Feshbach resonance in dense ultracold Fermi gases

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We propose a coherent framework allowing to deal with many-body effects in dense ultracold Fermi gases in the presence of a Feshbach resonance. We show that the simple effect of Pauli exclusion induces a strong modification of the basic scattering properties, leading in particular to an energy dependence of the effective scattering length on the scale of the chemical potential. This results in a smearing of the Feshbach resonance and provides a natural explanation for recent experimental findings.

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Besides the continuing progress in understanding Bose Einstein condensation in ultracold bosonic atomic gases, the exploration of similar dense [1] fermionic systems has received recently a strong impetus from experiments reaching the strongly degenerate regime with mixtures of fermions in two different hyperfine states [2]. A main purpose in exploring these systems is the search for a transition to a BCS superfluid [3]. A particularly fascinating possibility of experimentally controlling the strength of the interaction, already demonstrated in Bose systems, has been used in these last experiments. It consists in working in the vicinity of a Feshbach resonance [4] where the scattering length, directly linked to the interaction, depends strongly on the applied magnetic field. It has been emphasized recently [5] that the strong interaction obtained in the vicinity of this resonance, together with the Bose condensation of the molecules corresponding to the underlying bound state, could be of major interest for the BCS transition.

In the present paper we set up a theoretical framework for handling many-body effects in the presence of a Feshbach resonance. As a first consequence we show that the simple effect of Pauli exclusion explains qualitatively that the Feshbach resonance is strongly smeared for degenerate gases, as it appears experimentally [2]. Here we will restrict ourselves for simplicity to the case where the (quasi) bound state responsible for the resonance is not thermally occupied, which corresponds to a negative effective scattering length. Similarly we will consider only the normal state although our formalism can be extended to the superfluid state.

First we model the Feshbach resonance in the following way. The Feshbach resonance [4] is actually produced by the somewhat complex interplay between the spin (electronic and nuclear) and orbital degrees of freedom. However in order to have an understanding of the physics linked to this resonance, it is convenient to use a simple modeling where the spin degrees of freedom are no longer involved. One can think that the resonance occurs because there is a (quasi) bound state caused by the existence of a deep well in the atomic interaction potential at short distances. One will indeed have a bound state, corresponding physically to the formation of a molecule, if this well is essentially isolated from the large distance region by a high barrier with very small transmission probability. Clearly this model behaves phenomenologically exactly in the same way as a Feshbach resonance [6].

On the other hand we are only interested in the effect of this molecular state on the scattering of two atoms, and we will ignore the effect of the other atoms on these two when they are close together. This is reasonable since these other atoms will be most of the time far away and will not perturb the two atoms we consider. In other words we make use of the fact that the gas is dilute on the scale of the molecular state. Naturally this means that we ignore for example the possibility that three atoms are close together, which would require additional ingredients in the description.

We further simplify our description by separating the possible distance between the two particles in two domains. Either they are far away and interact by the long range part of the potential (this range will be denoted by index 1). Or they are quite close and interact through the deep well of the potential (this is noted by index 2). More precisely one can define the boundary between the two domains as being at some distance $R$, large compared to the molecular size but small with respect to interparticle distance. Then instead of describing exactly the transition from domain 1 to domain 2, we assume that a term in the Hamiltonian gives rise to a matrix element producing this transition. We note that this problem is actually quite similar to the one raised by tunneling of electrons between two metallic electrodes through an insulating barrier and our approach is at the level of the tunneling Hamiltonian [7]. It is actually known that this simple modeling can be improved up to the exact problem, and that many-body effects can also be included in this theory [8]. However this does not seem necessary in the present case and our simple modeling should be a quite enough.

To be more specific now consider first the problem with the center of mass of the two atoms at rest, so we deal with a one body problem with interparticle separation $r$ and reduced mass $m_r = m/2$. The parts of the Hamiltonian $H$ corresponding respectively to domain 1 and 2 are:
Carrying Eq.(4) into Eq.(3) gives:
\[ H_{12}(\mathbf{r}, \mathbf{r'}) = t(\mathbf{r}, \mathbf{r'}) \]
with \( H_{21} = H_{12}^* \). Since the purpose of \( t(\mathbf{r}, \mathbf{r'}) \) is just to make the particle cross the boundary between domain 1 and 2, we can assume it to be short-ranged around this boundary.

Let now \( G_{11}^0(\mathbf{r}, \mathbf{r'}, \omega) \) be the propagator corresponding to \( H_{11} \), at frequency \( \omega \) (we take \( h = 1 \)) and similarly \( G_{22}^0(\mathbf{r}, \mathbf{r'}, \omega) \) the propagator corresponding to \( H_{22} \). Physically they describe the motion either at long or short distance, without the possibility to hop between the two domains. We treat now exactly the effect of the hopping term. We introduce the full propagator \( G(\mathbf{r}, \mathbf{r'}, \omega) \) corresponding to \( H \). If \( \mathbf{r} \) and \( \mathbf{r'} \) are large (we call again \( G_{11} \) the corresponding propagator), the particle can propagate either by staying in domain 1 (this is described by \( G_{11}^0 \)) or, after a stay in domain 1, by making a first hop to domain 2 and then propagating by any means back to domain 1. This leads to the following equation between operators:
\[ G_{11} = G_{11}^0 + G_{11}^0 t G_{21} \]
where a same frequency is understood in all the propagators. We have a similar relation for propagation between domain 2 and 1, except that hopping is now required (because \( G_{21}^0 = 0 \)):
\[ G_{21} = G_{22}^0 t^\dagger G_{11} \]
Carrying Eq.(4) into Eq.(3) gives:
\[ G_{11} = G_{11}^0 + G_{11}^0 t G_{22}^0 t^\dagger G_{11} \]
which is an integral equation for \( G_{11} \).

This can now be simplified if we take into account that a single bound state of \( H_{22} \), corresponding to the Feshbach resonance we are interested in, is relevant. All the other bound states are supposed to be very far away. This allows us to make, in the energy range we are interested in, a single pole approximation for \( G_{22}^0 \):
\[ G_{22}^0(\mathbf{r}, \mathbf{r'}, \omega) = \varphi(\mathbf{r}) \varphi^\dagger(\mathbf{r'}) / (\omega - E_0 + i\epsilon) \]
where \( \varphi(\mathbf{r}) \) is the wavefunction of the bound state and \( E_0 \) its energy. This makes Eq.(5) explicitly soluble because \( G_{22}^0 \) becomes basically a projector on the bound state. One finds:
\[ G_{11} = G_{11}^0 + \frac{1}{\omega - E_0 - \delta E_0} G_{11}^0 t |\varphi > < \varphi| t^\dagger G_{11}^0 \]
where \( \delta E_0 = < \varphi| t^\dagger G_{11}^0 t |\varphi > \) is a complex quantity.

Let us assume for simplicity that there is no background scattering, i.e. the long distance potential \( V_1 \) is zero. In this case \( G_{11}^0 \) is just the free particle propagator. The corresponding T-matrix is then given by the last term in Eq.(7) without the \( G_{11}^0 \) operators. For the scattering we are interested in, we look for matrix elements between plane waves with very small wavevectors compared to the molecular scale. Since \( \varphi(\mathbf{r}) \) and \( t(\mathbf{r}, \mathbf{r'}) \) are short-ranged we can as well take these wavevectors to be zero. This leads to a numerator equal to \( |w|^2 \) with \( w = \int d\mathbf{r} d\mathbf{r'} t(\mathbf{r}, \mathbf{r'}) \varphi(\mathbf{r'}) \). The denominator gives a pole for \( \omega = E \) with \( E = E_0 + \delta E_0 \), corresponding to the resonance produced by the bound state. The real part \( \text{Re}\delta E_0 \) gives the physical energy \( \omega_0 \) of the resonance, which is the one actually measured experimentally. So we do not have to worry about calculating \( \text{Re}\delta E_0 \). The imaginary part gives the width of the resonance due physically to the possible decay, induced by \( t \), of the molecule into two atoms. Introducing the Fourier transform \( G^0_k \) of the free particle propagator, this imaginary part will come from \( \text{Im} G^0_k = -\pi \delta(\omega - \epsilon_k) \) with \( \epsilon_k = k^2/2m_r \), physically linked to the density of final states for the decay. Since we are concerned with low energy \( \omega \), the wavevector must be small and the matrix elements coming from \( t|\varphi > \) in the above expression of \( \delta E_0 \) can again be evaluated for zero wavevector, which introduces again \( |w|^2 \). Finally we obtain for the corresponding scattering amplitude:
\[ f(\kappa) = -\frac{1}{(\omega - \omega_0)/\gamma + i\kappa} \]
to be evaluated on the shell $\omega = \kappa^2/2m_r$. In this expression we have set $\gamma = m_r|w|^2/2\pi$. We find in particular in Eq.(8) that $\text{Im} f^{-1}(\kappa) = -\kappa$ as required by unitarity. Evaluating Eq.(8) at zero energy gives the scattering length $a = -\gamma/\omega_0$. Strictly speaking the Feshbach resonance corresponds to the situation where the above resonance occurs at zero energy $\omega = 0$. This occurs for $\omega_0 = 0$, i.e. for an infinite scattering length. Experimentally $\omega_0$ is controlled by the applied magnetic field. Naturally this result for the scattering amplitude is well known [6], as well as this general way of modeling the Feshbach resonance [4] as a simple switch between molecular state and diffusion states. We have just reformulated this approach in a way which lends itself conveniently to generalization in order to include many body effects.

We turn now to the case of a dense Fermi gas and assume again for simplicity that there is no background scattering. As we have already mentionned we take advantage that the gas is dilute on the molecular scale to neglect the effect of the other atoms when two atoms are scattering due to the Feshbach resonance. In other words we will take for the effective interaction the same as the one we had only two atoms present, namely $\Gamma_{00} = |w|^2/(\omega - E_0)$ as it results from Eq.(5). This is equivalent to retain only ladder diagrams for the short range potential. We note that this effective interaction is analogous to the one due to phonon exchange in standard superconductors, although there are differences. Actually we believe that this description should still be correct even if we take into account the body effects.

We turn now to the case of a dense Fermi gas and assume again for simplicity that there is no background scattering.

We will now explore the simplest consequences of this interaction by ignoring fluctuation-like effects and analogous terms, and taking merely $\Gamma_{00}$ as irreducible vertex. With this assumption we can write the Bethe-Salpeter equation for the full vertex $\Gamma(\omega, K)$, which is directly related to the scattering amplitude, as:

$$\Gamma(\omega, K) = \Gamma_{00}(\Omega) + \Gamma_{00}(\Omega)\Pi(\omega, K)\Gamma(\omega, K)$$

where $\Pi(\omega, K)$ describes the propagation of two atoms and is given, in terms of the full thermal propagator of an atom $G(\omega, k)$, by:

$$\Pi(\omega, K) = -T \sum_n \int \frac{dK}{(2\pi)^3} G(-i\omega - \omega_n, K - k)G(\omega_n, k)$$

with $\omega_n = (2n + 1)\pi T$ being the Matsubara frequency. We have written Eq.(9) in a simple way by taking already into account that the full vertex $\Gamma$ depends only, in our case, on the total energy $\omega$ and the total momentum $K$ of the scattering atoms. This results from the fact that the irreducible vertex $\Gamma_{00}(\Omega)$ has itself this property. We can more simply rewrite Eq.(9) as:

$$\Gamma_{00}^{-1}(\Omega) = \Gamma^{-1}(\omega, K) + \Pi(\omega, K)$$

We will now eliminate the pole location $E_0$ in $\Gamma_{00}$, which is not an observable quantity, in favor of the physical energy $\omega_0$ of the resonance, which is directly related to the scattering length as we have seen. This is done by writing Eq.(11), at zero temperature T, for the case of two atoms in vacuum (implying $\mu = 0$), at zero energy $\omega = 0$ and momentum $K = 0$. In this case $G(\omega_0, k)$ becomes the free propagator $(i\omega_n - \epsilon_k)^{-1}$ and the frequency summation in $\Pi$ becomes an easy integration. On the other hand for two atoms in vacuum $\Gamma(\omega, K)$ becomes $\Gamma_0(\Omega) \equiv |w|^2/(\Omega - \omega_0)$, which is essentially the T-matrix. Hence in this particular situation Eq.(11) reduces to:

$$-E_0/|w|^2 = -\omega_0/|w|^2 - \int \frac{dK}{(2\pi)^3} \frac{1}{2\epsilon_k}$$

Actually this equation is just equivalent to $\omega_0 = E_0 + \text{Re} \delta E_0$. Subtracting Eq.(12) from Eq.(11) we obtain:

$$\Gamma^{-1}(\omega, K) = \Gamma_0^{-1}(\Omega) - \Pi(\omega, K) - \frac{dK}{(2\pi)^3} \frac{1}{2\epsilon_k}$$

Taken together the last two terms of the r.h.s. of Eq.(13) give an integral which converges for large values of $k$, while each term separately is divergent. However this divergence is not a real problem. It would not be present if we had
kept the $k$ dependence of $<\mathbf{k}|\tilde{t}|\varphi>$ instead of making $\mathbf{k} = 0$ at the outset. Eq.(13) makes clear a general feature, namely the scattering amplitude depends not only on the total energy $\omega$ of the two particles, but also on their total momentum. This is due to the term $\Pi(\omega, K)$ which gives the effect of the other fermions on the scattering process. In other words Galilean invariance for this process is obviously lost because of the presence of the Fermi sea. It is clear physically that the existence of the Fermi sea will be unimportant when $K$ is very large. On the other hand we expect this feature will be most important for $K = 0$ and we will consider only this situation in the following.

Quite remarkably the modifications produced by the other fermions are already very important when the effect of the interactions is omitted. This corresponds to the modification of the scattering due to Pauli exclusion. We will restrict ourselves to this particular problem in the rest of the paper. In this case we have $G(\omega_n, k) = (\omega_n - \epsilon + \mu)^{-1}$ and the calculation of $\Pi(\omega, K)$ can be reduced to a single integration over the momentum $k$. It is convenient to use reduced units to display this result. We take $\mu$ as our energy scale and $k_0$ as a scale for wavevector defined by $\mu = k_0^2/2m$ (this is the Fermi wavevector at $T = 0$ and not much different at low temperature). We introduce the reduced wavevector $x = k/k_0$, the reduced energy $\bar{\omega} = \omega/\mu$ and reduced temperature $\tilde{t} = T/\mu$. Then Eq.(13) becomes:

$$
-\frac{2\pi^2}{mk_0} \frac{1}{\Gamma(\omega, 0)} = \frac{1}{\lambda} - \bar{\omega} + \frac{2}{W} + \int_{0}^{\infty} dx \left[ 1 - \frac{x^2}{x^2 - 1 - \bar{\omega}/2} \tanh \frac{x^2 - 1}{2\tilde{t}} \right]
$$

where in the last term $\bar{\omega}$ has to be understood with an infinitesimal positive imaginary part. Except for the factor $\pi/2k_0$ this is just the inverse $f^{-1}$ of the effective scattering amplitude for our problem. We have introduced the coupling constant $\lambda = 2k_0|a|/\pi$, also related to the detuning $\omega_0$ by $\lambda = (2/\pi)W/\omega_0$ with $W = \gamma k_0$ being the energetic (half) width of the resonance line for a wavevector $k_0$. We have used the reduced width $W = (2/\pi)W/\mu$. If we consider the specific case of $^6$Li, the most heavily explored experimentally, the standard energy width of the Feshbach resonance is given [4] by $\gamma/|a_{bg}|$ where $a_{bg}$ is the high field limit of the scattering length, of order of 100 nm. It is experimentally of order of 100 G, which translates into an energy of 10 mK. If we consider dense gases for which we have $k_0|a_{bg}| \sim 1$, this gives $W \sim 10$ mK. Since we will have at most experimentally $\mu \sim 10\mu K$, we see that $W \sim 10^3$. Since we are interested in reduced energy $\bar{\omega}$ of order 1, this makes the second term of the r.h.s. completely negligible and we omit it from now on. The same is likely to be true in most useful cases of Feshbach resonance. Note however that this term is necessary if we want to find in the lower complex plane the pole corresponding to the Feshbach resonance.

Let us call $I(\bar{\omega})$ the integral in Eq.(14). The imaginary part of the r.h.s. is easily found to be $\text{Im}I(\bar{\omega}) = -(\pi/2)R \tanh(\bar{\omega}/4t)$ with $R = (1 + \bar{\omega}/2)^{1/2}$, and is plotted in Fig. 1. At zero temperature with no Fermi sea, this would give us back the imaginary part in Eq.(8). We see that, in addition to $\bar{\omega} = -2$ corresponding to zero kinetic energy, this imaginary part is zero for $\bar{\omega} = 0$, that is at the chemical potential. This is expected on general grounds since injecting particles at this energy does not perturb equilibrium and so does not lead to decay. More generally the $\tanh(\bar{\omega}/4t)$ can be understood as the decrease of the scattering resulting from Pauli exclusion on the final state, together with the existence of reverse processes, both due to thermal occupation.

![FIG. 1. Imaginary and real part of the integral $I(\bar{\omega})$ in Eq.(14), as a function of reduced energy $\bar{\omega} = \omega/\mu$ for various reduced temperature $\tilde{t} = T/\mu$ indicated in the figure.](image)

Re$I(\bar{\omega})$ is plotted in Fig. 1 for various reduced temperatures. After adding the term $1/\lambda$ and multiplying by the factor $-\pi/2k_0$, we can consider the result as the inverse of an effective scattering length $a_{eff}^{-1}$ for two atoms. When $\lambda$ is of order of unity or larger, we see as naturally expected that the scale for this scattering length is the only one left in the problem, namely $1/k_0$. As seen in the figure $a_{eff}^{-1}(\bar{\omega})$ has a strong energy dependence on the scale of the Fermi
energy $E_F$. This is in contrast with the case of two isolated atoms seen in Eq.(8), where in the same energy range the real part of $-f^{-1}$ is a constant equal to the scattering length $a^{-1}$ (except if $\omega_0$ is of order $E_F$ that is extremely near the Feshbach resonance). This means that an essential simplification in the scattering properties effectively disappears. Indeed for ultracold atoms scattering is characterized by a single parameter, namely the scattering length $a$. Now because of the Fermi sea the energy scale $E_F$ appears and the scattering amplitude gets a complex energy dependence, which depends also on temperature. An immediate consequence is that physically the Feshbach resonance is actually washed out by the Fermi sea. Indeed instead of having for all possible scattering atoms a diverging scattering length, and correspondingly a zero $\text{Re}f^{-1}$, we have a $\text{Re}f^{-1}$ which is of order $1/k_F$ and depends on the energy of the two considered atoms (as well as their momentum as we have seen). This occurs as soon as $\lambda$ is not small. In particular nothing special occurs right at the Feshbach resonance when $\lambda^{-1} = 0$. This provides a simple explanation to the experimental observations [2] that the resonance is not seen when the magnetic field is swept through its assumed location when the gas is dense enough to be in the degenerate regime. Naturally the inhomogeneity due to the varying trapping potential is an additional source of smearing since the energy scale $\mu$ for the scattering is space dependent.

We look now more strictly for a resonance where the scattering amplitude diverges, which for two isolated atoms occurs at zero energy at the Feshbach resonance $a^{-1} = 0$. So we require that both the real and the imaginary part of $\Gamma(\omega,0)^{-1}$ are zero in Eq.(14). It is easy to see that, for $\bar{\omega} = -2$, the real part of the integral in Eq.(14) is always positive so $\text{Re}f^{-1} > 0$ for $a < 0$. So the only possible resonance occurs at the chemical potential $\bar{\omega} = 0$. In this case the condition that $\text{Re}f^{-1} = 0$ in Eq.(14) coincides with the well-known condition for the BCS pairing instability. In particular, at $T = 0$, the logarithmic divergence of $\text{Re}f^{-1}$ which occurs for $\bar{\omega} = 0$ is a mark of this instability. It is known that this pairing instability is basically due to Pauli exclusion by the Fermi sea on low energy states, which produces a shift from a 3D situation to an effective 2D physics. We can understand qualitatively the strong energy dependence of the scattering amplitude we have found above as a manifestation of this 2D physics. Naturally, since we have not included interactions, the value of the critical temperature $T_c$ we have for the pairing instability is just the standard one [3], and it does not contain lower order fluctuation effects [9] nor higher orders and self-energy effects considered in recent calculations [10]. Obviously our calculation is no longer strictly valid below $T_c$ since we should deal with the superfluid state, which can be done as we have already mentioned. However this is not an important restriction for our present purpose since we want to stress the strong frequency dependence of $\text{Re}f^{-1}$ on the scale of $E_F$, which will clearly remain at least qualitatively valid in the superfluid state. In the same spirit we have not included interactions, but they will not change the basic Pauli exclusion physics. We can not expect interactions to remove the energy dependence of the scattering and our qualitative conclusion will remain unchanged.

In conclusion we have presented a coherent framework which allows to deal with many-body effects in the presence of a Feshbach resonance. As a simple consequence we have shown that the mere result of Pauli exclusion, which results from Fermi statistics, induces a strong modification of the scattering properties. It is clear that this modification is a necessary ingredient in the physical understanding of these systems since Pauli exclusion can not be ignored. This modification results in a smearing of the Feshbach resonance and provides a natural explanation for recent experimental findings.

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