psi}_{m,k_1}) \). Considering the second order processes that exchange bosonic fluctuations between fermions, an effective interaction between f.a. and h.m. will be induced\([19]\), which can be described by following effective Hamiltonian

\[
\hat{H}_{\text{int}} = \sum_{k_1,k_2,k} \frac{1}{4g_0} \left( \frac{\alpha^2}{2m_1} \right) \left( \hat{\psi}_{m,k_1} \hat{\psi}_{m,k_2} - \hat{\psi}_{m,k_2} \hat{\psi}_{m,k_1} \right) \hat{\psi}_{a,k_1} \hat{\psi}_{a,k_2},
\]

Given the typical values of \( g_1 \) and \( g_2 \), when the density of bosonic atoms \( n_0 \) is as large as \( 10^{10} \text{cm}^{-3} \) for the width of resonance around 1G, or when the width of the res-
onance is as narrow as 10mG for the density of bosonic atoms around $10^4$cm$^{-3}$, $2g_1g_2n_0$ will be larger than $\alpha^2$ and the interaction between atoms and molecules will be attractive. This attraction will lead to the formation of atom-molecule pairs, and consequently the superfluid order $\langle \hat{\Psi}_a \hat{\Psi}_m \rangle$.

Before proceeding, we should remark that not only the attraction between f.a. and h.m., but also the attraction between f.a. (h.m.) themselves will be induced. Indeed these terms will result in an atom (or molecule-molecule) pairing order $\langle \sum_k \hat{\Psi}_{a,k} \hat{\Psi}_{a,-k} \rangle$. However, in this work we focus on the pairing structure and superfluid properties of atom-molecule paired state because the $p$-wave pairing between atoms (molecules) is usually weak.

**Atom-molecule pairing.** The following discussion on the pairing problem is based on the effective Hamiltonian for the low-energy fermionic degrees of freedom, that is, $\hat{H}_{\text{eff}} = \hat{H}_0 + \hat{H}_{\text{int}}$. For the low-energy scattering processes where the exchanged momentum $k$ is much smaller than $\sqrt{8g_0n_0}/\hbar$, we can approximate $\hat{H}_{\text{int}}$ by $-V \sum_{k,k',m,k_2} \hat{\Psi}_{a,k} \hat{\Psi}_{a,k_1} \hat{\Psi}_{m,k_2} \hat{\Psi}_{m,k_1}$, with $V$ denoting $(2g_1g_2n_0 - \alpha^2)/(4gn_0)$. Following the idea of FF and LO[6, 7, 14], we start with a generalized BCS order parameter $\Delta_q = V \langle \sum_k \hat{\Psi}_{a,k+q} \hat{\Psi}_{m,-k+q} \rangle$, where $q$ is introduced as a variational parameter characterizing the center-of-mass momentum of pairs. With the standard BCS mean-field theory, we can obtain the excitation spectrums $E_{\pm}(k)$ as

$$E_{\pm}(k) = \pm \frac{\epsilon_0(k+q) - \epsilon_m(-k+q)}{2} + \sqrt{\left(\frac{\epsilon_0(k+q) + \epsilon_m(-k+q)}{2} - \mu\right)^2 + \Delta_q^2},$$

where $\mu$ is the chemical potential. Contrary to the conventional BCS superconductor case, here $E_{\pm}(k)$ are not always positive for arbitrary $\Delta_q$, and the pairs will break where the quasi-particle excitation energy is negative. Therefore the wave function should be taken as

$$|\varphi\rangle = \prod_{\{k\}|E_{+}(k)|<0} \hat{\Psi}_{a,k+q}^\dagger \prod_{\{k\}|E_{-}(k)|<0} \hat{\Psi}_{m,-k+q}^\dagger \prod_{\{k\}|E_{\pm}(k)|>0} \left( u_k + v_k \hat{\Psi}_{a,k+q}^\dagger \hat{\Psi}_{m,-k+q}^\dagger \right) |0\rangle,$$

The order parameter $\Delta_q$, as well as the depairing regions, should be determined self-consistently from following gap equation

$$1 = V \sum_k \frac{1 - \Theta(E_{+}(k)) - \Theta(E_{-}(k))}{\sqrt{(\epsilon_0(k+q) + \epsilon_m(-k+q) - \mu)^2 + \Delta_q^2}},$$

where $\Theta(x)$ is the step function, with $\Theta(x) = 1$ for $x < 0$ and $\Theta(x) = 0$ for $x > 0$.

In the Fig.3(a) we plot the right-hand side of the gap equation Eq.(3) as a function of $\Delta_q$ with different values of $q$, from which we can know all the possible solutions to the gap equation. We find that the equation for $\Delta_0$ has two solutions. The one of large $\Delta$ is the BCS solution, where Cooper pairs are formed around $k_F = [(k_{F_a}^3 + k_{F_m}^3)/2]^{1/3}$ and the excitation spectrums are all gapped; and another of small $\Delta$ corresponds to the breached-pair state. The energy of the breached-pair state has been extensively studied before for similar model[12] and will not be repeated here. The curves with small $q$, such as $q = 0.175k_Fa$, are similar to the curve with $q = 0$. However, as $q$ increases the gap equation has only one solution at small $\Delta$, which corresponds to the FFLO states. The values of $\Delta_q$ are obtained numerically for different $q$, and shown in Fig.3(b). The small $\Delta$ solutions, including the breached-pair state and the FFLO states, are all characterized by the existence of the depairing region, which can be found from Fig.4 where the particle populations of a typical FFLO state are shown.
In the FFLO state, the center of Fermi sphere moves to $q$. The atoms pair with molecules at the small momentum side of the Fermi sphere, while the pairs at the high-momentum side will break. In this way, the FFLO states find a proper balance between lowering the interaction energy and not costing too much kinetic energy, and the nonzero momentum carried by the pairs can be cancelled out by the depaired normal molecules, producing an energetic stable FFLO state with the total momentum $Q$ vanishing. We calculate the total momentum of the FFLO states for different values of $q$ and find stable state exists for large $\Delta k_F$, such as $\Delta k_F = 0.41k_F$, as shown in Fig. 5(a), and in Fig. 5(b) we also compare the energy of two FFLO states with the BCS state, and find the FFLO state will dominate over the BCS state with the increase of $\Delta k_F$.

Remark. Although we have demonstrated the existence of non-BCS type pairing state in certain region, the phase diagram of this system in the full parameter region is much richer. With the increase of $E_b$, the system will enter a pure atomic phase, the atom-molecule pairing will be replaced by the $p$-wave pairing between fermionic atoms. Provided that the electric moments of these heteronuclear molecules are polarized by an external electric field, the direct dipole-dipole interactions between molecules can not be neglected, and it will lead to the pairing between molecules. The competition between these different superfluid orders will manifest itself in quantum phase transitions, and more fruitful physics is expected from the interplay of these phases, which will be a subject for further investigations.

The authors would like to thank Professor C. N. Yang for encouragement and valuable support, and we thank L. Chang, T. L. Ho, F. Zhou, Z. Z. Chen, R. Li and M. Zhang for helpful discussions, and we would like to thank Q. Zhou for critical reading the manuscript. This work is supported by NSF China (No. 10247002 and 10404015).

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FIG. 5: (color online) (a) The momentum per particle $Q/N$ of the FFLO states for different values of $q$. $\Delta k_F$ is fixed at $0.14k_F$. (b) The free energy per particle $F = E/N - \mu$ as a function of $\Delta k_F$ for BCS state (dotted line) and the FFLO states with $q = 0.255k_F$ (solid line) and $q = 0.30k_F$ (dash line). We change $\Delta k_F$ by tuning $E_b$. Both figures are plotted for $V = 8 \times 10^{-4}E_F$. The units of $q$, $Q$, and $\Delta k_F$ is $k_F$, and the unit of $F$ is $E_F$. 

\[ \text{References} \]