A generalized molecule approach capturing the Feshbach-induced pairing physics in the BEC–BCS crossover

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Received 24 February 2021, revised 25 March 2021
Accepted for publication 13 April 2021
Published 19 May 2021

Abstract
By including the effect of a trap with characteristic energy given by the Fermi temperature $T_F$ in a two-body two-channel model for Feshbach resonances, we reproduce the measured binding energy of ultracold molecules in a $^{40}$K atomic Fermi gas. We also reproduce the experimental closed-channel fraction $Z$ across the BEC–BCS crossover and into the BCS regime of a $^6$Li atomic Fermi gas. We obtain the expected behavior $Z \propto \sqrt{T_F}$ at unitarity, together with the recently measured proportionality constant. Our results are also in agreement with recent measurements of the $Z$ dependency on $T_F$ on the BCS side, where a significant quantitative discrepancy between experimental data and theory’s predictions has been repeatedly reported. In order to contrast with future experiments we report the proportionality constant at unitarity between $Z$ and $\sqrt{T_F}$ predicted by our model for a $^{40}$K atomic Fermi gas.

Keywords: ultracold atoms, Fermi gases, BEC–BCS crossover, Feshbach molecules

(Some figures may appear in colour only in the online journal)

1. Introduction
Magnetic-field tunable Feshbach resonances provide the essential tool to control the interaction between atoms in ultracold quantum gases. In current ultracold gases experiments these resonances are induced by varying the strength of an external magnetic field used to tune the relative energy between the collision energy of two atoms and that of a quasibound molecular state via the Zeeman effect. The resonant interactions allow not only to control the strength of the atomic interactions but also if they are effectively repulsive or attractive [1, 2]. Over the last twenty years, this precise generation and control of interactions has been a crucial ingredient in the understanding of the behavior of quantum matter, leading to many breakthroughs such as the generation of fermionic Bose–Einstein condensates (BECs) [3–6], the observation of a reversible crossover to a degenerate Fermi gas [7, 8], measurements of collective excitation modes as well as pairing in a strongly interacting Fermi gas of atoms [9, 10], and proofs of superfluidity in Fermi gases [11–14].

The crossover from a molecular BEC to atomic Cooper pairs in the Bardeen–Cooper–Schrieffer (BCS) state (namely, the BEC–BCS crossover) near a Feshbach resonance has been widely studied through several theoretical approaches, such as quantum Monte Carlo methods [15–17], field theory [18, 19], and multi- or two-channel calculations [20–23]. However, as it is pointed out in references [19, 24, 25], most of these theories fail to reproduce the measured closed-channel fraction and show a significant disagreement when compared to the available above-resonance experimental data [24, 25]. The recent experiments of reference [25] reinforce that even in very satisfactory matches (as the achieved in references [19, 26] by developing a functional integral formalism for...
atom and molecule field, or in references [25, 27] within a two-channel pairing fluctuation theory there is a considerable quantitative discrepancy between theory and experiments in the near-BCS regime.

In this work we present a quite simple two-channel model for two harmonically trapped atoms with finite-range interaction near a Feshbach resonance. We show that when including an effective trap which accounts not only for the optical trap and its geometry but also for the nontrivial many-body correlations the considered two-body model leads to handy general and near-resonance formulas for the binding energy and the closed-channel contribution, as well as to intuitive and accurate results. Our results reproduce the measured binding energy of ultracold molecules in a $^{40}$K atomic Fermi gas. Our results also reproduce the measured closed-channel fraction $Z$ across the BEC–BCS crossover and into the BCS regime of a $^{6}$Li atomic Fermi gas [24, 25]. We obtained the expected dependency of $Z$ on the Fermi temperature $T_F$ at unitarity: $Z \propto T_F^{-1}$, together with a proportionality constant in close agreement with the recently measured value (see reference [25]). Moreover, our calculated closed-channel fraction is in agreement with the measurements of the $Z$ dependency on $T_F$ on the near-BCS side reported in reference [25].

The structure of the paper is as follows. The proposed effective model is presented in section 2. In section 3 we show that our model reproduces several experimental measurements, as well as previous theoretical results. Finally, a summary and conclusions are given in section 4, which also includes a discussion about some applications and extensions of our work.

## 2. The proposed effective model

The qualitative essence of the BEC–BCS crossover involves a continual change between a BEC of diatomic molecules (that in the case of a Fermi gas implies the emergence of a bosonic degree of freedom) and a BCS loosely correlated Cooper pairing state. This simple idea points to the need of considering diatomic molecules that are more and more weakly bound. In other words, we need to consider generalized molecules or pairs stabilized by many-body effects [28]. A simple model that enables such a pairing of atoms consists of two channels (open and closed) in which a two-body bound state can be created. The open-channel corresponds to two atoms while the closed-channel supports bare molecular states [24]. Then, the complete picture consists of a pair or dressed molecule in a superposition of the open- and closed-channel states,

$$|\psi_{\text{pair}}\rangle = |\psi_{\text{m}}\rangle_{\text{closed}} + |\psi_{\text{aa}}\rangle_{\text{open}},$$

with normalization $1 = \int |\psi_{\text{m}}|^2 \, d^3r + \int |\psi_{\text{aa}}|^2 \, d^3r$ [2, 29]. Therefore, $\int |\psi_{\text{m}}|^2 \, d^3r$ gives the probability of the generalized molecule or pair to be in the closed-channel, i.e. the closed-channel population or closed-channel fraction which is usually denoted by $Z$. Here the simple idea is that each possible pair in the system behaves as our modeled generalized molecule. Then the number of pairs in the closed-channel satisfies $N_{cc} = N_{pp} \int |\psi_{\text{m}}|^2 \, d^3r = (N/2) \int |\psi_{\text{m}}|^2 \, d^3r$, where $N_{pp}$ is the number of possible pairs in the system and $N$ the number of atoms (notice that $N_{pp} = N/2$ for an unpolarized gas), being equivalent to $\int |\psi_{\text{m}}|^2 \, d^3r = 2 N_{cc}/N = Z$ [27, 30]. Notice that our previous qualitative formulation of the crossover requires $Z \sim 1$ deep into the BEC side and $Z \sim 0$ on the BCS side.

Translating all the above into equations, the wave function of two trapped atoms with mass $m$ on an open-channel supporting the threshold of the two-atom state and a closed-channel supporting a bound state $E_c$ magnetically tuned close to the threshold satisfies

$$E |\psi_{\text{pair}}\rangle = \left( -\frac{\hbar^2}{m} \nabla^2 + \frac{m \omega^2}{4} \right) |\psi_{\text{pair}}\rangle,$$

$$\hat{\psi} = \begin{cases} \psi_{\text{open}} & \text{for } r \leq r_0, \\ \psi_{\text{closed}} & \text{for } r > r_0, \end{cases}$$

where we consider spherical attractive potentials with range $r_0$ and depths $-\hbar^2 \gamma/2m$, a coupling between channels given by $\Omega$, a trap frequency denoted by $\omega$, and the Zeeman shift $\mu B$.

To solve equation (1) one must introduce new superposition states, $|+\rangle = \cos \theta |\text{open}\rangle + \sin \theta |\text{closed}\rangle$ and $|-\rangle = -\sin \theta |\text{open}\rangle + \cos \theta |\text{closed}\rangle$, related to new dressed uncoupled channels [22, 23]. The scattering length $a$ is obtained by solving the free-trap zero-energy scattering equation (see references [31, 32]) and can be rewritten in terms of the magnetic field as

$$a = \frac{a_{bg} - r_0}{\Delta B},$$

with $\Delta B$ being the resonance width and $B_{\text{res}}$ the resonance position. These quantities are given by $\Delta B = -\hbar^2 \gamma (a_{bg} - r_0)/m \mu B$ and $B_{\text{res}} = -\hbar^2 \gamma/m \mu B + \Delta B$, where $a_{bg}$ is the background scattering length, $\gamma = 2 q_f^2 \Omega^2/2r_0$ is the Feshbach coupling, and $\theta$ is the mixing angle of the dressed states [22, 23]. The scattering length $a$ diverges when $B$ is tuned very close to the resonance. In this situation, known as the unitary limit, the scattering length changes its sign from positive ($a > 0$, molecular side -BEC) to negative ($a < 0$, atom–atom side -BCS).

The energy of the two-body state obtained when solving equation (1) without restrictions is determined by

$$\frac{\lambda}{D_{\text{inv}}(q_{\text{inv}})} = \cos \theta \frac{\lambda_+}{f_{\text{inv}}^{+}(q_{\text{inv}})} + \sin \theta \frac{\lambda_-}{f_{\text{inv}}^{-}(q_{\text{inv}})},$$

where $f^\pm(x) = D_+(x) \pm D_-(x)$ with $D_+(x)$ being the parabolic cylinder functions [33, 34], and $x_0 = \sqrt{m \omega/2r_0}$. These functions depend on $\lambda = \epsilon - 1/2$ where $\epsilon = E/\hbar \omega$,

\[\text{Notice that the total wave function is a product of the center of mass state (a three dimensional oscillator state) and the relative state satisfying the relative Schrödinger equation given by equation (1)}.\]
\( \lambda = \lambda + \frac{2 g^2}{m} \) and \( \lambda^\prime = \lambda - \frac{2 g^2}{m} - \epsilon_c - \mu B/\hbar \omega \). For the last expressions we used \( g^2 = g^2 \) and \( \mu = \hbar \omega \). We also used the weak coupled channels conditions, i.e. \( \Omega \ll \frac{g^2}{m} \) implying \( \theta \ll 1 \), which has been found to be an excellent approximation \[34, 35\]. Notice that all the parameters are divided by the trap’s characteristic length or energy. Taking into account several properties of the parabolic cylinder functions, assuming that the states are close to the threshold, and considering the experimental ranges of the involved quantities, equation (3) transforms into

\[
- \frac{\sqrt{2} \Gamma(\frac{1+i}{2})}{\Gamma(\frac{1-i}{2})} + \frac{1}{x_0 - \tilde{a}_{bg}} \left( \epsilon_c + \frac{\mu B}{\hbar \omega} - \lambda \right) = \gamma,
\]

where \( \tilde{a}_{bg} = \sqrt{m \omega} / \hbar \) and \( \gamma = \sqrt{m \omega} / (\hbar \omega) \). When the coupling between channels is absent (\( \gamma = 0 \)) equation (5) implies \( \lambda = \epsilon_c + \frac{\mu B}{\hbar \omega} \) and \( \sqrt{2} \Gamma(1/2 - \lambda/2) / \Gamma(-\lambda/2) = 1 / (\tilde{a}_{bg} - x_0) \). The former corresponds to the bound state in the closed-channel while the latter resembles the results obtained when considering a single channel in a trap \[34, 36\].

The closed-channel fraction \( Z \) can be obtained by direct integration of the closed-channel wave function \( Z = \int |\psi_m|^2 d^3 r \) (thus requiring numerical integration) or as the derivative of the energy on \( \epsilon_c \) (i.e. \( Z = \partial \lambda / \partial \epsilon_c \)) due to the Hellman–Feynman theorem \[2, 22, 30\]. Although both procedures provide the same result, the second one leads directly to

\[
Z = \frac{2 \gamma}{2 \gamma + (\epsilon_c + \frac{\mu B}{\hbar \omega} - \lambda)^2 / \Gamma(-\gamma/2) \cdot \left\{ \Psi (\frac{1}{4} - \frac{\gamma}{2}) - \Psi (-\frac{1}{4}) \right\}},
\]

where \( \Psi(z) \) denotes the digamma function \[33\]. For a given magnetic field, one must first solve equation (5) to obtain the ground state energy and then insert it in equation (6) in order to compute the closed-channel fraction.

It is possible to obtain even simpler near-resonance expressions. Expanding equation (5) for small \( \lambda \) and using equation (2), the dependence of the molecular binding energy on the scattering length and magnetic field reads

\[
\frac{\sqrt{2} \Gamma(\frac{1+i}{2})}{\Gamma(\frac{1-i}{2})} = \frac{1}{\tilde{a} - x_0} = \frac{\mu (B - B_{res})}{\hbar \omega \gamma (\tilde{a}_{bg} - x_0)^2},
\]

where \( \tilde{a} = \sqrt{m \omega} / \hbar a \). Since the characteristic length of the trap is larger than the range of the interaction, the obtained dependence of the molecular binding energy on the scattering length is essentially the same obtained for a delta potential plus a correction due to the interaction range.

Although the free-trap two-body theory predicts that the closed-channel fraction vanishes when the resonance is reached (due to the absence of a two-body bound state for \( a < 0 \) in free space), the experimental evidence shows that it continues smoothly across the resonance \[22, 24, 25, 27, 37\]. Using the near-resonance approximation of equation (7) given by \( \lambda = \mu (B - B_{res}) / (\hbar \omega) \) in a first order expansion of equation (6) in the variable \( \lambda \), it is straightforward to see that the non-vanishing closed-channel contribution in the resonance is

\[
\frac{Z_{res}}{1} = \frac{1}{1 + \sqrt{\frac{\pi \hbar}{2 m \omega^2}} (\tilde{a}_{bg} - r_0)^2}.
\]

Now the naive idea is that the trap in our model is an effective trap accounting not only for the optical trap but also for the nontrivial many-body correlations. The effective trap frequency is given by \( \hbar \omega_{eq} = k_B T_F / \hbar \omega (3 N)^{1/3}, \) where \( k_B \) is the Boltzmann constant, \( T_F \) the Fermi temperature, and \( \omega \) the geometric mean of the three frequencies of the external trap \[30, 32\]. In other words, the characteristic energy of the trap is given by the Fermi temperature of a harmonically trapped ideal Fermi gas, and its characteristic length is comparable to the interparticle spacing. The effective trap takes into account the geometry of the optical trap (present in \( \omega \)) as well as the number of atoms \( N \). For vanishing \( \omega (3 N)^{1/3} \) the trap is absent and \( Z_{res} \) goes to zero recovering the results of the free-trap model of reference \[22\]. Numerical integration of the wave function gives \( \langle r \rangle = a/2 \) for fields below the resonance width, in consonance with the results of the regularized delta and two-channel free models \[32, 32\]. Deep into the BEC side the generalization of molecules or pairs behave as point-like composite bosons unaffected by the effective trap, while the pair size grows towards the resonance. When the available space defined by the effective trap is large compared to the size of the pairs (BEC side), the trap enhances the closed-channel fraction in line with the intuitive notion that the trap forces the
BEC–BCS crossover regime given by radius and magneton respectively. The vertical gray dashed lines indicate the black dashed line are the results obtained using equation (5). The free-trap model of reference [22] is depicted in gray solid line. The extracted from reference [8]. The calculated energy within the free model below the resonance and shows a good agreement with the dependency of \( Z \) on \( T_F \) at unitarity predicted in references [27, 30, 40] within different many-body approaches.

In what follows we contrast our results with the available experimental data for the binding energy measured in a \(^{40}\text{K} \) ultracold Fermi gas [8], as well as for the closed-channel fraction measured in a \(^{6}\text{Li} \) Fermi gas when crossing the so called \(^{6}\text{Li} \) broad resonance [24, 25] and with the theoretical results of reference [27]. The corresponding parameters are given in table 1.

Figure 1 depicts the binding energy of the molecules \( E_B \) vs magnetic field \( B \) in a \(^{40}\text{K} \) Fermi gas. The points are the experimental measurements extracted from reference [8]. The calculated energy within the free-trap model of reference [22] is depicted in gray solid line. The black dashed line are the results obtained using equation (5). The vertical gray dashed lines indicate the \( B_{\text{res}} \) value and the typical BEC–BCS crossover regime given by \( |a| > 3000a_0 \).

### Table 1. Parameters of the \(^{40}\text{K} \) and \(^{6}\text{Li} \) broad Feshbach resonances extracted from references [2, 22], where \( a_0 \) and \( \mu_B \) denote the Bohr radius and magneton respectively.

|        | \( r_0(a_0) \) | \( B_{\text{res}} \) (G) | \( \Delta B \) (G) | \( a_0(a_0) \) | \( \mu_B(\mu_B) \) | \( \gamma^{-1/2}(a_0) \) |
|--------|----------------|------------------|-----------------|----------------|-----------------|----------------|
| \(^{40}\text{K} \) | 62 | 224.2 | -9.7 | 174 | 1.68 | 76.25 |
| \(^{6}\text{Li} \) | 29.9 | 834.15 | 300 | -1405 | 2.0 | 101 |

Figure 2 shows the closed-channel fraction \( Z \) vs magnetic field \( B \) in a \(^{6}\text{Li} \) Fermi gas. The points are the experimental data of reference [24], whose size reflects the uncertainty in \( Z \). The closed-channel fraction obtained with the free-trap model of reference [22] is depicted in gray solid line while our results are depicted in black dashed line, see equation (6). The approximation calculated using equation (7) is shown in gray dot–dashed line. The horizontal lightgray dot–dashed line gives the closed-channel fraction in the resonance \( Z_{\text{res}} \). Vertical lightgray dashed lines indicate the \( B_{\text{res}} \) value and the typical BEC–BCS crossover regime \( |a| > 3000a_0 \). Notice that the 920 G point is identified in reference [24] as presenting some issues. The inset depicts the obtained \( Z \) for several \( T_F \) values.

### 3. Comparison with available experimental data and other theoretical approaches’ results

In the present section we intend to show that our effective model reproduces several theoretical and experimental results. First of all, by using \( \omega = \omega_{\text{eff}} = k_BT_f/h \) in a first order expansion of equation (8) in the variable \( \omega \), we obtain

\[
Z_{\text{res}} = \frac{\sqrt{2k_Bm}}{\gamma(a_{\text{bg}} - r_0)T_F} \sqrt{T_F},
\]

in agreement with the dependency of \( Z \) on \( T_F \) at unitarity predicted in references [27, 30, 40] within different many-body approaches.

In what follows we contrast our results with the available experimental data for the binding energy measured in a \(^{40}\text{K} \) ultracold Fermi gas [8], as well as for the closed-channel fraction measured in a \(^{6}\text{Li} \) Fermi gas when crossing the so called \(^{6}\text{Li} \) broad resonance [24, 25] and with the theoretical results of reference [27]. The corresponding parameters are given in table 1.
results are recovered when $T_F$ is small enough, the inset of the figure contains the obtained $Z$ for different values of $T_F$. Notice that in reference [24] the 920 G point is identified as presenting some issues (a deviation in the exponential approximation of the loss time dependency), which can be the reason for its deviation.

Figure 3 depicts the dependency of the closed-channel fraction on $T_F$ at unitarity for a $^6$Li Fermi gas. Our results (black line) are in close agreement with the experimental data (dots) and the datafit (gray dashed line) presented in reference [25]. From equation (9) we obtain $Z = 0.074\sqrt{T_F/K}$ at unitarity, while the experimental and theoretical proportionality constant reported in reference [25] are $0.074(12)/\sqrt{K}$ and $0.066/\sqrt{K}$ (gray dot–dashed line) respectively. Therefore, the proportionality constant predicted by our very simple theoretical model is closer to the experimental measures than the one obtained within the theoretical approach of references [25, 27]. To show that the obtained $Z$ is in qualitative agreement with previous theoretical results, the inset of figure 3 depicts its behavior for several magnetic fields in qualitative agreement with the results of reference [27] (we obtain a larger $Z$ on the BCS side which is in closer agreement with experimental measurements).

Figure 4 shows the agreement between our results (black line) and the experimental data of reference [25] (dots) for fields above resonance (near-BCS side) and $T_F = 0.45 \mu K$. The left-bottom inset depicts a comparison between our results and the theoretical closed-channel fraction (dot-dashed brown curve) reported in the inset of figure 4 of reference [25]. The curve obtained within the theoretical approach of references [25, 27] presents a significant quantitative discrepancy when compared to the experimental data varying from one to three orders of magnitude in the near-BCS regime, instead, our very simple model exhibits a remarkable agreement (regarding this it is important to notice that in their figure 4 the authors of reference [25] have multiplied their theoretical curve by 8 in order to reach the experimental data scale, see the corresponding caption). In other words, our theoretical Z which is larger than the one calculated in references [25, 27] on the BCS side (see the inset of figure 3 and the left-bottom inset of figure 4) presents a closer agreement with the experiments performed in that regime. Finally, the obtained agreement with measurements and the power law datafit (gray dashed line) reported in reference [25] for $B = 925$ G is shown in the right-top inset of figure 4. Notice that the deviation between our calculated $Z$ and the 920 G point of figure 2 can be disregarded at the light of the close agreement obtained with the recent measurements of reference [25], as depicted in the right-top inset of figure 4 for 925 G.

Before moving to the last section we would like to add that using the parameters given in references [2, 22] our model predicts that $Z = 13.5549\sqrt{T_F/K}$ at unitarity for the 224.2 G resonance of $^{40}$K. To the best of our knowledge measurements focusing on the closed-channel fraction with $^{40}$K have not been yet performed, even so, we leave this result in order to contrast with future experiments.

4. Summary and conclusions

In conclusion, by adding a trap with characteristic energy given by the Fermi temperature $T_F$ to a very simple two-channel two-body model for Feshbach resonances, we were able to reproduce the measured binding energy of ultracold molecules in a $^{40}$K atomic Fermi gas as well as the measured closed-channel
fraction $Z$ across the BEC–BCS crossover and into the BCS regime of a $^6\text{Li}$ atomic Fermi gas [24, 25]. We derived general and near-resonance simple formulas which show remarkable agreement with experimental measurements and previous theoretical results [27, 30, 40]. We obtained the expected dependency $Z \propto \sqrt{T_F}$ at unitarity, together with a proportionality constant that reproduces the value reported in the recent experiments of reference [25]. Our results are also in agreement with the measurements of the $Z$ dependency on $T_F$ on the near-BCS side, where a significant quantitative discrepancy between the experimental data and theory’s predictions has been repeatedly observed [19, 24, 25].

Our interpretation of the model presented in this work is as follows. The effective trap accounts not only for the optical trap and its geometry but also for the nontrivial many-body fermionic correlations. Our naive picture is that all the remaining fermions and their correlations act as a trap supporting a bound state for the generalized molecule or pair which leads, in turn, to a non-vanishing closed-channel fraction for fields above resonance. In other words, the generalized molecules or pairs are stabilized by the many-body effects which are included in the model as an effective trap (in this sense the trap averages the effects of all the remaining fermions as in a mean-field approach). We would like to stress the simplicity of the model as well as its intuitive and accurate results. The effective trap simulates the remaining fermions because it emulates the insufficient physical space that favors the interaction between pairs and provides a mechanism for Pauli blocking [38, 39]. This paves the way for studying the many-body unitarity physics by adding the exchange interactions within the composite boson ansatz [41–44], whose construction of the many-particle state relies upon the availability of an accurate pairing model.

Since the results obtained within our very simple model based on the intuitive idea of generalized molecules or pairs stabilized by many-body effects shows a remarkable agreement with several experimental data as well as with other theoretical approaches (moreover, our calculated closed-channel fraction depicts a closer agreement with the measured values in the near-BCS regime than the agreement depicted by the closed-channel fraction obtained in previous theoretical works), we strongly believe that our model deserves some attention. Even so, the model must be exposed to further contrast and evaluation. Our predicted proportionality constant for the closed-channel fraction at unitarity for a $^{40}\text{K}$ Fermi gas must be compared with future experiments keeping in mind that any potential deviation between our calculations and future experimental data most probably will arise from the interactions and many-body effects that are not being considered in our very simple model. We are also engaged in the study of the thermodynamics of the generalized molecules or pairs in order to compare the results obtained with our model and those of reference [27, 45, 46]. In this context, a complete characterization of the closed-channel fraction for any temperature $T$ and magnetic field $B$ – i.e. having $Z(T, B)$ – could lead to a new thermometry method in a Fermi gas, meaning that from a measure of $Z$ for a given $B$ one could determine the temperature $T$ of the system.

We would like to finish by suggesting that including this accurate two-body model in others approaches (as in the trial functions used in Monte Carlo studies [15–17]) may imply a considerable gain in the understanding of the many-body interacting quantum system, which is constructed upon a complete insight of the microscopic two-body physics.

Acknowledgments

We are extremely grateful to R G Hulet for helpful comments on the manuscript. We are also grateful to P A Bouvrie for introducing us in these questions. We thank J I Robledo for discussions. We acknowledge funding from Grant PICT-BID 2017-2583 from ANPCyT and Grant GRFT-2018 MINCYT-Córdoba, as well as financial support from SeCyT-UNC and CONICET. We would like to make a last unusual acknowledge: to C Chin for his generosity regarding knowledge, because his arXiv-published work, reference [22], inspired the present discussions.

Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

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