Feshbach Resonance in Dense Ultracold Fermi Gases

R. Combescot

Laboratoire de Physique Statistique, Ecole Normale Supérieure, 24 rue Lhomond, 75231 Paris Cedex 05, France*

(Received 12 February 2003; published 17 September 2003)

We propose a coherent framework allowing one to treat 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. In particular, this washes out the Feshbach resonance and provides a natural explanation for recent experimental findings.

DOI: 10.1103/PhysRevLett.91.120401 PACS numbers: 03.75.Ss, 05.30.Fk, 32.80.Pj, 67.90.+z

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 has been used in these last experiments. It consists of working in the vicinity of a Feshbach resonance [4] where the scattering length 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 [6] in the presence of a Feshbach resonance. As a first consequence we show why there is no resonant feature appearing in ^{6}Li at 860 G for degenerate gases, where it has been predicted to appear for collisions between two atoms in vacuum [7]. There is no need to modify this prediction. The simple effect of Pauli exclusion explains that the Feshbach resonance is washed out, as it appears experimentally [2]. Here we will restrict ourselves to the case where the (quasi) bound state responsible for the resonance is not thermally occupied, which corresponds to a negative scattering length. Similarly we will consider only the normal state although our formalism can be extended to the superfluid state.

Let us consider modeling the Feshbach resonance [4] which is actually produced by the somewhat complex interplay between the spin (electronic and nuclear) and orbital degrees of freedom. In order to have an understanding of the physics, it is convenient to get rid of the spin degrees of freedom and think that the resonance occurs because there is a (quasi) bound state caused by a deep well in the atomic interaction potential at short distances. Indeed one will 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 [8]. On the other hand we are interested only in the effect of this molecular state on the scattering of two atoms, and we ignore the effect of the other atoms on these two when they are close together, because the gas is dilute on the scale of the molecular state. So 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 interparticle distance in two domains. Either particles are far away and interact by the long range part of the potential (denoted by index 1) or they are quite close and interact through the deep well potential (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. This problem is quite similar to the one of electrons tunneling between two metallic electrodes through an insulating barrier and our approach is at the level of the tunneling Hamiltonian [9]. 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 [10], but this does not seem necessary in the present case and our simple modeling should be quite enough.

Now consider first the atoms with their center of mass at rest, so we deal with a one body problem with interparticle distance $\mathbf{r}$ and reduced mass $m_r = m/2$. The parts of the Hamiltonian H corresponding, respectively, to domains 1 and 2 are $H_{11} = \mathbf{p}^2/2m_r + V_1(\mathbf{r})$ and $H_{22} = \mathbf{p}^2/2m_r + V_2(\mathbf{r})$, where V_1 and V_2 are the interaction potential at long and short distances, respectively. For example, V_1 gives rise to a scattering length a_{bg} while V_2 produces the molecular state. Then we describe hopping between the two domains by the nonlocal term $H_{12}(\mathbf{r}, \mathbf{r}') = t(\mathbf{r}, \mathbf{r}')$ with $H_{21} = H_{12}^\dagger$. Since the purpose of $t(\mathbf{r}, \mathbf{r}')$ is just to make the particle cross the boundary between domains 1

and 2, we can assume it to be short ranged around this boundary.

Now let $G_{11}^0(\mathbf{r}, \mathbf{r}', \omega)$ be the propagator corresponding to H_{11}, at frequency ω ($\hbar = 1$), and similarly $G_{22}^0(\mathbf{r}, \mathbf{r}', \omega)$ the H_{22} propagator. Physically they describe the motion either at long or short distances, without the possibility to hop between the two domains. We now treat exactly the effect of the hopping term. Let $G(\mathbf{r}, \mathbf{r}', \omega)$ be the full propagator corresponding to H. If $\mathbf{r}$ and $\mathbf{r}'$ are large (we call 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 (giving again G_{11}^0), by making a first hop (produced by t) to domain 2 and then propagating back by any means to domain 1 (described by G_{21}). This leads to the following equation between operators:

$$G_{11} = G_{11}^0 + G_{11}^0 t G_{21}, \tag{1}$$

where the same frequency is understood in all propagators. Similarly, since $G_{21}^0 = 0$, we have $G_{21} = G_{22}^0 t^\dagger G_{11}$ for propagation between domains 2 and 1. Carrying this into Eq. (1) gives

$$G_{11} = G_{11}^0 + G_{11}^0 t G_{22}^0 t^\dagger G_{11} \tag{2}$$

which is an integral equation for G_{11}.

This can now be simplified by keeping only the bound state of H_{22} corresponding to the Feshbach resonance. All the other bound states are supposed to be very far away energetically. This allows one to make, in the relevant energy range, a single pole approximation for G_{22}^0:

$$G_{22}^0(\mathbf{r}, \mathbf{r}', \omega) = \frac{\varphi(\mathbf{r})\varphi^*(\mathbf{r}')}{\omega - E_0 + i\epsilon} \tag{3}$$

with $\epsilon \to 0_+$ and where $\varphi(\mathbf{r})$ is the wave function of the bound state and E_0 its energy. This makes Eq. (2) explicitly soluble because G_{22}^0 becomes basically a projector on the bound state. One finds the explicit solution:

$$G_{11} = G_{11}^0 + \frac{1}{\omega - E_0 - \delta E_0} G_{11}^0 t|\varphi\rangle\langle\varphi| t^\dagger G_{11}^0, \tag{4}$$

where $\delta E_0 = \langle\varphi| t^\dagger G_{11}^0 t|\varphi\rangle$ is a complex quantity.

Let us assume for simplicity that there is no background scattering, i.e., $V_1 = 0$, so G_{11}^0 is just the free particle propagator. The corresponding T matrix is then given by the last term in Eq. (4) without the G_{11}^0 operators. For the scattering we are interested in, we look for matrix elements between plane waves with very small wave vectors compared to the molecular scale [4,6]. Since $\varphi(\mathbf{r})$ and $t(\mathbf{r}, \mathbf{r}')$ are short ranged we can take these wave vectors 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 $\mathrm{Re}E$ gives the physical energy ω_0 of the resonance, which is the one measured experimentally. So we do not have to worry about calculating $\mathrm{Re}\delta E_0$. 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 $G_{\mathbf{k}}^0$ of the free particle propagator, this imaginary part will come from $\mathrm{Im}G_{\mathbf{k}}^0 = -\pi\delta(\omega - \epsilon_{\mathbf{k}})$ with $\epsilon_{\mathbf{k}} = k^2/2m_r$, physically linked to the density of final states for the decay. Since we are concerned with low energy ω, the wave vector must be small and the matrix elements coming from $t|\varphi\rangle$ in the above expression of δE_0 can again be evaluated for zero wave vector, which introduces again $|w|^2$. Finally we obtain for the corresponding scattering amplitude

$$f(\kappa) = -\frac{1}{(\omega - \omega_0)/\gamma + i\kappa} \tag{5}$$

to be evaluated on the shell $\omega = \kappa^2/2m_r$. We have set $\gamma = m_r|w|^2/2\pi$. Equation (5) gives in particular $\mathrm{Im}f^{-1}(\kappa) = -\kappa$ as required by unitarity. Evaluating Eq. (5) 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 $\omega = 0$, implying an infinite scattering length, i.e., $\omega_0 = 0$. Experimentally ω_0 is controlled by the applied magnetic field. Naturally this result for the scattering amplitude is well known [8], as well as this general way of modeling the Feshbach resonance [4] as a simple switch between molecular and diffusion states. We have just reformulated this approach in a way convenient for generalization in order to include many-body effects.

We turn now to the case of a dense Fermi gas and assume again no background scattering. As already mentioned we neglect the effect of the other atoms when two atoms are scattering due to the Feshbach resonance since the gas is dilute on the molecular scale. In other words we take for the effective interaction the same as the one we had for only two atoms present, namely, $\Gamma_{00} = |w|^2/(\omega - E_0)$, as results from Eq. (2). This is equivalent to retain only ladder diagrams for the short range potential. Actually we believe that this description should still be correct even if we take into account the perturbation due to the other atoms, provided it is not too strong. Indeed this should change only the effective parameters energy position, width, and coupling strength of the resonance which are already present in our description. Naturally ω in our expression for Γ_{00} is the energy for the center of mass of the two atoms at rest. If their total momentum is $\mathbf{K}$ and their total energy ω we have to discount the energy associated with the center of mass motion and write $\Gamma_{00}(\Omega) = |w|^2/(\Omega - E_0)$, with $\Omega = \omega + 2\mu - K^2/4m$. Here, as in the following, we take the origin of the single particle energy at the chemical potential μ, which produces a shift 2μ for the energy of two atoms.

We will now explore the simplest consequences of this interaction by ignoring fluctuationlike effects and analogous terms, and taking merely Γ_{00} as an irreducible vertex. With this assumption we can write the Bethe-Salpeter equation [6] for the full vertex $\Gamma(\omega, K)$, which is directly related to the scattering amplitude, as

$$\Gamma(\omega, K) = \Gamma_{00}(\Omega) + \Gamma_{00}(\Omega)\Pi(\omega, K)\Gamma(\omega, K), \quad (6)$$

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

$$\Pi(\omega, K) = -T\sum_n \int \frac{d\mathbf{k}}{(2\pi)^3} G(-i\omega - \omega_n, \mathbf{K} - \mathbf{k})G(\omega_n, \mathbf{k}) \quad (7)$$

with [6] $\omega_n = (2n + 1)\pi T$. We have written Eq. (6) in a simple way by already taking into account that the full vertex Γ depends only, in our case, on the total energy ω and the total momentum $\mathbf{K}$ of the scattering atoms, because $\Gamma_{00}(\Omega)$ has itself this property. Equation (6) gives

$$\Gamma_{00}^{-1}(\Omega) = \Gamma^{-1}(\omega, K) + \Pi(\omega, K). \quad (8)$$

We now eliminate the pole location E_0 in Γ_{00}, in favor of the physical energy ω_0 of the resonance. This is done by writing Eq. (8), at $T = 0$, for the case of two atoms in vacuum (implying $\mu = 0$), at zero energy $\omega = 0$ and momentum $\mathbf{K} = 0$. In this case $G(\omega_n, \mathbf{k})$ becomes the free propagator $(i\omega_n - \epsilon_k)^{-1}$ and the frequency summation in Π gets easy. On the other hand for two atoms in vacuum $\Gamma(\omega, K)$ becomes $|w|^2/(\Omega - E)$, which is essentially the T matrix. Hence in this case Eq. (8) reduces to

$$-E_0/|w|^2 = -\omega_0/|w|^2 - \int \frac{d\mathbf{k}}{(2\pi)^3}\frac{1}{2\epsilon_k}. \quad (9)$$

Actually this equation is just equivalent to $\omega_0 = E_0 + \mathrm{Re}\delta E_0$. Subtracting Eq. (9) from Eq. (8) we obtain

$$\Gamma^{-1}(\omega, K) = \Gamma_0^{-1}(\Omega) - \Pi(\omega, K) - \int \frac{d\mathbf{k}}{(2\pi)^3}\frac{1}{2\epsilon_k}, \quad (10)$$

where $\Gamma_0(\Omega) \equiv |w|^2/(\Omega - \omega_0)$. Taken together the last two terms on the right-hand side (r.h.s.) of Eq. (10) give a convergent integral for large values of k, while each term separately diverges. However this divergence would not be present if we had kept the k dependence of $\langle \mathbf{k}|t|\varphi\rangle$ instead of making $\mathbf{k} = 0$ at the outset. Equation (10) makes clear a general feature, namely, the scattering amplitude depends not only on the total energy ω of the two particles, but also on their total momentum, due to the term $\Pi(\omega, K)$ which gives the effect of the other fermions on the scattering process: 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 $\mathbf{K}$ is very large, while we expect it to be most important for $\mathbf{K} = 0$. We consider only this situation in the following.

Remarkably the modifications produced by the other fermions are already very important when interactions are omitted in $\Pi(\omega, K)$. This corresponds to the modification of the scattering due to the Pauli exclusion. We restrict ourselves to this problem in the following. In this case we have $G(\omega_n, \mathbf{k}) = (i\omega_n - \epsilon_k + \mu)^{-1}$ and the calculation of Π can be reduced to a single integration over the momentum. It is convenient to use reduced units to display the result. We take μ as the energy scale and k_0, defined by $\mu = k_0^2/2m$, as the wave vector scale (this is the Fermi wave vector at $T = 0$). Introducing the reduced wave vector $x = k/k_0$, reduced energy $\bar{\omega} = \omega/\mu$, and reduced temperature $\bar{t} = T/\mu$, Eq. (10) becomes

$$-\frac{2\pi^2}{mk_0}\frac{1}{\Gamma(\omega, 0)} = \frac{1}{\lambda} - \frac{\bar{\omega} + 2}{\bar{W}} + I(\bar{\omega}),$$

$$I(\bar{\omega}) = \int_0^\infty dx\left[1 - \frac{x^2}{x^2 - 1 - \bar{\omega}/2}\tanh\frac{x^2 - 1}{2\bar{t}}\right], \quad (11)$$

where $\bar{\omega}$ means $\bar{\omega} + i\epsilon$. Except for the factor $\pi/2k_0$ this is just the inverse f^{-1} of the effective scattering amplitude for our problem. The coupling constant $\lambda = 2k_0|a|/\pi$ is also related to the detuning ω_0 by $\lambda = (2/\pi)W/\omega_0$ with $W = \gamma k_0$ being the energetic (half) width of the resonance line for a wave vector k_0. We have used the reduced width $\bar{W} = (2/\pi)W/\mu$. In 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 the order of 100 nm. It is experimentally of the order of 100 G, corresponding to an energy of 10 mK. For dense gases we have $k_0|a_{bg}| \sim 1$, which gives $W \sim 10$ mK. Since we have at most experimentally $\mu \sim 10\ \mu$K, we see that $\bar{W} \sim 10^3$. Since we are interested in reduced energy $\bar{\omega}$ of the order of 1, this makes the second term on the r.h.s. completely negligible and we omit it from now on. However this term is necessary if we want to find in the lower complex plane the pole corresponding to the Feshbach resonance.

The imaginary part of the r.h.s. is simply $\mathrm{Im}I(\bar{\omega}) = -(\pi/2)R\tanh(\bar{\omega}/4\bar{t})$ with $R = (1 + \bar{\omega}/2)^{1/2}$ and is plotted in Fig. 1. At $T = 0$ with no Fermi sea, this would give us back the imaginary part in Eq. (5). 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 $\tanh(\bar{\omega}/4\bar{t})$ can be understood as the decrease of the scattering resulting from the Pauli exclusion on the final state, together with the existence of reverse processes, both due to thermal occupation.

$\mathrm{Re}I(\bar{\omega})$ 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 λ is of the 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, $1/k_0$. One sees from Fig. 1 that $a_{\mathrm{eff}}^{-1}(\bar{\omega})$ has a strong energy dependence on the scale of the Fermi energy E_F. This is in contrast to the case of two isolated atoms seen in Eq. (5), where in the same energy range the real part of $-f^{-1}$ is a constant

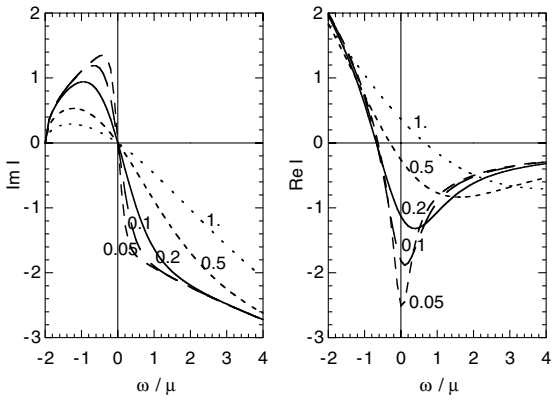

FIG. 1. Imaginary and real parts of the integral $I(\bar{\omega})$ in Eq. (11), as a function of reduced energy $\bar{\omega} = \omega/\mu$ for various reduced temperatures $\bar{t} = T/\mu$ indicated in the figure.

equal to the scattering length a^{-1}. This means that an essential simplification in the scattering properties effectively disappears. Indeed for ultracold atoms scattering is characterized by a single parameter, 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 $\mathrm{Re}f^{-1}$, we have a $\mathrm{Re}f^{-1}$ which is of the 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 λ 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 (see [2], for example, Fig. 4 of Bourdel *et al.*). Naturally the inhomogeneity due to the varying trapping potential is an additional source of smearing since the energy scale μ is space dependent.

We now look more strictly, in the domain $a \leq 0$, 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 $\mathrm{Im}\Gamma^{-1}(\bar{\omega}, 0) = \mathrm{Re}\Gamma^{-1}(\bar{\omega}, 0) = 0$ in Eq. (11). Since for $\bar{\omega} = -2$, $\mathrm{Re}I > 0$, $\mathrm{Re}f^{-1} > 0$, and the only possible resonance occurs at the chemical potential $\bar{\omega} = 0$. In this case $\mathrm{Re}f^{-1} = 0$ in Eq. (11) coincides with the well-known condition for the BCS pairing instability. In particular, at $T = 0$, the logarithmic divergence of $\mathrm{Re}f^{-1}$ which occurs for $\bar{\omega} = 0$ is a mark of this instability. It is known that this pairing instability is basically due to the 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 [11] nor higher orders and self-energy effects considered in recent calculations [12]. Note that we have not included interactions in $I(\bar{\omega})$, but they will not change the basic Pauli exclusion physics. We cannot expect interactions to remove the energy dependence of the scattering and our qualitative conclusion will remain unchanged. Finally for $a > 0$ we can use Eq. (11) to find the field at which the molecular bound state appears and relate it to the atom losses found [2] around 700 G. This will be reported elsewhere [13].

In conclusion we have presented a coherent framework which allows one 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 the 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 cannot be ignored. This modification results in washing out the Feshbach resonance and provides a natural explanation for recent experimental findings.

We are very grateful to Y. Castin, C. Cohen-Tannoudji, J. Dalibard, R. Hulet, X. Leyronas, C. Mora, and C. Salomon for very stimulating discussions.

*Laboratoire associé au Centre National de la Recherche Scientifique et aux Universités Paris 6 et Paris 7.

[1] B. DeMarco and D. S. Jin, Science **285**, 1703 (1999); A. G. Truscott *et al.*, Science **291**, 2570 (2001); F. Schreck *et al.*, Phys. Rev. Lett. **87**, 080403 (2001).
[2] K. Dieckmann *et al.*, Phys. Rev. Lett. **89**, 203201 (2002); K. M. O'Hara *et al.*, Science **298**, 2179 (2002); T. Bourdel *et al.*, Phys. Rev. Lett. **91**, 020402 (2003).
[3] H. T. C. Stoof *et al.*, Phys. Rev. Lett. **76**, 10 (1996).
[4] E. Timmermans *et al.*, Phys. Rep. **315**, 199 (1999), and references therein.
[5] M. Holland *et al.*, Phys. Rev. Lett. **87**, 120406 (2001).
[6] For a general introduction to many-body effects, see, for example, A. L. Fetter and J. D. Walecka, *Quantum Theory of Many-Particle Systems* (McGraw-Hill, New York, 1971).
[7] M. Houbiers *et al.*, Phys. Rev. A **57**, R1497 (1998).
[8] L. D. Landau and E. M. Lifshitz, *Quantum Mechanics* (Pergamon Press, Oxford, 1980).
[9] J. Bardeen, Phys. Rev. Lett. **6**, 57 (1961).
[10] C. Caroli *et al.*, J. Phys. C **5**, 21 (1972).
[11] L. P. Gorkov and T. K. Melik-Barkhudarov, Sov. Phys. JETP **13**, 1018 (1961).
[12] R. Combescot, Phys. Rev. Lett. **83**, 3766 (1999).
[13] R. Combescot, New J. Phys. **5**, 86 (2003).