BCS-BEC crossover in a gas of Fermi atoms with a p-wave Feshbach resonance

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Abstract

We investigate unconventional superfluidity in a gas of Fermi atoms with an anisotropic p-wave Feshbach resonance. Including the p-wave Feshbach resonance as well as the associated three kinds of quasi-molecules with finite orbital angular momenta $L_z = \pm 1, 0$, we calculate the transition temperature of the superfluid phase. As one passes through the p-wave Feshbach resonance, we find the usual BCS-BEC crossover phenomenon. The p-wave BCS state continuously changes into the BEC of bound molecules with $L = 1$. Our calculation includes the effect of fluctuations associated with Cooper-pairs and molecules which are not Bose-condensed.

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The search for $p$-wave superfluidity is the next big challenge in a trapped Fermi gas, after the discovery of $s$-wave superfluidity in $^{40}$K and $^{6}$Li\cite{1, 2, 3, 4, 5}. Recently, $p$-wave Feshbach resonances have been observed\cite{6, 7, 8}. The discovery of $p$-wave superfluidity will be the first realization of pseudo-spin triplet superfluidity in a Fermi atomic gas, quite different from the recently discovered singlet $s$-wave superfluidity\cite{1, 2, 3, 4, 5}. Since the pairing interaction associated with a Feshbach resonance can be tuned by varying the threshold energy $2\nu$ of the resonance (see below), one can probe the $p$-wave BCS-BEC crossover. The superfluidity will continuously change from $p$-wave BCS-type to a BEC-type of bound molecules with a finite angular momentum $L = 1$, as one passes through the Feshbach resonance.

As a useful first step, we calculate the superfluid phase transition temperature $T_c$ over the entire $p$-wave BCS-BEC crossover regime. We explicitly include the $p$-wave Feshbach resonance and associated molecules with three values of $L_z = \pm 1, 0$. To describe the BCS-BEC crossover\cite{9, 10}, it is necessary to include the fluctuations in the three $p$-wave Cooper-channels and their coupling due to the strong pairing interaction associated with the Feshbach resonance. Our work is a generalization of Ref. [10]. We consider both a single-component Fermi gas (where a Feshbach resonance occurs in the same hyperfine state) as well as a two-component Fermi gas (where a Feshbach resonance occurs between different hyperfine states). The Feshbach resonances in both cases have been recently observed\cite{6, 7, 8}. We deal with both a narrow and a broad Feshbach resonance. Although we mainly consider a uniform gas in this letter, we discuss $T_c$ in a trapped gas in the BEC limit.

$p$-wave superfluidity in trapped Fermi gases was discussed in the BCS regime at $T_c$\cite{11, 12}. Very recently, the $p$-wave gap equation for the order parameter of the superfluid phase in the crossover region was solved in Ref. [13] at $T = 0$. An attractive interaction in the $L \neq 0$ partial wave channel was considered. An interesting phase transition in a two-dimensional Fermi gas has also been predicted\cite{14}. In contrast to these recent papers, our starting point explicitly introduces the molecules which form as a result of the Feshbach resonance. We thus emphasize the physical nature of the $p$-wave bound states which form the Bose condensate in the crossover region. We also remark that a $p$-wave pairing mechanism has been proposed using the dipole interaction\cite{15}.

We extend the coupled fermion-boson (CFB) model for a $s$-wave Feshbach resonance\cite{10,}.
describe three kinds of molecular bosons (labelled by $H$ into (1) by considering the grand-canonical Hamiltonian

\[ H = \sum_p \varepsilon_p c_p^\dagger c_p + \sum_{q,j} [\varepsilon_q^B + 2\nu] b_{q,j}^\dagger b_{q,j} \]

\[ - \frac{U}{2} \sum_{p,p',q,j} \mathbf{p} \cdot \mathbf{p}' c_{p+q/2}^\dagger c_{-p+q/2}^\dagger b_{q+q/2} c_{p'+q/2}^\dagger b_{q'+q/2} + \frac{g_r}{\sqrt{2}} \sum_{p,q,j} p_j [b_{q,j}^\dagger c_{p+q/2}^\dagger c_{-p+q/2}^\dagger + h.c.]. \]

(1)

Here $c_p^\dagger$ is a creation operator of a Fermi atom with the kinetic energy $\varepsilon_p \equiv p^2/2m$. $b_{q,j}$ describe three kinds of molecular bosons (labelled by $j = x, y, z$), all with the center of mass momentum $\mathbf{q}$, associated with the $p$-wave Feshbach resonance. The threshold energy $2\nu$ in the molecular kinetic energy $\varepsilon_q^B + 2\nu \equiv q/2M + 2\nu$ is independent of $j$, due to the spherical symmetry of the system we are considering. In the last term, $g_r$ is the coupling constant of a $p$-wave Feshbach resonance, with $p_j$ characterizing the $p$-wave symmetry [18].

The Feshbach resonance term in (1) is obtained from a more general Hamiltonian $H_{F,R} \equiv \int d\mathbf{r} d\mathbf{r}' [g_r (\mathbf{r} - \mathbf{r}') \Phi(\mathbf{r}, \mathbf{r}') \Psi(\mathbf{r}) \Psi^\dagger(\mathbf{r}') + h.c.]$. Here $\Psi(\mathbf{r}) \equiv \sum_p e^{ip \cdot \mathbf{r}} c_p$ is a fermion field operator, and

\[ \Phi(\mathbf{r}, \mathbf{r}') \equiv \sum_q e^{i\mathbf{q} \cdot \mathbf{R}} \sum_{n,L,L_z} u_{nL}(\tilde{\mathbf{r}}) Y_{L,L_z}^\dagger(\theta, \phi) b_{q,n,L,L_z} \]

(2)

describes molecules with center of mass $\mathbf{R} \equiv (\mathbf{r} + \mathbf{r}')/2$, and relative coordinate $\tilde{\mathbf{r}} \equiv \mathbf{r} - \mathbf{r}'$. $b_{q,n,L,L_z}$ is an annihilation operator of a bound molecular state, described by the eigenfunction $u_{nL}(\tilde{\mathbf{r}}) Y_{L,L_z}^\dagger(\theta, \phi)$. The last term in (1) is obtained when we retain the terms in $\Psi(\mathbf{r})$ to leading order in $\mathbf{p}$, in the $L = 1$ channel ($b_{qL_z} \equiv b_{q,n,L=1,L_z}$) for a Feshbach resonance state specified by a radial quantum number $n$. We note that $p_x \propto Y_{11} + Y_{1,-1}$, $p_y \propto Y_{11} - Y_{1,-1}$ and $p_z \propto Y_{1,0}$. Thus the molecular operators $b_{q,j}$ in (1) are related to $b_{q,L_z}$, with azimuthal angular momentum components $L_z = \pm 1, 0$, as follows

$$(b_{q,x}, b_{q,y}, b_{q,z}) = (\frac{1}{\sqrt{2}}[b_{q,1} + b_{q,-1}], \frac{1}{\sqrt{2}}[b_{q,1} - b_{q,-1}], b_{q,0}).$$

Equation (1) also includes a non-resonant $p$-wave interaction $U$ [18], which we take to be attractive ($-U < 0$).

In the $p$-wave Feshbach resonance, since two Fermi atoms form one of the three kinds of quasi-molecular bosons described by $b_{q,j}^\dagger$ ($j = x, y, z$) and this bound state can dissociate into two Fermi atoms, we take $M = 2m$ and impose the conservation of the total number of Fermi atoms as $N = N_F + 2 \sum_{j=x,y,z} N_{B_j}^j$. Here $N_F$ is the number of Fermi atoms and $N_{B_j}^j$ is the number of Bose molecules in the $j$-th component. This constraint can be actually absorbed into (1) by considering the grand-canonical Hamiltonian $H \equiv H - \mu N$. The resulting
Hamiltonian has the same form as (1), where \( \varepsilon_p \) and \( \varepsilon_q^B \) are replaced by \( \xi_p \equiv \varepsilon_p - \mu \) and \( \xi_q^B \equiv \varepsilon_q^B - 2\mu \), respectively.

The superfluid phase is characterized by three anisotropic \( p \)-wave Cooper-pairs \( \Delta_j(p) \equiv U \sum_{p'} p_j p_j' \langle c_{-p} c_{p'} \rangle \) and three molecular BEC order parameters \( \phi_j \equiv \langle b_{q=0,j} \rangle (j = x, y, z) \). In the equilibrium state, these are related to each other through the identity \[10\]

\[ p_j \phi_j = -\frac{g_t}{\sqrt{2}U/2\nu - 2\mu} \Delta_j(p). \]

The single-particle excitations have the BCS spectrum \( E_p = \sqrt{\xi_p^2 + |\sum_j \Delta_j(p)|^2} \) with the composite order parameter, given by \( \tilde{\Delta}_j(p) \equiv \Delta_j(p) - \sqrt{2} g_t p_j \phi_j \). The angular dependence of \( \tilde{\Delta}_j(p) \) is proportional to \( p_j \). This composite order parameter is self-consistently determined by the BCS gap equation, \( 1 = \frac{1}{3} U_{\text{eff}} \sum_p \frac{p_j^2}{2E_p} \tanh \frac{E_p}{2T} \), where the factor \( p_j^2 / 3 \) comes from the angular integration of \( p_j^2 \). The effective pairing interaction \( U_{\text{eff}} \equiv U + g_t^2 / (2\nu - 2\mu) \) includes the effect of Feshbach resonance \[10\]. In the weak-coupling or BCS regime, \( \mu \simeq \varepsilon_F \) (where \( \varepsilon_F \) is the Fermi energy).

The analogous \( p \)-wave CFB model for a two-component Fermi gas (\( \equiv \uparrow, \downarrow \)) is described by

\[
H = \sum_{p,\sigma} \varepsilon_p c_{p\sigma}^\dagger c_{p\sigma} + \sum_{q,ij} [\varepsilon_q^B + 2\nu] b_{q,j}^\dagger b_{q,j} - U \sum_{p, p', q, j} \mathbf{P} \cdot \mathbf{P}' \langle \phi_{q+p/2}^\dagger \phi_{-q+p/2} \phi_{q+p/2} \phi_{-q+p/2} \rangle + g_t \sum_{p, q, j} p_j \langle b_{q,j} c_{q+p/2}^\dagger c_{q-p/2} + h.c. \rangle.
\]

In a mean field pairing approximation, we again obtain the same single-particle excitations \( E_p \) and the gap equation as those in the single-component case. The Cooper-pair order parameter is \( \Delta_j(p) \equiv U \sum_{p'} p_j p_j' \langle c_{-p} c_{p'} \rangle \).

We now present the \( p \)-wave strong-coupling theory at \( T_c \) for the single-component (spin polarized) model defined in (1). The discussion is easily extended to the two-component case. The equation for \( T_c \) is obtained by employing the Thouless criterion \[3, 10\], the temperature when the particle-particle scattering matrix first develops a pole at \( \omega = q = 0 \). In the \( t \)-matrix approximation, the \( p \)-wave scattering matrix has the form \( \tilde{\Gamma}_{ij}(p, p', q, \omega) = p_i \Gamma_{ij}(q, \omega) p_j \), which is shown diagrammatically in Fig. 1(a). In this figure, the first and the second lines, respectively, describe the effects of non-resonant interaction \( U \) and the \( p \)-wave Feshbach resonance, that give \( \tilde{\Gamma}(q, \omega) \equiv \{ \Gamma_{ij} \} = -[1 - U_{\text{eff}}(q, \omega) \tilde{\Pi}(q, \omega)]^{-1} U_{\text{eff}}(q, \omega) (i, j = x, y, z) \). Here, \( U_{\text{eff}}(q, \omega) \equiv U - g_t^2 D_0(q, \omega) \) is an atom-atom interaction including dynamical effects described by the bare molecular Bose propagator \( D_0^{-1}(q, \omega) \equiv \omega + i\delta - [\varepsilon_q^B + 2\nu] \). The correlation functions \( \tilde{\Pi} \equiv \{ \Pi_{ij} \} \) are obtained from the analytic continuation \( iv_n \to \omega + i\delta \).
of the two-particle thermal Green’s function,
\[ \Pi_{ij}(q, i\nu_n) \equiv \frac{1}{\beta} \sum_{p_i, p_j} p_i p_j \frac{1 - f(\xi_{p+q/2}) - f(\xi_{p-q/2})}{\xi_{p+q/2} + \xi_{p-q/2} - i\nu_n}, \tag{4} \]
where \( f(\varepsilon) \) is the Fermi distribution function. The diagonal components \( \Pi_{ii} \) \((i = x, y, z)\) describe superfluid fluctuations in the \( i \)-th Cooper-channel, while the off-diagonal components give the coupling of fluctuations in different channels. Noting that \( \Pi_{i \neq j}(0, 0) = 0 \) in our approximation, the Thouless criterion gives the equation for \( T_c \) as
\[ 1 = U_{\text{eff}} \Pi_{ii}(0, 0) = \frac{1}{3} U_{\text{eff}} \sum_{p} \frac{p^2}{2(\varepsilon_p - \mu)} \tanh \frac{\varepsilon_p - \mu}{2T}. \tag{5} \]
This has the same form as the mean-field gap equation at \( T = T_c \), with \( \tilde{\Delta}_j(p) \rightarrow 0 \). However, the chemical potential \( \mu \) in (5) can be quite different from the Fermi energy \( \varepsilon_F \) in the crossover regime\cite{9, 10, 19, 20}, and one needs an additional equation to determine \( \mu \).

The chemical potential \( \mu \) is determined from the equation for the number of atoms \( N \), which is calculated from the thermodynamic potential \( \Omega \) using the formula \( N = -\frac{\partial \Omega}{\partial \mu} \). Figure 1(b) shows the fluctuation correction to \( \Omega \), where the diagrams on the left and right describe fluctuations in the \( p \)-wave Cooper-channels and the Feshbach resonance, respectively. Summing up these diagrams, we obtain
\[ N = N_F - \frac{1}{\beta} \sum_{q, i\nu_n} \frac{\partial}{\partial \mu} \text{tr} \left[ \log \hat{D}(q, i\nu_n) \right] \\
- \frac{1}{\beta} \sum_{q, i\nu_n} \frac{\partial}{\partial \mu} \text{tr} \left[ \log [1 - U \hat{\Pi}(q, i\nu_n)] \right] \\
\equiv N_F + 2N_B + 2N_C, \tag{6} \]
where the trace is taken over the \( L = 1 \) space \((j = x, y, z)\). \( N_F \equiv \sum_p f(\xi_p) \) is the number of free Fermi atoms. \( N_B \) is the number of Feshbach molecules, given as the poles of the renormalized (matrix) molecular Bose Green’s function \( \hat{D}^{-1}(q, i\nu_n) \equiv i\nu_n - (\xi_q^B + 2\nu) - \hat{\Sigma}(q) \). The molecular self-energy \( \hat{\Sigma}(q, i\nu_n) \equiv -g_r^2\hat{\Pi}/(1 - U\hat{\Pi}) \) describes the fluctuation effects in the \( p \)-wave Cooper-channels. As in Refs. \cite{9, 10}, \( N_C \) can be interpreted as the contribution of preformed \( p \)-wave Cooper-pairs as well as particle-particle scattering states. We note that superfluid fluctuations in the three \( p \)-wave Cooper-channels are strongly coupled to one another through \( \Pi_{ij} \) \((i \neq j)\). Equations (5) and (6) are the basic coupled equations describing \( T_c \) of a uniform \( p \)-wave superfluid over the entire BCS-BEC crossover.
The same equations are obtained in the two-component case in (3), with $N_F$ replaced by $N_F = 2 \sum_p f(\xi_p)$, reflecting the two Fermi hyperfine states.

Figure 2 shows the self-consistent numerical solutions of (5) and (6). In this figure, we have introduced a $p$-wave scattering length $a_p$ for the renormalized interaction $U_{\text{eff}}^R$ which occurs in the gap equation when written in a cutoff-independent way [21]. This is defined [11, 12] by $-4\pi(3a_p^3)/m \equiv U_{\text{eff}}^R = U_{\text{eff}}/(1 - U_{\text{eff}}^3 \sum_{0,\omega < \omega_c} \frac{\gamma^2}{2\omega_0^2})$, where $\omega_c$ is a high-energy cutoff. The increase of $(k_F a_p)^{-3}$ corresponds to a decrease of bare threshold energy $2\nu$. Since the chemical potential also decreases to approach $\nu$ [see the inset in panel 2(b)], the bare interaction $U_{\text{eff}} = U + g^2/(2\nu - 2\mu)$ becomes stronger for larger $(k_F a_p)^{-3}$. In the BCS regime $[(k_F a_p)^{-3} \lesssim -1]$, $T_c$ agrees well with the standard weak-coupling BCS theory ['BCS' in Fig. 2(a)]. On the other hand, in the crossover regime $[-1 \lesssim (k_F a_p)^{-3} \lesssim 0]$, the deviation of $T_c$ from the weak-coupling result is large. The chemical potential $\mu$ also begins to strongly deviate from the Fermi energy $\varepsilon_F$, as shown in Fig. 2(b). Figure 3 shows that the gas continuously changes from a gas of Fermi atoms (dominated by $N_F$) into a Bose gas of bound states (dominated by $N_M = N_B + N_C$). In the BEC regime $[(k_F a_p)^{-3} \lesssim 0]$, free Fermi atoms are almost absent, and $T_c$ approaches a constant value. Its precise value depending on whether one is dealing with a single-component gas ($\uparrow\uparrow$) or a two-component gas ($\uparrow\downarrow$).

This difference is due to different Fermi energies in the two cases (see TABLE I). The peak in $T_c$ in Fig. 2(a) would be absent if the coupling to the bound states [10, 22] was properly included in the self-energies of the Fermi atoms.

In the extreme BEC limit, where all the atoms have formed Feshbach molecules ($N_F, N_C = 0$), the gas can be regarded as a non-interacting Bose gas mixture with three kinds of Feshbach molecules, with $L_z = \pm 1, 0$. In this case, rewriting Eq. 5 as $2\mu = 2\nu - g^2\Pi_{ii}(0,0)/[1 - U\Pi_{ii}(0,0)]$, we find $2\mu \to 2\nu$, because $\Pi_{ii}(0,0) = 0$ in this BEC limit. This result is consistent with the inset in Fig. 2(b). Since $2\mu$ is the chemical potential of the molecular Bose gas and $2\nu$ is the threshold energy of molecular excitations, the condition $2\mu = 2\nu$ is that required for BEC in a non-interacting Bose gas. That is to say, $T_c$ in this extreme case is simply determined by $N = 3 \sum_q n_B(\varepsilon_q^B)$, where $n_B(\varepsilon)$ is the Bose distribution function. The factor 3 comes from the presence of three kinds of molecules, which is characteristic of $p$-wave superfluidity. Because of this factor, $T_c$ in the $p$-wave case is lower than the $s$-wave case, as shown in TABLE I. TABLE I also shows $T_c$ in the BEC limit in a trapped gas, evaluated within the LDA. These values for $T_c$ in a trapped gas
seems accessible in current experiments. The crossover behavior of $T_c$ shown in Fig. 2(a) is a general result valid for any type of $p$-wave superfluidity.

Figures 2 and 3 indicate that the crossover behavior of $T_c$, $\mu$, and the number of Fermi atoms $N_F$ and that of Bose molecules $N_M$ show quasi-universal behavior when plotted as a function of $(k_Fa_s)^{-3}$, irrespective of whether the Feshbach resonance is narrow ($\tilde{g}_r < \varepsilon_F$) or broad ($\tilde{g}_r > \varepsilon_F$). On the other hand, the character of the bound state bosons is different between the two. In a narrow Feshbach resonance, the Feshbach molecules ($N_B$) are dominant in the crossover regime, while Cooper-pairs ($N_C$) are dominant in a broad Feshbach resonance (see Fig. 3). However, Feshbach molecules always dominate in the extreme BEC limit.

We note that the phase diagrams in trapped Fermi gases[1, 2, 3, 4, 5] which experiments measure involve passing through the resonance in an adiabatic (constant entropy) manner. In the case of a $s$-wave Feshbach resonance, Ref. [23] has discussed how one can calculate such phase diagrams using a simple ideal gas model. This could be extended to the $p$-wave Feshbach resonance case.

To summarize, we have discussed the BCS-BEC crossover in the presence of a $p$-wave Feshbach resonance. Generalizing earlier work on the $s$-wave BCS-BEC crossover[10], we have included fluctuation effects in the three $p$-wave Cooper-channels, as well as the three kinds of Feshbach molecules with $L_z = \pm 1, 0$. Observation of the molecular condensate in the BEC regime[1, 2, 3, 4, 5] would be a first step in the study of $p$-wave superfluidity.

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FIG. 1: (a) Particle-particle scattering matrix in the $t$-matrix approximation in terms of the non-resonant interaction $U$ (first line) and the $p$-wave Feshbach resonance $g_r$ (second line). $G_0$ and $D_0$ are the bare single-particle Fermi and Bose Green’s function, respectively. (b) Corrections to the thermodynamic potential originating from fluctuations in the $p$-wave Cooper-channels (left diagram) and the Feshbach resonance (right diagram).

FIG. 2: (a) $T_c$ in the $p$-wave BCS-BEC crossover. ↑↑: single-component Fermi gas, with $\bar{U} \equiv N p_F^2 U = 0.4\varepsilon_F$. ↑↓: two-component Fermi gas, with $\bar{U} = 0.8\varepsilon_F$. Results for a narrow Feshbach resonance ($\bar{g}_r \equiv \sqrt{N p_F^2} g_r = 0.6\varepsilon_F$) and a broad Feshbach resonance ($\bar{g}_r = 5\varepsilon_F$) are shown. ‘BCS’ shows a weak-coupling result in the two-component case with $\mu$ being fixed at the value at $\nu = 2.5\varepsilon_F$. (b) Chemical potential $\mu(T_c)$ in a single component Fermi gas. The solid and dashed lines show the results for a narrow and a broad Feshbach resonance, respectively. The inset shows $\mu(T_c)$ as a function of the threshold energy $2\nu$ for a narrow Feshbach resonance.

FIG. 3: Numbers for various kinds of particles at $T_c$ in a single-component Fermi gas. (a) narrow Feshbach resonance, and (b) broad Feshbach resonance. $N_M \equiv N_B + N_C$, where $N_B$ describes Feshbach molecules and $N_C$ gives the contribution from Cooper-pairs (stable and unstable).
TABLE I: \( T_c \) in the BEC limit. (S) and (T) show the single- and two-component Fermi gas, respectively. \( T_c \) in a uniform gas is given by
\[
T_c = \frac{2T_F}{6\alpha \sqrt{\pi \zeta(3/2)^{2/3}}}
\]
(where \( \zeta(z) \) is the zeta-function), with \( \alpha = 1 \) (s-wave), \( \alpha = 6 \) (S), and \( \alpha = 3 \) (T). In a harmonic trap, \( T_c = \frac{T_F}{6\alpha \zeta(3)^{1/3}} \) is evaluated using the LDA. \( T_F = \varepsilon_F \) is obtained from
\[
N = \eta \sum_{\varepsilon \leq \varepsilon_F} 1
\]
where \( \eta = 1 \) (\( \eta = 2 \)) for the single (two) component case.

| symmetry | uniform gas \([T_F]\) | trapped gas \([T_F]\) |
|----------|-------------------------|--------------------------|
| s-wave   | 0.218                   | 0.518                    |
| p-wave (S)| 0.066                   | 0.285                    |
| p-wave (T)| 0.105                   | 0.359                    |
\( \Gamma = p + q/2 = p' + q/2 \)

\[ \mathcal{G} = \sum \mathcal{G}_0 \]

\[ \delta \Omega = \left( \begin{array}{c}
G_0 \\
\mathcal{G}_0 \\
\end{array} \right) + \left( \begin{array}{c}
g_r p_i \\
g_r p_i \\
\end{array} \right) \]
(a) $g_r = 0.6 \varepsilon_F$

(b) $g_r = 5.0 \varepsilon_F$