# Population of Closed-Channel Molecules in Trapped Fermi Gases with Broad Feshbach Resonances

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We compute the fraction of closed-channel molecules in trapped atomic Fermi gases, over the entire range of accessible fields and temperatures. We use a two-channel model of Bardeen-Cooper-Schrieffer–Bose-Einstein-condensation crossover theory at general temperature $T$, and show that this fraction provides a measure of the $T$-dependent pairing gap. Our calculations, containing no free parameters, are in good quantitative agreement with recent low-$T$ measurements in $^6$Li. We present readily testable predictions for the dependencies of the closed-channel fraction on temperature and Fermi momentum.

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The superfluid phases of ultracold, trapped atomic Fermi gases present an exciting opportunity to study how superfluidity is changed as the system evolves from the weak attraction limit of Bardeen-Cooper-Schrieffer (BCS) state to the strong attraction Bose-Einstein condensation (BEC) regime [1]. Feshbach resonances arise when a bound state (''closed-channel molecules'') of a two-body spin-singlet potential lies near the continuum onset of a spin-triplet scattering state (''open channel''). As a consequence of an applied magnetic field $B$, proximity to these resonances can profoundly change the two-body ($s$-wave) scattering lengths $a$. The well-studied Feshbach resonances in both $^6$Li and $^{40}$K are very wide as a function of $B$, compared to the Fermi energy. Moreover, the focus is on unitary scattering where $a$ diverges. For these reasons one often resorts to a one-channel version of BCS-BEC crossover theory [1,2], although attention has also been paid to the two-channel variant [3–7] for Feshbach resonances.

In recent experiments [8] on the broad resonance in $^6$Li at low temperatures, $T$, a laser drives transitions between dressed molecules (hybridized with open-channel atom pairs) and an excited molecular singlet, in the process removing excited atoms from the trap. The exponentially decreasing number of remaining trapped atoms as a function of probe duration time is used to determine that fraction $\mathcal{Z}$ of dressed molecules/pairs corresponding to the closed channel. Here we present the analogous theoretical calculations of $\mathcal{Z}$, as a function of $a$ and for general $T$. We demonstrate very good agreement with experiment, and provide predictions for future finite $T$ experiments. The small size of this fraction means that for many properties the two-channel model reduces to the single-channel description. We emphasize, however, that the two-channel model contains more information, making it capable of addressing a wider range of physical systems and experiments, and of testing the fundamentals of BCS-BEC crossover theory.

Our theoretical approach reduces to the generalized Leggett-BCS theory [1] at $T = 0$. At finite $T$, the noncondensed as well as condensed contributions enter in the appropriate combinations, so that a future measurement of the total closed-channel fraction will provide a measure of the $T$-dependent pairing gap $\Delta(T)$. This gap is, in general, distinct from the superfluid order parameter, $\tilde{\Delta}_{sc}(T)$, except at $T = 0$. Finally, we present results for the closed-channel fraction as a function of the global Fermi wave vector $k_F$, at different fields $B$. At unitarity, the dependence is a simple proportionality.

We begin with a discussion of the superfluid phase. A gas of Fermi atoms in the presence of a Feshbach resonance contains open-channel fermionic atoms as well as closed-channel molecules. Because of coupling $g$ between the open and closed channels the three propagators for the open-channel fermion pairs $[t_{pg}(Q)]$, the closed-channel molecules $[D(Q)]$ and the single (open-channel) fermion states $[G(K)]$ are all highly interconnected. Here and throughout, we use a four-momentum notation: $K \equiv (i\omega_n, \mathbf{k})$ and $Q \equiv (i\Omega_m, \mathbf{q})$, $\sum_K \equiv k_B T \sum_n \sum_{\mathbf{k}}$, and their analytical continuation, $i\omega_n \rightarrow \omega + i0^+$, $i\Omega_m \rightarrow \Omega + i0^+$, where $\omega_n = (2n+1)\pi k_B T/\hbar$, $\Omega_n = 2n\pi k_B T/\hbar$ are the odd and even Matsubara frequencies. The $T$-matrix scheme we employ to treat these coupled propagators is derived from the equations of motion for the Green's functions, and, importantly, it naturally leads to the self-consistency conditions of the standard $T = 0$ mean-field theory [1]. It can be shown [9] that the pairs are described by the pair susceptibility $\chi(Q) = \sum_K G_0(Q - K)G(K)\varphi^2_{\mathbf{k}-\mathbf{q}/2}$ where $G$ depends on a BCS-like self-energy $\Sigma(K) \approx -\Delta^2 G_0(-K)\varphi^2_{\mathbf{k}}$. Here $G_0(K)$ is the noninteracting fermion Green's function. Throughout this Letter $\varphi_{\mathbf{k}} \equiv \exp\{-k^2/2k_0^2\}$ introduces a momentum cutoff, where $k_0$ represents the inverse range of interaction, which is assumed infinite for a contact interaction.

Our Hamiltonian is the standard boson-fermion model [3,5,10] in which there are only fermion-boson and fermion-fermion interactions. Central to our analysis at finite $T$ are noncondensed pairs [9] which we characterize by a $T$ matrix $t_{pg}(Q) = U_{eff}(Q)/[1 + U_{eff}(Q)\chi(Q)]$, where

 

$U_{\rm eff}$ is the effective pairing interaction which involves the direct two-body interaction $U$ as well as virtual excitation processes associated with the Feshbach resonance [5,9]. At small $Q$, $t_{\rm pg}$ can be expanded as

$$t_{\rm pg}(Q) \approx \frac{Z^{-1}}{\Omega - \Omega_q + \mu_{\rm pair} + i\Gamma_Q}. \quad (1)$$

The parameters appearing in Eq. (1) are discussed in more detail in Ref. [10]. Here $Z^{-1}$ is a residue and $\Omega_q$ the pair dispersion. The latter parameter as well as the effective pair chemical potential $\mu_{\rm pair}$ both depend on the important but unknown gap parameter $\Delta$ through the fermion self-energy $\Sigma$. The decay width $\Gamma_Q$ is negligibly small for small $Q$ below $T_c$. We caution here that the inverse residue "$Z$" appearing in Eq. (1) is not the same as the quantity $\mathcal{Z}$ used in Ref. [8]. More technical details about the various residues can be found in Ref. [10].

To determine $\Delta$, one imposes the BEC-like constraint $\mu_{\rm pair} = 0$ which yields $t_{\rm pg}^{-1}(Q \to 0) = 0$, i.e.,

$$U_{\rm eff}^{-1}(0) + \sum_{\mathbf{k}} \frac{1 - 2f(E_{\mathbf{k}})}{2E_{\mathbf{k}}} \varphi_{\mathbf{k}}^2 = 0, \quad (2)$$

so that $\Delta$ formally satisfies the usual BCS gap equation with quasiparticle dispersion $E_{\mathbf{k}} = \sqrt{(\epsilon_{\mathbf{k}} - \mu)^2 + \Delta^2 \varphi_{\mathbf{k}}^2}$, where $\epsilon_{\mathbf{k}} = \hbar^2 k^2/2m$ is the fermion kinetic energy, $\mu$ is the fermionic chemical potential, and $f(x)$ is the Fermi distribution function.

Physically, one should view $\Delta$ as reflecting the presence of bosonic degrees of freedom. In the fermionic regime ($\mu > 0$), it represents the energy required to break the pairs. It contains contributions from both noncondensed and condensed pairs, whose densities are proportional to $\Delta_{\rm pg}^2(T)$ and $\tilde{\Delta}_{\rm sc}^2(T)$, respectively. One has a constraint on the *number of pairs* [10] which can be viewed as analogous to the usual BEC number constraint

$$\Delta^2(T) = \tilde{\Delta}_{\rm sc}^2(T) + \Delta_{\rm pg}^2(T). \quad (3)$$

The total contribution of noncondensed pairs is readily computed in terms of $\Delta$ via

$$\Delta_{\rm pg}^2 \equiv -\sum_Q t_{\rm pg}(Q). \quad (4)$$

One can then compute the number of condensed pairs associated with $\tilde{\Delta}_{\rm sc}$.

Fermions are the fundamental particles in this system, so that their chemical potential $\mu$ is determined from the number conservation constraint

$$n = n_f + 2n_{b0} + 2n_b \equiv n_f + 2n_b^{\rm tot}, \quad (5)$$

where $n_{b0}$ and $n_b$ represent the density of condensed and noncondensed closed-channel molecules, respectively, $n_b^{\rm tot}$ is their sum, and $n_f = 2\sum_K G(K)$ is the atomic density associated with the open-channel fermions. Here

$$n_b = -\sum_Q D(Q) \approx Z_b \sum_{\mathbf{q}} b(\Omega_{\mathbf{q}} - \mu_{\rm pair}), \quad (6)$$

where $b(x)$ is the Bose distribution function. The renormalized closed-channel molecule propagator $D(Q)$ is given by the same equation as Eq. (1) with a different residue $Z^{-1} \to Z_b$. We compute $\Delta$ (and $\mu$) via Eqs. (2) and (5), to determine the contribution from the condensate $\tilde{\Delta}_{\rm sc}$ via Eqs. (3) and (4). Note that at $T = 0$, $\Delta_{\rm pg} = 0$ so that all pairs are condensed.

At $T = 0$, a nonzero excitation gap for all $\mathbf{k}$ constrains $n_f$ so that one can identify our closed-channel fraction $2n_b^{\rm tot}/n = 2n_{b0}/n$ with the quantity $\mathcal{Z}$ in experiment. In this picture the ground state consists of $n/2$ pairs with fraction $2n_{b0}/n$ in the closed channel. A short range attractive interaction (appropriate for cold Fermi gases) leads to a picture in which all fermions are paired, since the attraction extends to the entire Fermi sphere. Importantly, this is consistent, at least at unitarity, with the observed exponential behavior of the remaining total particle number in the trap found in Ref. [8]. Thus, we presume here that the ground state has no unpaired fermions.

The interaction parameters $U$ and $g$ which appear in the Hamiltonian can be related to their experimental counterparts $U_0$ and $g_0$. The latter are, in turn, determined by the open-channel background scattering length $a_{\rm bg}$ and the Feshbach resonance width $W$: $U_0 = 4\pi a_{\rm bg}\hbar^2/m = 8\pi k_F a_{\rm bg}(E_F/k_F^3)$ and $g_0^2 = |U_0 W|$. Here $E_F = \hbar^2 k_F^2/2m$ is the global noninteracting Fermi energy. From the Lippmann-Schwinger equation [11] we obtain $1/U_0 = 1/U - 1/U_c$, where $1/U_c \equiv -\sum_{\mathbf{k}}(\varphi_{\mathbf{k}}^2/2\epsilon_{\mathbf{k}})$ is the value of the interaction corresponding to unitary scattering ($a = \infty$). Similarly, we define $U^* \equiv 4\pi a^* \hbar^2/m$ and the "experimental" magnetic detuning $\nu_0$ such that

$$U^* = U_0 + \frac{g_0^2}{2\mu - \nu_0}, \qquad \frac{1}{U^*} = \frac{1}{U_{\rm eff}} - \frac{1}{U_c}. \quad (7)$$

As in Ref. [11], defining $\Gamma = 1/(1 + U_0/U_c)$, one has $U = \Gamma U_0$, $g = \Gamma g_0$, and $\nu = \nu_0 - \Gamma g_0^2/U_c$. In order to make contact with experiment, it is convenient to define a two-body counterpart of $U^*$ in Eq. (7):

$$U_{2B} \equiv 4\pi a \hbar^2/m = U_0 - g_0^2/\nu_0, \quad (8)$$

which diverges at $\nu_0 = 0$. Here $\nu_0 = (B - B_0)\Delta\mu^0$, where $B_0$ is the resonance field, and $\Delta\mu^0 = 2\mu_B$ for $^6$Li is the difference in the magnetic moment between open-channel pairs and the closed-channel molecules [12]. Here $\mu_B$ is the Bohr magneton. For the wide Feshbach resonances in $^{40}$K and $^6$Li, the dimensionless parameters $1/k_F a$ and $1/k_F a^*$ are very close to each other for the magnetic fields addressed in Ref. [8].

It is useful now to rewrite the closed-channel density in terms of more physically accessible parameters. One can show [9] $n_{b0} \propto \tilde{\Delta}_{\rm sc}^2$. It follows from our $T \neq 0$ formalism [10] that when a condensate is present

$$n_{b0} = Z_g \tilde{\Delta}_{\rm sc}^2, \qquad n_b = Z_g \Delta_{\rm pg}^2 = \frac{\Delta_{\rm pg}^2}{g_0^2}\left(1 - \frac{a_{\rm bg}}{a^*}\right)^2, \quad (9)$$

where we have used some simple algebra to rewrite $Z_g \equiv g^2/[(2\mu - \nu)U + g^2]^2$. Importantly, in this way we can conclude from Eq. (3) that the total closed-channel contribution $n_b^{\rm tot} = Z_g \Delta^2$. The simplicity of this last result reflects the fact that $D(Q)$ and $t_{\rm pg}(Q)$ [of Eq. (1)] share the same denominator. The relative probabilities for the (hybridized) pairs to live in the closed and open channels are essentially fixed for all $T \leq T_c$ and given by $Z_b = Z_g/Z$ and $1 - Z_b$, respectively.

To represent the trap, we use the local density approximation (LDA) by replacing $\mu \rightarrow \mu(r) \equiv \mu - V(r)$. Here $\mu$ is the global chemical potential and $V(r) = m\omega^2 r^2/2$ for a harmonic trap with angular frequency $\omega$. We solve Eqs. (4) and (2) at each $r$ for given $\mu$ and then self-consistently adjust $\mu$ to satisfy the total number constraint $N = \int d^3 r n(r)$. We define $N_{b0} \equiv \int d^3 r n_{b0}(r)$ and similarly for the noncondensed molecules $N_b$, and the total $N_b^{\rm tot} = N_{b0} + N_b$. Here $N_{b0}$ represents the trap average of the superfluid order parameter. Moreover, this trap average is proportional to the order parameter at the center so that $N_{b0}/N \propto \tilde{\Delta}_{\rm sc}^2(r = 0)$. Thus, this full two-channel calculation provides a theoretical underpinning for the simple interpretation, provided in Ref. [8], of their experiments.

In the unitary regime where $|a_{\rm bg}/a^*| \ll 1$, Eq. (9) implies $n_{b0} \approx \tilde{\Delta}_{\rm sc}^2/g_0^2$, at each point $r$. Therefore, we can deduce that at unitarity

$$\frac{2N_{b0}}{N} = \int d^3 r \frac{\tilde{\Delta}_{\rm sc}^2(r)}{g_0^2 N} \propto \frac{\int d^3 r \tilde{\Delta}_{\rm sc}^2(r)/E_F^2}{\int d^3 r n(r)/n(0)} \frac{\sqrt{E_F}}{g_0^2} \propto \sqrt{T_F}. \quad (10)$$

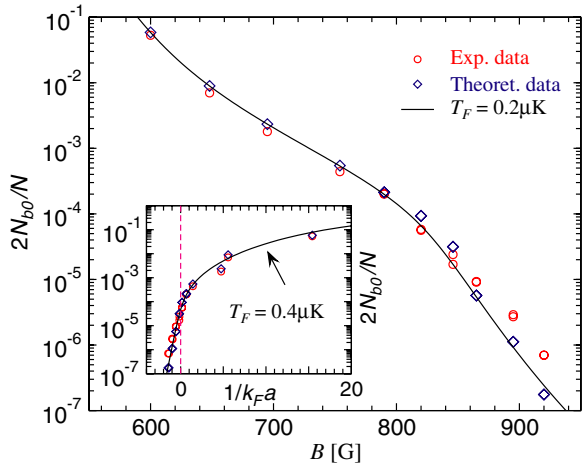


FIG. 1 (color online). Calculated closed-channel fraction $2N_b^{\rm tot}/N = 2N_{b0}/N$ at $T = 0$ as a function of magnetic field $B$ (main figure) at $T_F = 0.2$ $\mu$K for $^6$Li in a harmonic trap. The inset shows $2N_{b0}/N$ as a function of $1/k_F a$ (black curve) at $T_F = 0.4$ $\mu$K. The red circles are experimental measurements from Ref. [8], and the blue diamonds are theoretically calculated data using specific values of $T_F$ from experiment [13], which vary between 0.18–0.662 $\mu$K.

At unitarity, $2N_{b0}/N$ scales with $k_F$. Here we have used the relationship $N = n(0) \int d^3 r[n(r)/n(0)]$ and $n(0) \propto E_F^{3/2}$. The fraction in front of $\sqrt{E_F}/g_0^2$ is dimensionless and independent of $T_F$.

In Fig. 1, we plot the calculated molecular fraction $2N_{b0}/N$ at $T = 0$ for $^6$Li (black curve and blue diamonds) as a function of the magnetic field $B$ as compared with experimental data (red circles) from Ref. [8]. The experimental values for $T_F$ vary from one data point to another. Our calculations at each field value use as input the specific experimental value for $T_F$, plotted as blue diamonds, in the figure and inset. However, for the continuous curve plotted in the main figure, we use $T_F = 0.2$ $\mu$K which better represents the values in the BCS regime [13]. In the inset we used $T_F = 0.4$ $\mu$K, since this best reflects the average value over the entire range of data points. These slightly different choices for $T_F$ reflect the fact that the two plots have different horizontal axes, and, therefore, amplify small errors in different ways. As will be shown below, in the BCS regime the results are particularly sensitive to $T_F$. We take the parameters for the Feshbach resonance from Ref. [14]: $W = 300$ G and a field-dependent $a_{\rm bg} = a_{\rm bg}^0/[1 + \alpha(B - B_0)]$, where $a_{\rm bg}^0 = -1405 a_0$, $\alpha = 0.0004$ G$^{-1}$, $B_0 = 834.15$ G, and $a_0 = 0.529$ Å is the Bohr radius. For $T_F = 0.4$ $\mu$K, this uniquely determines $U_0 = -5.90 E_F/k_F^3$ and $g_0 = -771 E_F/k_F^{3/2}$ at unitarity.

In Fig. 1 the roughly a factor of 3 difference between theory and experiment in the BCS regime may in part be associated with the observed deviation from an exponential time dependence [8]. Because of the extremely small gap ($\lesssim T$) at these high fields, unpaired fermions may be thermally excited. However, it should be noted that this particular thermal "correction" alone would be in the wrong direction (see below). This may point to the need

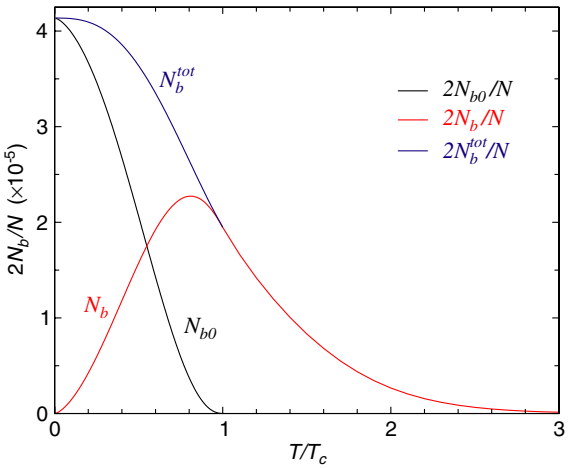


FIG. 2 (color online). Closed-channel fraction as a function of $T/T_c$ at unitarity for $T_F = 0.4$ $\mu$K for $^6$Li in a harmonic trap. The black, red, and blue curves are the condensed ($2N_{b0}/N$), noncondensed ($2N_b/N$), and total ($2N_b^{\rm tot}/N$) fractions, respectively. Here $T_c = 0.273 T_F$. In the BEC regime $2N_b^{\rm tot}/N$ is relatively $T$ independent below $T_c$.

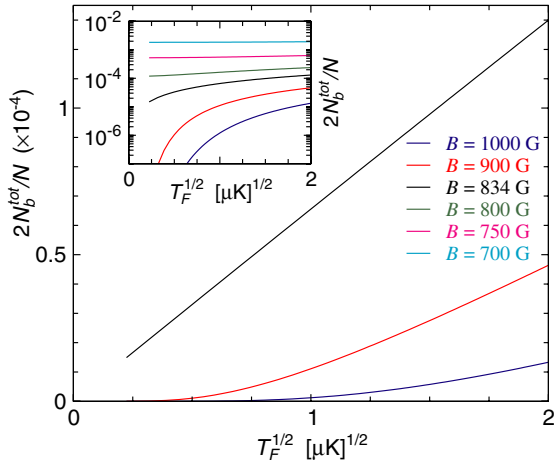


FIG. 3 (color online). Predicted closed-channel fraction $2N_{b0}/N$ at $T = 0$ as a function of $\sqrt{T_F} \propto k_F$ at different fields for $^6$Li in a harmonic trap. At unitarity ($B = 834$ G, black line), $2N_{b0}/N \propto k_F$. On the BCS side ($B = 900$ G, red, and $B = 1000$ G, blue), this becomes a higher power law. On the BEC side ($B < 834$ G, see the inset, $B$ increases from top to bottom), the fraction becomes less sensitive to $T_F$, and is determined by two-body physics in the deep BEC limit.

for a more systematic treatment of dynamical effects in this regime. Overall, agreement with the data is quantitatively very good [8] everywhere but in the BCS regime; there are no adjustable parameters [15].

We turn to the $T$ dependence of the closed-channel fraction, which is plotted at unitarity in Fig. 2. This fraction was shown above to be proportional to the pairing gap squared $\Delta^2(T)$. The condensed fraction $2N_{b0}/N$ (black curve) decreases as $T$ increases from zero and vanishes at $T_c$. At the same time, the noncondensed fraction $2N_b/N$ (red) increases from zero, as determined by Eq. (6). It has a maximum slightly below $T_c$. The total fraction $2N_b^{\rm tot}/N$ (blue) decreases monotonically with $T$. Note that it decreases very slowly at low $T$. This justifies our comparison in Fig. 1 between the $T = 0$ calculations and the low-$T$ measurements. Using Eqs. (9) and (10), and in conjunction with the temperature insensitivity of the various residues ($Z_g$ and $Z_b$), one can measure the $T$ dependence of the pairing gap, presuming that $T$ is determined from isentropic sweeps [16]. The sensitivity of the total fraction to temperature increases with field.

In Fig. 3, we plot $2N_{b0}/N$ at $T = 0$ as a function of $\sqrt{T_F} \propto k_F$ for different magnetic fields, from the weak pairing BCS ($B = 1000$ G, blue curve) to the strong pairing BEC ($B = 700$ G, cyan curve). It can be seen that the plots reflect our earlier theoretical prediction that $2N_{b0}/N \propto k_F$ at unitarity. As the field increases, $2N_{b0}/N$ varies as a higher power of $k_F$. In contrast, as the field decreases in the BEC regime, it becomes less sensitive to $k_F$. For $^6$Li, it approaches unity in the deep BEC limit, where it is dominated by two-body physics. More generally, $2N_{b0}/N$ increases faster (slower) on the BCS (BEC) side than the simple proportionality found at unitarity, as is confirmed by Fig. 3.

In summary, we find that the wider the resonance is, the more readily the closed-channel molecules decay into the open channel so that the steady state molecular fraction remains small, as observed experimentally. We have shown here that measurements of the closed-channel fraction will complement other techniques for obtaining the pairing gap. While broad Feshbach resonances often lead to universal behavior at unitarity [17], a single dimensionless parameter $k_F a$ is inadequate for determining quantities such as $2N_{b0}/N$, which is intrinsically associated with two-channel physics.

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*Note added.*—After submission of this Letter, two papers appeared on the $T = 0$ closed-channel fraction within a homogeneous system based on a different model for the ground state [18] and on a limiting case [19] of the present theory in which direct interfermion interactions and the closed-channel self-energy are ignored.

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