Effective interaction between molecules in the BEC regime of a superfluid Fermi gas

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Abstract

We investigate the effective interaction between Cooper-pair molecules in the strong-coupling BEC regime of a superfluid Fermi gas with a Feshbach resonance. Our work uses a path integral formulation and a renormalization group (RG) analysis of fluctuations in a single-channel model. We show that a physical cutoff energy $\omega_c$ originating from the finite molecular binding energy is the key to understanding the interaction between molecules in the BEC regime. Our work thus clarifies recent results by showing that $a_M = 2a_F$ is a bare molecular scattering length while $a_M = (0.6 \sim 0.75)a_F$ is the low energy molecular scattering length renormalized to include high-energy scattering up to $\omega_c$ (here $a_F$ is the scattering length between Fermi atoms). We also include many-body effects at finite temperatures. We find that $a_M$ is strongly dependent on temperature, vanishing at $T_c$, consistent with the earlier Bose gas results of Bijlsma and Stoof.

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Recently, the interaction between bound molecules has attracted much attention in the strong-coupling BEC regime of a superfluid Fermi gas\[1, 2, 3, 4\]. In a trapped Fermi gas with a Feshbach resonance, one can tune the magnitude of a pairing interaction by varying the threshold energy of the Feshbach resonance\[5, 6, 7\]. Using this tunable interaction, the BCS-BEC crossover\[7\] has been observed in \(^{40}\)K and \(^{6}\)Li, where the character of superfluidity continuously changes from the weak-coupling BCS type to the BEC of tightly bound molecules, as one increases the pairing interaction\[1, 8\]. In the strong-coupling BEC regime, where the molecules already form above the superfluid phase transition temperature \(T_c\)[7], the system can be regarded as a molecular Bose gas.

The magnitude of the molecular interaction in the BEC regime was originally studied in the superconductivity literature\[1, 2\], where the result \(a_M = 2a_F\) was obtained using a Ginzburg-Landau (GL) type expansion. Here \(a_M\) is the molecular scattering length and \(a_F\) is the atomic \(s\)-wave two-body scattering length. Later, Pieri and Strinati\[3\] obtained \(a_M \approx 0.75a_F\) within a two-body \(t\)-matrix approximation. More recently, Petrov and co-workers\[4\] obtained \(a_M \approx 0.6a_F\) by solving a four-fermion problem. This last result is confirmed by a direct Monte-Carlo simulation for the ground state\[9\]. In addition, Grimm and co-workers also obtained \(a_M \approx 0.6a_F\) in superfluid \(^{6}\)Li\[10\], using a Thomas-Fermi fit to their molecular condensate density profile.

In this paper, we investigate this interaction between molecules in the strong-coupling BEC regime of a uniform Fermi gas, using a single-channel model. We show that the finite binding energy of a Cooper-pair “molecule” naturally leads to a physical cutoff energy \(\omega_c\), which is not present in the usual atomic BEC. In a two-molecule case, we show that \(\omega_c\) is the key to understanding the physics behind the difference between earlier results, namely, \(a_M = 2a_F\)[1, 2] and \(a_M = (0.6 \sim 0.75)a_F\)[3, 4]. We also calculate the many-body \(t\)-matrix at finite temperatures, extending the renormalization group analysis\[11\] for an atomic BEC to the BEC regime of a superfluid Fermi gas. In a many-particle system, we show that \(a_M\) depends strongly on temperature, vanishing in the region near \(T_c\).

In the functional integral formalism, the action \(S\) in the partition function \(Z = \sum_\sigma \int \mathcal{D}\Psi_\sigma \mathcal{D}\Psi_\sigma^\dagger e^{-S}\) has the form\[2\],

\[
S = \int_0^\beta d\tau \int d\mathbf{r} \left[ \sum_\sigma \Psi_\sigma^\dagger \left( \frac{\partial}{\partial \tau} + \frac{\mathbf{p}^2}{2m} - \mu \right) \Psi_\sigma - U \Psi_\uparrow \Psi_\downarrow \right].
\]

Here, \(\Psi_\sigma(\mathbf{r}, \tau)\) and \(\Psi_\sigma^\dagger(\mathbf{r}, \tau)\) are a Grassmann variable and its conjugate, describing Fermi atoms with pseudo-spin \(\sigma = \uparrow, \downarrow\). \(\mu\) is the atomic chemical potential. In \(^{40}\)K and \(^{6}\)Li Fermi...
gases, the tunable pairing interaction $U$ is associated with the Feshbach resonance\cite{2,4,7}. We simply treat $U$ as a tunable parameter in a single channel formulation. This is valid for a broad Feshbach resonance.

To discuss the strong-coupling BEC regime, it is convenient to introduce a Cooper-pair Bose field $\Delta(r, \tau)$, using the usual Stratonovich-Hubbard transformation\cite{2}. After functional integrations over $\Psi_\sigma$ and $\Psi_\sigma^\dagger$, we obtain $Z = \int \mathcal{D}\Delta^\dagger \mathcal{D}\Delta e^{-S_\Delta}$, where $S_\Delta = \int_0^\beta d\tau \int d r |\Delta|^2 - Tr[\ln[-\hat{G}^{-1}]]$\cite{2}. The fermion single-particle Green’s function is given by

$$\hat{G}^{-1} \equiv -\frac{\partial}{\partial \tau} - (\frac{\hat{p}^2}{2m} - \mu)\tau_3 + \begin{pmatrix} 0 & \Delta(r, \tau) \\ \Delta^\dagger(r, \tau) & 0 \end{pmatrix},$$ (1)

where $\tau_j$ ($j = 1, 2, 3$) is the Pauli matrices. The mean-field gap equation is obtained from the saddle point solution for $\Delta_{MF}$ determined by $\partial S_\Delta/\partial \Delta = 0$. Expanding the action $S_\Delta$ around this mean-field solution ($\Delta_{MF}$), we obtain

$$S_\Delta = \int_0^\beta d\tau \int d r \frac{|\delta \Delta|^2}{U} + \sum_{n=2}^\infty \frac{(-1)^n}{n} Tr\left[[\hat{G}^0 \begin{pmatrix} 0 & \delta \Delta \\ \delta \Delta^\dagger & 0 \end{pmatrix}]^n\right],$$ (2)

where $\delta \Delta(r, \tau) \equiv \Delta(r, \tau) - \Delta_{MF}$ describes fluctuations in the particle-particle channel. The mean-field $2 \times 2$ matrix Green’s function $\hat{G}^0$ has the standard BCS form,

$$\hat{G}^0(p, i\omega_m) = \frac{-i\omega_m + (\varepsilon_p - \mu)\tau_3 - \Delta_{MF}\tau_1}{\omega_m^2 + E_p^2}.$$ (3)

Here, $i\omega_m$ is the fermion Matsubara frequency. $E_p \equiv \sqrt{(\varepsilon_p - \mu)^2 + \Delta_{MF}^2}$ is the single-particle excitation spectrum, where $\varepsilon_p$ is the kinetic energy of a Fermi atom.

In the BEC regime, the atomic chemical potential $\mu$ is related to the atomic scattering length $a_F$ by the formula $\bar{\mu} \equiv -1/2ma_F^2$\cite{1,2}. We note that $\bar{\mu}$ is large and negative as we approach the BEC limit ($a_F \to +0$). In this regime, since the BCS order parameter at $T = 0$ is given by $\Delta_{MF} = \sqrt{16/3\pi} |\bar{\mu}|^{1/4} \varepsilon_F^{3/4}$\cite{2}, we find $|\bar{\mu}| \gg \Delta_{MF}$. Thus, we can use approximation $E_p \simeq \varepsilon_p + |\bar{\mu}|$ in (3). In addition, the energy gap $E_g$ is given by $E_g = \sqrt{|\mu|^2 + \Delta_{MF}^2} \simeq |\bar{\mu}|$, so that the binding energy $E_{bind}$ of a Cooper-pair is given by $E_{bind} = 2E_g = 2|\bar{\mu}|$.

In the BEC regime, we expand (2) in powers of $\delta \Delta$, retaining terms up to $n = 4$. We recall that the Gaussian approximation\cite{1,2,7,8,9} only keeps fluctuation terms to order...
FIG. 1: (a) Interaction between molecules $V_{\text{eff}}^{(4)} (q, q', K)$ mediated by Fermi atoms. The dotted lines describe the molecular Boson propagator. (b) Particle-non-conserving interaction $V_{\text{eff}}^{(3)} (q, K)$.

In the superfluid phase, we find

$$S_\Delta = \frac{1}{\beta} \sum_q \Phi_q^\dagger (-i\nu_n + \varepsilon_q^M + U_M n_e) \Phi_q$$

$$+ \frac{n_c U_M}{2} \sum_q \left( \Phi_{q+q/2} \Phi_{q-q/2} \Phi_{K+q/2} \Phi_{K-q/2} \Phi_{K+q/2} \Phi_{K-q/2} \right)$$

$$+ \frac{1}{\beta^2} \sum_{q,K} V_{\text{eff}}^{(3)} (q, K) \left( \Phi_{-q/2+q} \Phi_{-q/2-q} \Phi_K \Phi_{K+q/2} \Phi_{K-q/2} \Phi_{K+q/2} \Phi_{K-q/2} \right)$$

$$+ \frac{1}{2\beta^3} \sum_{q,q',K} V_{\text{eff}}^{(4)} (q, q', K) \left( \Phi_{q+q/2} \Phi_{q+q/2} \Phi_{K+q/2} \Phi_{K+q/2} \Phi_{K+q/2} \Phi_{K+q/2} \right).$$

Here, $U_M \equiv 4\pi(2\sigma_F)/M$ (where $M = 2m$) is the bare $s$-wave molecular interaction obtained in what amounts to the time-dependent GL theory \cite{1, 2}; $\varepsilon_q^M \equiv q^2/2M$ is the kinetic energy of a free molecule, and $i\nu_n$ is the pair boson Matsubara frequency, with $p \equiv (p, i\omega_m)$. In the BEC limit of interest, the fluctuations in the order parameter $\delta \Delta_q$ involve the molecular condensate. We introduce a renormalized molecular field $\Phi_q \equiv \delta \Delta_q/\eta$, where $\eta = [\sum_p 1/4(\varepsilon_p - \bar{\mu})^2]^{-1/2}$. Defining $\phi_M \equiv \Delta_{\text{MF}}/\eta$ as the equilibrium value of the Bose-condensate order parameter, at $T = 0$, one can show that $n_c \equiv \phi_M^2 = n_F/2$ (where $n_F$ is the number of Fermi atoms) gives the number of Bose-condensed molecules.

$V_{\text{eff}}^{(4)}$ in (4) describes an interaction between molecules mediated by the Fermi gas [see Fig. 1(a)], given by

$$V_{\text{eff}}^{(4)} (q, q', K) = \frac{\eta^4}{\beta} \sum_p G_{11}^0 (p + \frac{q - q'}{2} + \frac{K}{4}) G_{11}^0 (-p + \frac{q + q'}{2} + \frac{K}{4}).$$
The calculated momentum dependence of the boson-boson interaction $V^{(4)}_{\text{eff}}(q,0,0)$ (solid line). The dashed line is the Lorentzian fit given by $U_M/(1 + (q/\Lambda)^2)$. The vertical dotted line shows the position of the cutoff momentum $\Lambda$.

$$\times \ G_{11}^0(-p - \frac{q + q'}{2} + \frac{K}{4}) G_{11}^0(p - \frac{q - q'}{2} + \frac{K}{4}).$$

(5)

Here, $G_{11}^0$ is the diagonal $(1,1)$-component of the BCS mean-field Green’s function defined in (3). $V^{(3)}_{\text{eff}}$ in (4) represents a particle-non-conserving interaction, given by [see also Fig. 1(b)]

$$V^{(3)}_{\text{eff}}(q, K) = -\frac{\eta^3}{\beta} \sum_p G_{11}^0(p + \frac{K}{2}) G_{11}^0(-p + \frac{K}{2}) G_{12}^0(p + q).$$

(6)

This interaction involves the off-diagonal (anomalous) Green’s function $G_{12}^0$ defined in (3), so that $V^{(3)}_{\text{eff}}$ only exists in the superfluid phase.

For $q = q' = K = 0$, one can show that $V^{(4)}_{\text{eff}}(0,0,0) = U_M$ and $V^{(3)}_{\text{eff}}(0,0) = \sqrt{n_c}U_M$, where $U_M = 4\pi(2a_F)/M$. Using these results in place of $V^{(4)}_{\text{eff}}(q, q', K)$ and $V^{(3)}_{\text{eff}}(q, K)$ in (4), we reproduce the previous results obtained in the literature, namely, $a_M = 2a_F [1, 2]$. However, $V^{(4)}_{\text{eff}}$ and $V^{(3)}_{\text{eff}}$ actually depend on momentum, and go to zero with a characteristic cutoff momentum $\Lambda$. To calculate this cutoff momentum $\Lambda$, we expand (5) and (6) in terms of the relative momentum (taking the center-of-mass-momentum $K$ to be zero [12]), keeping terms of $O(q^2)$. We obtain $V^{(4)}_{\text{eff}}(q, q', 0) \simeq U_M F(q) F(q')$ and $V^{(3)}_{\text{eff}}(q, 0) \simeq \sqrt{n_c}U_M F(q)$, where $F(q) = 1 - (q/\Lambda)^2$. The characteristic momentum is found to be $\Lambda = 4/\sqrt{5a_F}$. For larger values of the momentum, we replace $F(q)$ by the Lorentzian $[1 + (q/\Lambda)^2]^{-1}$. This gives a very good fit to the momentum dependent interaction, as shown in Fig. 2. In terms of energy, we
can write $F(q) = \left[1 + \varepsilon_q^M / \omega_c\right]^{-1}$, where the interaction or molecular cutoff energy is defined by

$$\omega_c \equiv \frac{\Lambda^2}{2M} = \frac{8}{5} |\bar{\mu}|. \quad (7)$$

We note that $\omega_c$ is comparable to the binding energy $E_{\text{bind}} = 2|\bar{\mu}|$ of a molecule in the BEC limit. Thus we conclude that $\omega_c$ is a physical cutoff determined by the dissociation energy of a molecule in the BEC phase.

To summarize, when we replace $V_{\text{eff}}(q, q', K)$ and $V_{\text{eff}}(q, K)$ in (4) with $V_{\text{eff}}(0, 0, 0)$ and $V_{\text{eff}}(3) (0, 0)$, respectively, we have to include the physical momentum cutoff $\Lambda$, as discussed above. We recall that $\Phi_q = \delta \Delta_q / \eta$ describes excitations from the Bose-condensate. The molecular Bose field involving the condensate part is given by $\phi_q \equiv \Phi_q + \phi_M$. Using $\phi_q$ in (4), we obtain

$$S_\Delta = \frac{1}{\beta} \sum_q \phi_q^\dagger (-i\nu_n + \varepsilon_q^M - \mu_M) \phi_q$$

$$+ \frac{1}{2\beta^3} \frac{4\pi(2a_F)}{M} \sum_{q, q', K} \phi_q^\dagger \phi_{q+q'}^\dagger \phi_{q+q} \phi_{q}$$

where $\mu_M \equiv U_M n_c$ is the molecular chemical potential. We note that $V_{\text{eff}}^3$ has been absorbed into the last term of (8). The corresponding Hamiltonian has the form

$$H_{\text{BEC}} = \sum_q \phi_q^\dagger (\varepsilon_q^M - \mu_M) \phi_q$$

$$+ \frac{4\pi(2a_F)}{M} \sum_{q, q', K} \phi_q^\dagger \phi_{q+q'}^\dagger \phi_{q-q'} \phi_{K} \phi_{K+q}$$

This Hamiltonian is also obtained in the normal phase, but now with $\mu_M = 4(\mu + \sqrt{|\mu||\bar{\mu}|})$.

The effective Hamiltonian in (9) gives a clear physical picture of the two different molecular scattering lengths found in earlier literature, namely $a_M = 2a_F \[1, 2\]$ and $a_M = (0.6 \sim 0.75)a_F \[3, 4\]$. Although $U_M = 4\pi(2a_F)/M$ looks like the low-energy expression for s-wave interaction, (9) shows that $U_M$ is actually a bare interaction involving a cutoff energy $\omega_c$. In the case of two molecules in a vacuum, to obtain the low-energy interaction $U_M^{2b} \equiv 4\pi a_M^{2b}/2M$, we have to renormalize $U_M$ to remove the need for a high-energy cutoff \[13\]. In the usual manner, this is given by

$$\frac{4\pi a_M^{2b}}{M} = \frac{4\pi(2a_F)}{M} \sum_{q, q'} \frac{1}{2|\varepsilon_q^M|} \frac{1}{2|\varepsilon_{q'}^M|} = \frac{4\pi}{M} \frac{2a_F}{1 + 2.28}$$

$$= \frac{4\pi(0.61a_F)}{M}. \quad (10)$$
Here we note that $a_F$ in the denominator has been canceled out by the $a_F$ involved in $\omega_c$, defined in (7). The resulting renormalized Hamiltonian has the same form as (9), but now with $0.61a_F$ in place of $2a_F$. Eq. (10) agrees with the recent four-fermion (two-molecule) analysis, which gives $a_M = 0.6a_F$. Thus, we find that $a_M = 2a_F$ is the bare molecular scattering length before renormalization, while $a_M = (0.6 \sim 0.75)a_F$ is the renormalized two-molecule scattering length in which the high-energy processes up to $\omega_c$ have been incorporated.

The effective action in (8) is also useful to calculate the molecular scattering length $a_M$ in a many-particle system. In this case, $a_M$ is affected by many-body effects, as well as by temperature, which are not included in the $T = 0$ two-molecule result in (10). To include these effects, we apply the RG theory developed for an atomic Bose-condensed gas[11] to deal with (8), including the physical cutoff $\Lambda$. In the 1-loop level, the RG equations are given by[11], for $\mu_M < 0$,

$$\frac{d\mu_M}{dl} = 2\mu_M - \frac{\Lambda^3}{\pi^2} U_M N(\varepsilon^M_A - \mu_M), \quad (11)$$

$$\frac{dU_M}{dl} = -U_M - \frac{\Lambda^3}{2\pi^2} U_M^2 \left[ \frac{2N(\varepsilon^M_A - \mu_M) + 1}{2(\varepsilon^M_A - \mu_M)} + 4\beta N(\varepsilon^M_A - \mu_M)[N(\varepsilon^M_A - \mu_M) + 1] \right] \quad (12)$$

and for $\mu_M \geq 0$[15],

$$\frac{d\mu_M}{dl} = 2\mu_M - \frac{\Lambda^3}{2\pi^2} U_M \left[ \frac{\varepsilon^M_A + \mu_M}{E^M_A} \left[ 2N(E^M_A) + 1 \right] - 1 + 4\beta N(E^M_A)[N(E^M_A) + 1] \right], \quad (13)$$

$$\frac{dU_M}{dl} = -U_M - \frac{\Lambda^3}{2\pi^2} U_M^2 \left[ \frac{2N(E^M_A) + 1}{2E^M_A} + 4\beta N(E^M_A)[N(E^M_A) + 1] \right].$$

Here, $E^M_A = \sqrt{\varepsilon^M_A (\varepsilon^M_A + 2\mu_M)}$, and $N(\varepsilon)$ is the Bose distribution function. $\mu_M$, $U_M$, and $T$ involve the trivial scaling as $\mu_M(l) = \mu_M e^{2l}$, $U_M(l) = U_M e^{-l}$, $T(l) = T e^{2l}$. We solve the RG equations together with the equations for the number of molecules $n_M = n_F/2 = n_c + n_n$. Here, $n_c = \lim_{l \to \infty} \mu_M(l)/U_M(l)e^{-3l} \ (\mu_M(l) > 0)$ is the number of Bose-condensed molecules, and the number of non-condensate molecules $n_n$ is determined by[11],

$$n_n = \frac{\Lambda^3}{2\pi^2} \int_0^\infty dl N(\varepsilon^M_A - \mu_M)e^{-3l} \quad (\mu_M < 0), \quad (15)$$
FIG. 3: Many-body molecular scattering length $a_M$ as a function of temperature. $p_F$ is the Fermi momentum for a free Fermi gas. We show results down to $T = 0$, although the RG equations (13) and (14) are not valid for temperatures such that $T/T_F \lesssim 0.1(p_F a_F)$, The inset shows $T_c$ in the BEC regime determined from the fixed points of the RG equations (13) and (14). The dashed line shows $T_{c\text{ideal}} = 0.218T_F$.

$$n_n = \frac{\Lambda^3}{2\pi^2} \int_0^\infty dl \left[ \frac{\varepsilon_n^M + \mu_M}{2E_n^M} \right] \left[ N(\varepsilon_n^M - \mu_M) + 1 \right] - \frac{1}{2} e^{-\frac{\Lambda^2}{4l}}.$$  

(16)

Figure 3 shows the many-body molecular scattering length $a_M$ at finite temperatures. The scattering length $a_M$ depends on temperature, and the temperature dependence is stronger as one approaches the crossover regime. At $T_c$, $a_M$ vanishes. This is expected since if molecules are to be stable at $T_c$, the scattering between them must vanish at $T_c$. We note that a similar $T$-dependent scattering length was also obtained earlier in the study of Bose-condensed gases. However, in the present situation, one may have such large values of $a_F$ near the resonance that the decrease in the effective value of $a_M$ may have observable consequences at finite temperatures. In atomic Bose gases, the small size of the scattering length meant this region was restricted to temperatures very close to $T_c$ and hence of less interest.

As shown in the inset in Fig.3, the many-body effects enhance $T_c$ compared with $T_{c\text{ideal}} = 0.218T_F$ for the transition temperature of a non-interacting Bose gas. In the extreme BEC limit, we find $\Delta T_c \equiv T_c - T_{c\text{ideal}} \propto (p_F a_F) \propto (n_M^{1/3} a_M)$, consistent with the previous work on
the BEC in Bose gases\[1, 17, 18, 19\]. Although $T_c$ in the inset initially increases with $p_F a_F$ from the BEC side, it will eventually decrease in the crossover region, smoothly going into the weak-coupling BCS result\[2\].

Our theory is only valid in so far as the effect of fluctuations involving terms higher order than $n = 4$ in (2) is small. Comparing the fourth order term with the sixth order term above $T_c$, we find that the fourth order term is dominant as long as $(p_F a_F)^{-1} \gtrsim 1$, i.e., we are not in the unitarity region.

To conclude, we have studied the effective interaction between bound molecules in the BEC regime of a superfluid Fermi gas. We have included the binding energy of a molecule, which naturally leads to a physical cutoff energy in the molecular Bose gas. For the two-molecule case, we showed that this cutoff gives a simple physical explanation of the difference between the two molecular scattering lengths, the bare value $a_M = 2a_F[1, 2]$ and the renormalized value $a_M = (0.6 \sim 0.75)a_F[3, 4]$. We have also shown that the many-body scattering length deviates considerably from the two-body scattering length as the temperature approaches $T_c$ if we are close to the unitarity limit. By employing the RG technique, the present paper includes fluctuations past the mean-field BCS theory in a more sophisticated way than the original crossover theory developed by Nozières and Schmitt-Rink\[8\].

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