Shift of the molecular bound state threshold in dense ultracold Fermi gases with Feshbach resonance

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Abstract. We consider a dense ultracold Fermi gas in the presence of a Feshbach resonance. We investigate how the threshold for bound state formation, which is just at the Feshbach resonance for a dilute gas, is modified due to the presence of the Fermi sea. We make use of a preceding framework of handling this many-body problem. We restrict ourselves to the simple case where the chemical potential $\mu$ is negative, which allows us to cover in particular the classical limit where the effect is seen to disappear. We show that, within a simple approach where basically only the effect of Pauli exclusion is included, the Fermi sea produces a large shift of the threshold, which is of the order of the width of the Feshbach resonance. This is in agreement with very recent experimental findings.

After the original breakthrough in the production of Bose–Einstein condensates in ultracold bosonic atomic gases and the remarkable progress in understanding the underlying physics of these superfluids [1, 2], the exploration of similar dense [3]–[5] fermionic systems has taken off recently. A first series of experiments have reached the strongly degenerate regime with mixtures of fermions in two different hyperfine states [6]–[9]. One of the major goals in exploring these systems is the search for a transition to a BCS superfluid [10, 11], which is the equivalent of Bose condensation for these fermionic gases. A major advantage of these gaseous systems is the possibility of a direct experimental control of the interaction, through electric fields or laser induced resonance for example. However, the most used method currently is to apply a static magnetic field and go to the vicinity of a Feshbach resonance [12] where the scattering length, directly linked to the interaction, is strongly varying.

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In this paper we consider how the threshold for formation of the molecular bound state linked to this Feshbach resonance is modified by the presence of the Fermi sea. The standard Feshbach resonance is due to the coupling of an open channel, corresponding to two atoms with nuclear and electronic spin degrees of freedom corresponding to a long distance situation, with a closed channel where these degrees of freedom are in another configuration corresponding to a bound state with atoms at short distance, i.e. a molecular state. Actually, when the energy of this bound state is positive (this corresponds to a positive detuning), this bound state is only a quasi-bound state because the molecular state can decay into two free atoms, precisely because of the small coupling between the two channels. On the other hand, when the energy of the molecular state is negative (negative detuning), we have a true bound state since there is no decay energetically allowed. Naturally, the existence of this molecular state is important both for fundamental and for practical reasons. On the fundamental side it has been emphasized recently [13] that the strong interaction produced by the vicinity of this resonance could be a major help for the BCS transition. Moreover, the physics would become richer, due to the appearance of a Bose condensate of the molecules corresponding to the bound state. On the practical side the production of this molecular state is a first step in the decay of the whole metastable atomic gas, produced by three-body recombination [14]. Therefore, it is of clear interest to investigate what happens to this molecular state due to the influence of the Fermi sea.

Quite recently [15], we have considered how the scattering amplitude due to a Feshbach resonance is modified by the presence of the dense Fermi gas. Note that the problem of the modification of scattering by interactions in cold quantum gases has already been addressed by Stoof [16]. Although the formalism we used [15] is quite general, its application in this paper has been strongly simplified. First, the irreducible vertex has been taken merely as the simple scattering amplitude of two isolated atoms. Second, the effect of the Fermi gas has been taken into account by including only Pauli exclusion. Even so, the resulting scattering amplitude displays quite non-trivial features. First, in contrast with what happens in vacuum, it depends on the total momentum of the scattering atoms. This is easily understood since, for two atoms with very high momentum, the blocking of some states due to Pauli exclusion will only slightly alter their scattering. On the other hand, when the total momentum is zero and the energy of the atoms is of the order of a typical energy for atoms in the Fermi gas, many states which are relevant for the scattering of the two atoms in vacuum will be blocked due to Pauli exclusion and the scattering amplitude is deeply modified. In the following, we consider only this case of zero total momentum since it displays the strongest manifestation of Pauli exclusion. Also, just as in [15], we omit for simplicity any background scattering, so the scattering originates only from the Feshbach resonance.

In this case, the following result [15] is obtained for the inverse of the scattering amplitude $f(\omega)$ as a function of the total energy $\omega$ of the scattering particles (we take $\hbar = 1$ and $k_B = 1$):

$$\frac{1}{f(\omega)} = -\frac{1}{a} - \frac{\omega}{\gamma} + \frac{2}{\pi} \int_0^\infty dk \left[ 1 - \frac{k^2}{k^2 - m \omega} \tanh \frac{\epsilon_k - \mu}{2T} \right]$$

with $\epsilon_k = k^2/2m$. Here, the coupling parameter $\gamma$ is also a measure of the energetic width of the Feshbach resonance, while $a$ is the scattering length due to the Feshbach resonance which is directly linked to the detuning $\omega_0$ by $a = -\gamma/\omega_0$. In contrast with [15], the origin for the energy $\omega$ of the particles has not been shifted at the chemical potential. This energy $\omega$ has to be understood with an infinitesimal positive imaginary part. One recovers the case of two atoms in vacuum by setting the chemical potential $\mu = 0$ and looking at the $T = 0$ limit. Then the last
term gives only the contribution required by unitarity and one finds as expected
\[ f(\omega) = -\frac{1}{(\omega - \omega_0)/\gamma + i(m\omega)^{1/2}}. \] (2)

The standard Feshbach resonance, with a diverging scattering amplitude, is found at zero energy \( \omega = 0 \) when the detuning \( \omega_0 \) is equal to zero. This corresponds to an infinite scattering length \( a \). In contrast, nothing peculiar happens in equation (1) when one crosses the infinite scattering length \( a^{-1} = 0 \) situation. Actually, in the case of \( ^6\text{Li} \) the coupling \( \gamma \) is very large and we are left only with the last term in equation (1) which originates from the presence of the Fermi sea. Clearly, when \( a^{-1} \) becomes small, it also becomes irrelevant. This is in agreement with the recent experimental results of various groups [6]–[9] who do not see any accident when they cross the supposed location of the resonance. This finding is also completely coherent with a very recent calculation of Pitaevskii and Stringari [17] where they showed that the virial coefficient has no discontinuity when one goes across the unitary limit \( a^{-1} = 0 \).

In this paper we want to consider another immediate consequence of equation (1) which is also directly relevant for experiments. For the case (equation (2)) of two particles in vacuum the appearance of the bound state of these two particles, corresponding physically to the existence of a molecular state, occurs as soon as the detuning becomes negative, that is when the scattering length becomes positive, \( a > 0 \). Experimentally, this corresponds to a well defined magnetic field, since the detuning is directly controlled by the applied magnetic field. This molecular state appears as a pole in \( f(\omega) \) as given by equation (2) for negative values of the energy. One finds specifically for the binding energy \( \epsilon_b = -\omega \) of this state
\[ \epsilon_b = \frac{1}{ma^2} \frac{2}{1 + 2r + \sqrt{1 + 4r}} \] (3)
where \( r = (1/ma^2)/|\omega_0| = 1/(m\gamma a) \) is the ratio between the two limiting values of this binding energy. Indeed for \( r \ll 1 \) one finds the standard binding energy \( \epsilon_b = 1/ma^2 \) associated with the positive scattering length \( a \), while for \( r \gg 1 \) the binding energy is equal to the detuning \( \epsilon_b = |\omega_0| \).

Now it is clear that the existence of the Fermi sea will shift in general the magnetic field at which the molecular state appears. This is specifically produced by the last term in equation (1). Indeed, it is seen that for \( \omega = 0 \) one does not find a pole for \( a^{-1} = 0 \) since in this case the last term is always positive because \( \tanh x < 1 \). Here we restrict ourselves to the simple case where the chemical potential \( \mu \) is negative, which allows us to cover in particular the classical limit where the effect is seen to disappear. The extension to positive chemical potential will be considered elsewhere. In order to find the magnetic field \( B \) for which the molecules appear we look for the corresponding value of the scattering length \( a(B) \). We find it from equation (1) by assuming that the binding energy of the molecules is zero when they first appear. We will afterwards check this hypothesis. Since we are interested in non-positive values of the energy, the imaginary part in equation (1) is zero and we have only to deal with the real part. Setting \( \text{Re} f^{-1}(\omega) = 0 \) for \( \omega = 0 \) leads to
\[ a = \frac{4}{\pi} \int_0^\infty dk \frac{1}{e^{(\epsilon_k + |\mu|)/T} + 1}. \] (4)

At the level of our approximation the chemical potential \( \mu \) in equation (3) is merely linked to the single-species particle density \( n \) by the free particle equation:
\[ n = \frac{1}{2\pi^2} \int_0^\infty dk \frac{k^2}{e^{(\epsilon_k + |\mu|)/T} + 1}. \] (5)
In the classical limit $e^{\mu/T} \to \infty$ one finds easily from equation (4)

$$\frac{1}{a} = 4 \left( \frac{mT}{2\pi} \right)^{1/2} e^{-\mu/T} = \frac{4}{\Lambda_T} e^{-\mu/T}$$

(6)

where $\Lambda_T = (2\pi\hbar^2/mT)^{1/2}$ is the de Broglie thermal wavelength, while equation (5) gives the well known classical ideal gas relation:

$$n = \left( \frac{mT}{2\pi} \right)^{3/2} e^{-\mu/T} = \Lambda_T^{-3} e^{-\mu/T}.$$  

(7)

Together these results lead to

$$\frac{1}{a} = 8\pi \frac{n\hbar^2}{mT} = 4n\Lambda_T^2$$

(8)

where we have reintroduced the Planck constant. As expected $a^{-1}$ goes to zero in the limit of large temperature and low density, and we recover that the molecular state appears right below the Feshbach resonance. We can also rewrite this result by introducing a wavevector $k_F$ linked to the density $n$ by the same relation as in the $T = 0$ limit, namely $n = k_F^3/6\pi^2$. If we set $E_F = \hbar^2 k_F^2/2m$ for the corresponding energy we have

$$k_F a = \frac{3\pi}{8} \frac{T}{E_F}.$$  

(9)

Naturally, the classical regime corresponds to $T \gg E_F$, so the scattering length $a$ at the threshold for molecule formation gets very large, all the more since, for a trapped gas, the density $n$ decreases when the temperature increases, which makes the length scale $1/k_F$ (basically the interparticle distance) increase with $T$. On the other hand, the extrapolation of this simple formula in the regime $T \sim E_F$ shows immediately that the molecular threshold is shifted in this case to a scattering length $a \sim 1/k_F$. In the specific case of $^6$Li, one of the most studied experimentally, this gives for the degenerate conditions a scattering length of order of 100 nm. This implies a shift corresponding to a change of the magnetic field of the order of the width of the Feshbach resonance, which is typically 100 G. This large shift is in very good qualitative agreement, both in sign and in magnitude, with the very recent experimental results of Dieckmann et al [6] and of Bourdel et al [9].

In order to be more quantitative in the general case we have just to handle equations (4) and (5) numerically. This is done conveniently by taking $y = k/(2mT)^{1/2}$ as a new variable. Introducing $k_F$ as above, setting $R = T/E_F$ and $A = \exp(\mu/T)$, we see that equation (5) gives $R$ in terms of $A$ as

$$R^{-3/2} = 3 \int_0^{\infty} dy \frac{y^2}{Ae^{y^2} + 1}$$

(10)

while equation (4) then leads for the threshold scattering length $a$ to

$$\frac{1}{k_F a} = \frac{4}{\pi} R^{1/2} \int_0^{\infty} dy \frac{1}{Ae^{y^2} + 1}.$$  

(11)

For our range of interest $A \geq 1$, our degeneracy parameter $R$ is going from $\sim 1$ to $\infty$. The result for $1/k_F a$ as a function of $R = T/E_F$ is given in figure 1 with a logarithmic scale for $R$. We have also plotted the asymptotic result equation (9) which is seen still to give a reasonable estimate for $R = 1$. 

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Figure 1. Reduced inverse scattering length $1/(k_Fa) = (6\pi^2na^3)^{-1/3}$ at the bound state threshold as a function of the degeneracy parameter $R = T/E_F = (16/9\pi)^{1/3}/(n\Lambda_F^3)^{2/3}$, with a logarithmic scale for $R$. Full curve: numerical result, equations (10) and (11). Dashed curve: asymptotic result, equation (9).

We have still to check that the threshold corresponds to molecules with zero binding energy. If we look for a bound state with binding energy $\epsilon_b$ appearing for a scattering length $a_b$, we have from equation (1) with $\omega = -\epsilon_b$,

$$\frac{1}{a_b} = \frac{\epsilon_b}{\gamma} + \frac{2}{\pi} \int_0^\infty \mathrm{d}k \left[ 1 - \frac{k^2}{k^2 + m\epsilon_b} \tanh \frac{\epsilon_k + |\mu|}{2T} \right].$$

Taking the difference from equation (4) which gives the scattering length $a$ for zero binding energy, we find

$$\frac{1}{a_b} - \frac{1}{a} = \frac{\epsilon_b}{\gamma} + \frac{2}{\pi} \int_0^\infty \mathrm{d}k \frac{m\epsilon_b}{k^2 + m\epsilon_b} \tanh \frac{\epsilon_k + |\mu|}{2T},$$

which is positive. So, just as for the case of two particles in vacuum, molecules with non-zero binding energy correspond to lower scattering length than those with zero binding energy. Therefore, they appear later when one starts from the Feshbach resonance and decreases progressively the scattering length by lowering the magnetic field.

Naturally, we have to keep in mind that this result represents the maximum shift on the threshold for the molecular state, since it corresponds to the case where the total momentum is zero. There will be a similar shift for non-zero momentum, but it decreases with momentum as we have already mentioned since for very high momentum the blocking effect of the other fermions is clearly very weak. So there is actually a distribution of densities due to the trapping potential. So direct comparison with experiment should take into account these two distributions. Nevertheless, the maximum value of the threshold is given by equation (4) with the particle density equal to its maximum value at the centre of the trap. Starting from low positive values of the scattering length and increasing it, which corresponds for $^6\text{Li}$ to increasing the magnetic field starting from low values, our result, equation (4), corresponds therefore to the lowest magnetic field for which resonating conditions for the formation of molecules will occur. Of course, the molecular bound states appear later when one starts from the Feshbach resonance and decreases progressively the scattering length by lowering the magnetic field.
do exist for the whole range $a > 0$ but it is known that its formation through three-body recombination [14] is strongly enhanced in the immediate vicinity of the resonant situation. Note that important dynamical effects will necessarily occur in experiments, which will make quantitative comparison with theory even harder. In this respect it seems that direct spectroscopic observation of the molecules would provide the best investigation tool.

In conclusion, we have studied the effect of Pauli exclusion due to the Fermi sea on the Feshbach resonance. We have shown that, as a natural consequence, there is a shift of the threshold for the formation of molecules under resonating conditions. The sign and the size of the effect is in very good qualitative agreement with the very recent experimental findings of Dieckmann et al and of Bourdel et al [6, 9]. Naturally, it must be kept in mind that our theoretical treatment is rough since we only take into account Pauli exclusion and we have not included the effect of the interactions in the last term in equation (1). Nevertheless, we do not expect the physics linked to Pauli exclusion to disappear in the full solution of the problem. Proper account of the interactions is likely to modify quantitatively the size of the shift, but we do not expect it to modify it qualitatively. In particular, it is unlikely to suppress this effect and make this shift almost disappear. Therefore, we believe that our simple estimates already provide a proper physical understanding of the shift.

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