

Analytical theory of the dressed bound state in highly polarized Fermi gases

R. COMBESCOT^(a), S. GIRAUD and X. LEYRONAS

Laboratoire de Physique Statistique^(b), Ecole Normale Supérieure - 24 rue Lhomond, 75231 Paris Cedex 05, France, EU

received 23 September 2009; accepted in final form 2 December 2009

published online 8 January 2010

PACS 03.75.Ss – Degenerate Fermi gases

PACS 05.30.Fk – Fermion systems and electron gas

PACS 71.10.Ca – Electron gas, Fermi gas

Abstract – We present an analytical treatment of a single \downarrow -atom within a Fermi sea of \uparrow -atoms, when the interaction is strong enough to produce a bound state, dressed by the Fermi sea. Our method makes use of a diagrammatic analysis, with the involved diagrams taking only into account at most two particle-hole pairs excitations. The agreement with existing Monte Carlo results is excellent. In the BEC limit our equation reduces exactly to the Skorniakov and Ter-Martirosian equation. We present results for \uparrow - and \downarrow -atoms with different masses, which is of interest for experiments in progress.

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Introduction. – The past few years have seen an intense exploration of the field of ultracold Fermi gases [1]. Quite recently it has turned toward very interesting and unexplored physical domains for superfluidity. Indeed it is possible to have stable mixtures of two fermionic species with different particle numbers [2–4] (called polarized gases) and also different masses. When quantum degeneracy is reached, these fermions may form Cooper pairs when there is a weak attractive interaction between atoms of different fermionic species, leading to BCS-like superfluidity. In the opposite regime of very strong attractive interaction these pairs are very tightly bound, forming essentially small molecules, and one obtains the Bose-Einstein condensation (BEC) of these resulting bosons. Thanks to the existence of Feshbach resonances [1], the strength of the attractive interaction can be essentially controlled at will experimentally and one can explore the whole extent of the so-called BEC-BCS crossover [1] between these two extreme regimes, where the overlap between the pairs goes from very small to very large. Polarization has been shown to be detrimental to superfluidity in this crossover, but one could also hope to discover new superfluid phases, like the FFLO phases [5,6], although experimental results are up to now negative in this respect.

A particularly attractive limiting case is the one of very strong polarization, which is at the same time easier to handle but provides also the possibility to understand quantitatively the physics at lower polarization [7–9]. This is the situation where a single fermion (say \downarrow -atom) with mass m_{\downarrow} is in the presence of a Fermi sea of another, say \uparrow , fermion species with mass $m \equiv m_{\uparrow}$, Fermi wave vector k_F and scattering length a between \uparrow - and \downarrow -atoms. In the absence of bound state, we have shown recently [10] that the exact solution of this problem is obtained as the limit of an extremely rapidly convergent series of approximations. These successive approximations amount to restrict the Hilbert space of the excited states of the system to one, two, \dots , n , \dots particle-hole pairs. In practice the first-order approximation, which coincides with the standard ladder approximation is already quite satisfactory. The second-order one, where at most two particle-hole pairs are coming in, gives an essentially exact answer, as it may be confirmed by comparison with QMC calculations, when available. Note that very recently the effective mass of this polaron has been measured experimentally at unitarity [11], with results in good agreement with theory [10,12].

In this paper we address analytically, by a diagrammatic extension of the above treatment, the case where the attractive interaction is strong enough to lead to a bound state, which is merely a molecule in the “BEC” limit of very strong attraction $k_F a \rightarrow 0_+$. This regime is of essential importance [9] for the understanding of the

^(a)E-mail: combesco@lps.ens.fr

^(b)The “Laboratoire de Physique Statistique” is “Laboratoire associé au Centre National de la Recherche Scientifique et aux Universités Paris 6 et Paris 7”.

whole phase diagram, since when the density of \downarrow -atoms increases, the corresponding bound states form a Bose-Einstein condensate. We will calculate in this regime the chemical potential and the effective mass, with results for the case of equal masses $m_{\uparrow} = m_{\downarrow}$ in remarkable agreement with known results from QMC calculations [9,13]. This allows us to provide accurate answers in the case of very high current interest where the mass ratio $r = m_{\downarrow}/m_{\uparrow}$ is different from 1. In the BEC limit our results are exact, since they reduce to the Skorniakov and Ter-Martirosian [14–16] equation.

Derivation of the equation. – In this section we sketch the derivation of our essential equations (2) and (3). This derivation will be provided in much more details in a long paper in preparation. The reader uninterested in these technical details may skip them and go to the next section, where we analyze eq. (3), and provide and discuss the results for the binding energy (obtained from eq. (3)) and the effective mass (obtained from eq. (2)).

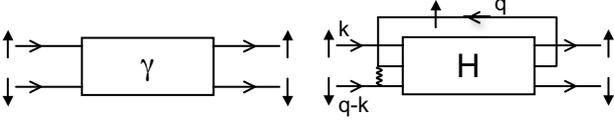
Since we have a single \downarrow -atom $N_{\downarrow} = 1$, we are, in the thermodynamic limit, just at the border between a zero density $n_{\downarrow} = 0$ and a non-zero density $n_{\downarrow} \neq 0$. Calculating this density by $n_{\downarrow} = \sum_{\mathbf{p}} \int (d\omega/2i\pi) G_{\downarrow}(\mathbf{p}, \omega)$, where the integration contour on ω encircles the $\text{Re } \omega < 0$ half-plane, this leads to the requirement that $G_{\downarrow}(\mathbf{p}, \omega)$ is analytic in this domain. But considering the evolution of its singularities when μ_{\downarrow} is increasing, starting from very large negative values, we reach the conclusion that, for $N_{\downarrow} = 1$, a singularity has reached $\omega = 0$. The simplest singularity to consider is just the explicit pole, corresponding to $G_{\downarrow}^{-1}(\mathbf{p}, 0) = G_{0\downarrow}^{-1}(\mathbf{p}, 0) - \Sigma(\mathbf{p}, 0) = \mu_{\downarrow} - E(p) - \Sigma(\mathbf{p}, 0) = 0$. Since the lowest energy for the \downarrow -atom is expected to occur for $\mathbf{p} = 0$, this leads to the expression $\mu_{\downarrow} = \Sigma(\mathbf{0}, 0)$ used in [12].

However there is also the possibility that the singularity arises from $\Sigma(\mathbf{p}, \omega)$ itself. This is the case which is of interest for us, and it is well known to occur in the "BEC" limit $1/k_F a \rightarrow \infty$, where a strongly bound state arises between the \downarrow -atom and an \uparrow -atom. Quite generally the existence of a bound state will appear as a pole in the vertex corresponding to the scattering of the \downarrow -atom and an \uparrow -atom. From the relation between the self-energy and this vertex, one can see that a pole occurring for a negative value of the total energy Ω of the two atoms will automatically give rise to singularities of $\Sigma(\mathbf{p}, \omega)$ for $\text{Re } \omega < 0$ and accordingly to $n_{\downarrow} \neq 0$. Hence, as it is physically obvious, we have to look for the chemical potential μ_{\downarrow} at which such a pole appears and compare it to the one corresponding to the condition found in the preceding paragraph. The lowest one will give the physical μ_{\downarrow} . Naturally the pole appears at zero energy $\Omega = 0$. Moreover, just as above, the limiting situation for the appearance of the \downarrow -atom is for $\omega = 0$, for the frequency variable in the self-energy. With respect to the momentum variables it is clear physically that the lowest energy for the pole is obtained when the total momentum

\mathbf{q} of the two atoms is zero. More precisely the dependence of the chemical potential on this momentum will give the effective mass, which is found positive in the physical range.

We make now the following approximation: in all the diagrams we draw, we restrict ourselves to have at most two explicit propagator lines corresponding to \uparrow -atoms running forward through the diagram. Naturally we have also the propagator line of our single \downarrow -atom which runs forward throughout the diagram. We could generalize to 3, 4 \dots explicit propagators, this series of approximations converging very rapidly to the exact result, just as in [10], but again the present approximation is quite enough. On completely general grounds all the diagrams we can draw for the vertex begin with an elementary interaction between our \downarrow -atom and an \uparrow -atom. However, since we let the strength g of this interaction go to zero $g \rightarrow 0$, we have to repeat this scattering an infinite number of times, any finite number giving a zero contribution. The summation of this series gives a factor $T_2(\mathbf{q}, \Omega)$, instead of the factor g we would have for a single interaction. It depends only on the total momentum \mathbf{q} and energy Ω of the two scattering atoms, and not on the variables of each atom separately. In vacuum we would have explicitly $T_2(\mathbf{q}, \Omega) = T_2^{(0)}(\mathbf{q}, \Omega) = (2\pi/m_r)[a^{-1} - \sqrt{2m_r(q^2/2M - \Omega)}]^{-1}$ (*i.e.* essentially the scattering amplitude of the two atoms with total mass M and reduced mass m_r), but here we have to calculate this quantity in the presence of the Fermi sea, with chemical potentials μ_{\uparrow} and μ_{\downarrow} . In a first-level approximation, where we would have at most a single propagator line for \uparrow -atoms, T_2 would be the only contribution. However at our second-level approximation, with two \uparrow -atoms propagators, we have also to consider processes where, as a first interaction or after T_2 , our single \downarrow -atom interacts with another \uparrow -atom.

Before proceeding let us consider first what happens when we calculate within our approximation the self-energy $\Sigma_{\downarrow}(\mathbf{0}, 0)$ relevant for the case without bound state [12]. In this case the essential difference is that, in order to obtain Σ from the vertex [17], we should not set $\Omega = 0$ but rather close all the diagrams by a \uparrow propagator running backward. This gives an additional factor $G_{0\uparrow}(\mathbf{q}, \Omega)$ and we have then to sum over \mathbf{q} and Ω . We sum over Ω by closing the Ω contour (which runs on the imaginary frequency axis) at infinity in the half-plane $\text{Re } \Omega < 0$. We do similarly for the other \uparrow propagator going backward. On the other hand, for all the explicit intermediate \uparrow propagators going forward (that is in the same direction as our entering \downarrow propagator), we close the contour in the $\text{Re } \omega > 0$ half-plane. It can then be seen that, due to the explicit \uparrow and \downarrow intermediate propagators, all the frequency integrations lead merely to on-the-shell evaluations for the remaining factors. This is naturally so only when these propagators give rise to poles in the corresponding frequency integration domain. Otherwise the result is zero. This leads to the constraint $k > k_F$ on the wave vectors for the forward propagators, and $q < k_F$


 Fig. 1: Diagrammatic representation of $\gamma_{\mathbf{k},\mathbf{q}}$ and $H_{\mathbf{k},\mathbf{q},\mathbf{q}'}$.

for the ones going backward. In this way we have been able to rederive exactly the equation ruling the self-energy in [10] and accordingly all the results of [10] for μ_\downarrow .

Coming back to our present problem, the only difference is that, instead of having the on-the-shell evaluation $\Omega = \epsilon_q - \mu_\uparrow$, with $\epsilon_q = \mathbf{q}^2/2m$, we have merely to set $\Omega = 0$. In the following we will have this implicit understanding for the variable named \mathbf{q} . Otherwise, by proceeding in the same way as above, we will have on-the-shell evaluations for all the other frequency variables entering our diagrams, with the same constraints $k_i > k_F$ and $q_i < k_F$ on the momenta. Hence, since all the frequencies are determined in this way, we refer in the following only to the momentum variables.

We need to write a general equation for the vertex $\gamma_{\mathbf{k}\mathbf{q}}$ with entering momenta \mathbf{k} for the \uparrow -atom and $\mathbf{q} - \mathbf{k}$ for the \downarrow -atom (see fig. 1). Except for a factor, this quantity is actually quite similar to $\alpha_{\mathbf{k}\mathbf{q}}$ in [10], the essential difference being the $\Omega = 0$, instead of on-the-shell, value for the \mathbf{q} variable. A first contribution is naturally $T_2(\mathbf{q}, 0)$. However we have also the possibility that the first interaction of the \downarrow -atom is with another \uparrow -atom, with momentum \mathbf{q}' . For fixed value of \mathbf{q}' , we call this contribution $H_{\mathbf{k}\mathbf{q}\mathbf{q}'}$ (see fig. 1). Since \mathbf{q}' is an internal variable, one has to sum over it to obtain the contribution to $\gamma_{\mathbf{k}\mathbf{q}}$. Finally, after the repeated scattering described by $T_2(\mathbf{q}, 0)$, we have the possibility to have the processes described by H . These two parts will be linked by an \uparrow and a \downarrow propagator. Integration over the frequency of the \uparrow propagator gives a factor $-1/\bar{E}_{\mathbf{k}\mathbf{q}}^{(1)}$ coming from the on-the-shell evaluation of the \downarrow one. In this way we obtain

$$\gamma_{\mathbf{k}\mathbf{q}} = T_2(\mathbf{q}, 0) \left[1 + \sum_{\mathbf{k}'\mathbf{q}'} \frac{H_{\mathbf{k}'\mathbf{q}\mathbf{q}'}}{\bar{E}_{\mathbf{k}'\mathbf{q}}^{(1)}} \right] - \sum_{\mathbf{q}'} H_{\mathbf{k}\mathbf{q}\mathbf{q}'} \quad (1)$$

with $\bar{E}_{\mathbf{k}\mathbf{q}}^{(1)} = |\mu_\downarrow| + E_{\mathbf{k}-\mathbf{q}} + \epsilon_{\mathbf{k}} - \mu_\uparrow$ and $E_{\mathbf{p}} = \mathbf{p}^2/2m_\downarrow$, quite analogous to $E_{\mathbf{k}\mathbf{q}}^{(1)}$ in [10].

We want to find under which conditions $\gamma_{\mathbf{k},0}$ diverges. This can naturally occur if $[T_2(\mathbf{0}, 0)]^{-1} = 0$, but this is just the first-level approximation. However this can also arise from a divergence of H , and we will look for the equation corresponding to this condition. Quite generally we have for γ and H a set of coupled linear equations. The divergence is obtained when there is a solution for the homogeneous part of these equations. In the following we retain only the terms contributing to this homogeneous part and we omit the other ones.

We have now to write for $H_{\mathbf{k}\mathbf{q}\mathbf{q}'}$ an equation analogous to eq. (1). However, since we accept only two \uparrow propagators, we do not have to go to higher-order vertices, and our equation will be closed. First, the \downarrow -atom and \uparrow -atom, having a first interaction, will interact repeatedly, giving rise to a common factor $T_2(\mathbf{q} + \mathbf{q}' - \mathbf{k}, \epsilon_{\mathbf{q}'} - \epsilon_{\mathbf{k}})$. Then, after this process, we may have another H vertex, giving rise to a term completely analogous to the second one in eq. (1). However we have also the possibility that, after this repeated interaction, the involved \uparrow -atom recombines with a hole (this corresponds to closing the T_2 by a backward \mathbf{q}' propagator). Afterwards the \mathbf{q}' \uparrow -atom has disappeared and all the possible remaining processes are described by $\gamma_{\mathbf{k}\mathbf{q}}$. There is a factor $-1/\bar{E}_{\mathbf{k}\mathbf{q}}^{(1)}$ coming from the propagator linking these two parts. Finally when we replace $\gamma_{\mathbf{k}\mathbf{q}}$ by its explicit expression from eq. (1), the first term does not contain H and is not retained. Hence, keeping only the homogeneous part of the equation, we obtain that the bound state appears when

$$[T_2(\mathbf{q} + \mathbf{q}' - \mathbf{k}, \epsilon_{\mathbf{q}'} - \epsilon_{\mathbf{k}})]^{-1} H_{\mathbf{k}\mathbf{q}\mathbf{q}'} = \sum_{\mathbf{k}'} \frac{H_{\mathbf{k}'\mathbf{q}\mathbf{q}'}}{\bar{E}_{\mathbf{k}\mathbf{k}'\mathbf{q}\mathbf{q}'}^{(2)}} - \frac{1}{\bar{E}_{\mathbf{k}\mathbf{q}}^{(1)}} \sum_{\mathbf{q}''} H_{\mathbf{k}\mathbf{q}\mathbf{q}''} + \frac{T_2(\mathbf{q}, 0)}{\bar{E}_{\mathbf{k}\mathbf{q}}^{(1)}} \sum_{\mathbf{k}'\mathbf{q}''} \frac{H_{\mathbf{k}'\mathbf{q}\mathbf{q}''}}{\bar{E}_{\mathbf{k}'\mathbf{q}}^{(1)}}, \quad (2)$$

with $\bar{E}_{\mathbf{k}\mathbf{k}'\mathbf{q}\mathbf{q}'}^{(2)} = |\mu_\downarrow| + E_{\mathbf{k}+\mathbf{k}'-\mathbf{q}-\mathbf{q}'} + \epsilon_{\mathbf{k}} + \epsilon_{\mathbf{k}'} - \epsilon_{\mathbf{q}} - \mu_\uparrow$. In this equation \mathbf{q} appears as a parameter and again the lowest energy bound state is obtained when $\mathbf{q} = \mathbf{0}$. Setting $H_{\mathbf{k},0,\mathbf{q}'} \equiv \bar{H}_{\mathbf{k}\mathbf{q}'}$ we find the following equation for the appearance of the lowest energy bound state:

$$[T_2(\mathbf{q} - \mathbf{k}, \epsilon_{\mathbf{q}} - \epsilon_{\mathbf{k}})]^{-1} \bar{H}_{\mathbf{k}\mathbf{q}} = \sum_{\mathbf{k}'} \frac{\bar{H}_{\mathbf{k}'\mathbf{q}}}{\bar{E}_{\mathbf{k}\mathbf{k}'\mathbf{0}\mathbf{q}}^{(2)}} - \frac{1}{\bar{E}_{\mathbf{k}\mathbf{0}}^{(1)}} \sum_{\mathbf{q}'} \bar{H}_{\mathbf{k}\mathbf{q}'} + \frac{T_2(\mathbf{0}, 0)}{\bar{E}_{\mathbf{k}\mathbf{0}}^{(1)}} \sum_{\mathbf{k}'\mathbf{q}'} \frac{\bar{H}_{\mathbf{k}'\mathbf{q}'}}{\bar{E}_{\mathbf{k}'\mathbf{0}}^{(1)}}. \quad (3)$$

Bound-state energy and effective mass. – We show now analytically that, in the BEC limit, our equation leads systematically to the exact result, whatever the mass ratio r . In this BEC limit our equation simplifies since it can be seen as the limit $k_F \rightarrow 0$ at fixed a . Since by definition $q \leq k_F$, we are left with a function $\bar{H}_{\mathbf{k},0} \equiv \bar{h}_{\mathbf{k}}$ of the single variable \mathbf{k} (actually only of its modulus for symmetry reasons). Then the summation over \mathbf{q}' in the last two terms of eq. (3) gives merely a factor $n_\uparrow = k_F^3/(6\pi^2)$. On the other hand, when we compare the first two terms in the right-hand side of eq. (3), the only difference is that the typical range for the summation over \mathbf{k}' is $k' \sim 1/a$ (as can be seen explicitly below) while it is $q' \sim k_F$ for the summation over \mathbf{q}' , as we have just seen. Hence the second term is of order $(k_F a)^3$ compared to the first, and accordingly completely negligible in the BEC limit (actually we find numerically that, even for the lowest relevant values of $1/k_F a$ this term gives a very small

contribution). Accordingly we are left with

$$[T_2(\mathbf{k}, -\epsilon_k)]^{-1} h_{\mathbf{k}} = \sum_{\mathbf{k}'} \frac{h_{\mathbf{k}'}}{\bar{E}_{\mathbf{k}\mathbf{k}'00}^{(2)}} + \frac{k_F^3}{6\pi^2} \frac{T_2(\mathbf{0}, 0)}{\bar{E}_{\mathbf{k}\mathbf{0}}^{(1)}} \sum_{\mathbf{k}'} \frac{h_{\mathbf{k}'}}{\bar{E}_{\mathbf{k}'0}^{(1)}}. \quad (4)$$

We are looking for a solution with the form $\rho \equiv |\mu_{\downarrow}|/E_F = \epsilon_b/E_F + 1 + \beta(m/m_r)k_F a$ which is an expansion in powers of $k_F a$, with $\epsilon_b = 1/2m_r a^2$ the molecule binding energy and $E_F = k_F^2/2m$ the Fermi energy. Taking into account the general expression of $T_2(\mathbf{k}, \omega)$ which gives $[m_r T_2(\mathbf{0}, 0)/(2\pi a)]^{-1} = 1 - (2k_F a/\pi)[1 + \sqrt{(\rho-1)m_r/m} \arctan(\sqrt{(\rho-1)m_r/m})]$ and substituting the expansion for ρ gives the expansion $[m_r T_2(\mathbf{0}, 0)/(2\pi a)]^{-1} = -(k_F a)^3[\beta/2 + 2/(3\pi)]$. The lowest-level approximation corresponds to write $[T_2(\mathbf{0}, 0)]^{-1} = 0$. This leads to $\beta = -4/(3\pi)$ which corresponds to the Born approximation for the \uparrow -atom-dimer scattering length.

While in the BEC limit we have, in the last term of eq. (4), to evaluate $T_2(\mathbf{0}, 0)$ carefully since it is large, all the other terms can be evaluated to lowest order. Hence we set $|\mu_{\downarrow}|/E_F = (m/m_r)/(k_F a)^2$ in $\bar{E}_{\mathbf{k}\mathbf{0}}^{(1)} = |\mu_{\downarrow}| + k^2/2m_r$ and in $\bar{E}_{\mathbf{k}\mathbf{k}'00}^{(2)} = |\mu_{\downarrow}| + (\mathbf{k} + \mathbf{k}')^2/2m_{\downarrow} + (k^2 + k'^2)/2m$. Similarly we have $[m_r T_2(\mathbf{k}, -\epsilon_k)/(2\pi a)]^{-1} = 1 - \sqrt{1 + R(ka)^2}$, where $R = m_r/m_r^T$ is the ratio of m_r to the reduced mass $m_r^T = m(m + m_{\downarrow})/(2m + m_{\downarrow})$ of the \uparrow -atom-dimer system ($R = 3/4$ for equal masses). We take the reduced variable $\mathbf{x} = a\mathbf{k}$ and make the change of function $h(\mathbf{k}) = C f(x)/x^2$ where C is a constant to be determined just below. We find from eq. (4)

$$\begin{aligned} \pi R \left[1 + \sqrt{1 + R x^2}\right]^{-1} f(x) = \\ -\frac{1}{2\pi} \int_0^{\infty} dy \int d\Omega_y \frac{f(y)}{1 + x^2 + y^2 + R' \mathbf{x} \cdot \mathbf{y}} \\ + \frac{8}{4 + 3\pi\beta} \frac{1}{1 + x^2} \int_0^{\infty} dy \frac{f(y)}{1 + y^2}, \end{aligned} \quad (5)$$

where $R' = 2m_r/m_{\downarrow}$ and the angular average over \mathbf{y} can be easily performed. We can choose C so that $f(0) = -3\pi\beta/(2R)$. Then, writing eq. (5) for $x=0$, we find that the coefficient of $1/(1+x^2)$ (including the integral) in the last term of eq. (5) is just equal to π . Hence eq. (5) coincides exactly with the equation, suitably generalized to the case of unequal masses, found by Skorniakov and Ter-Martirosian [14] for the scattering amplitude to obtain the fermion-dimer scattering length a_3 . Solving eq. (5) provides the exact result for $a_3 = a f(0)$. From the above relation this gives $\beta = -2R a_3/(3\pi a)$. When this is inserted in the above expression for $|\mu_{\downarrow}|$, we obtain a contribution $-2\pi n_{\uparrow} a_3/m_r^T$ from the fermion-dimer scattering, which is precisely the one resulting from a mean-field argument, exact in this limit. Hence our equation provides the exact answer in the BEC limit by reducing to the Skorniakov and Ter-Martirosian equation [14–16].

We have solved numerically eq. (3) in the general case. The results for μ_{\downarrow} are given in fig. 2, or rather we plot

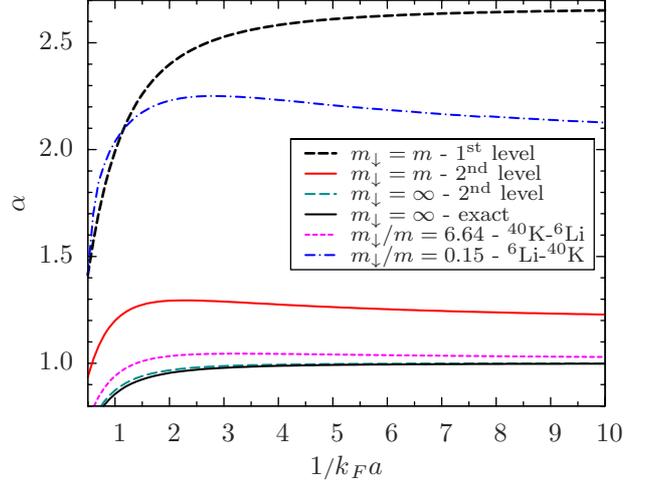


Fig. 2: (Colour on-line) Reduced chemical potential $\alpha \equiv (3\pi m_r^T/2m E_F k_F a) (\epsilon_b + E_F - |\mu_{\downarrow}|)$ as a function of $1/k_F a$ for various mass ratios.

$\alpha \equiv (3\pi m_r^T/2m E_F k_F a) (\epsilon_b + E_F - |\mu_{\downarrow}|)$ which reduces to a_3/a in the BEC limit and allows to magnify small differences. For equal masses $m_{\downarrow} = m$ we find that, basically down to $1/k_F a \sim 2$, α is essentially constant, almost equal to its BEC value $a_3/a = 1.18$ (we display also the first-level result $[T_2(\mathbf{0}, 0)]^{-1} = 0$ which goes to the Born result $a_3/a = 8/3$ in the BEC limit). This is exactly what is found by QMC calculations [9,13]. More precisely we find the actual value of α is slightly higher, the decrease toward the BEC limit being quite slow, behaving as $k_F a$. We also find that the bound state appears for $1/k_F a \simeq 0.88$ in perfect agreement with QMC [13] (all the more remarkable since the two chemical potential curves for the polaron and the bound state cross at a very small angle, which makes this value quite sensitive). Another very striking check of the precision of our results is found for $m_{\downarrow} = \infty$, where the exact result is known [12]. For most of the range the agreement for α is within a few 10^{-3} and the difference is barely seen even in our blown up fig. 2. A very interesting feature of this limit is that the convergence toward the BEC result $\alpha = 1$ is as $(k_F a)^2$, faster than in the general case. This allows to understand qualitatively why, for the equal mass case, which is not much different, one obtains also a fairly slow variation. The case of physical interest $r = 6.64$ for the ^{40}K - ^6Li mixture is also shown and is actually very close to this limit. We display also the $r = 1/6.64 \simeq 0.15$ result. Note finally that, in agreement with [10], the quite simple $\mathbf{q} = \mathbf{0}$ approximation of eq. (3) gives results in fairly good agreement with our exact numerical treatment.

Finally let us turn to our results for the effective mass m^* . Naturally we always obtain that, in the BEC limit, the effective mass of the bound state is equal to the molecular mass $M = m_{\downarrow} + m$. In fig. 3 we display our results for the inverse ratio of the effective mass to the bare mass m_{\downarrow}/m^* , in the case of equal masses $m_{\downarrow} = m$. We see that the effective mass increases when one goes away from this BEC limit. This is physically reasonable since in general

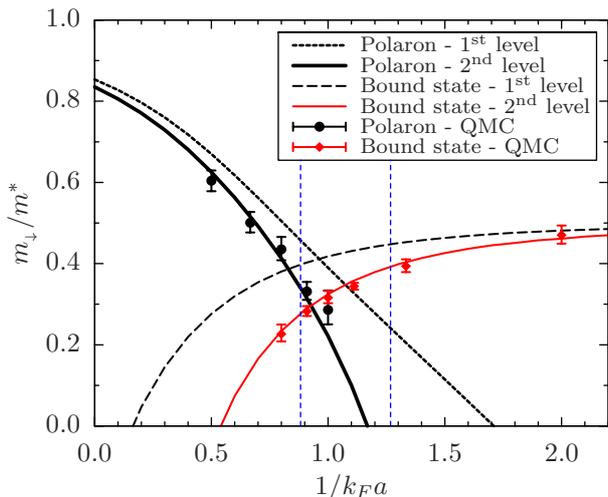


Fig. 3: (Colour on-line) Case $m_\downarrow = m$. Reduced inverse effective mass m_\downarrow/m^* of the polaron and of the bound state as a function of $1/k_F a$, at the first- and second-level approximations. The dashed lines indicate the location of the appearance of the bound state, both at the first-level $1/k_F a \simeq 1.27$ and the second-level $1/k_F a \simeq 0.88$ approximations.

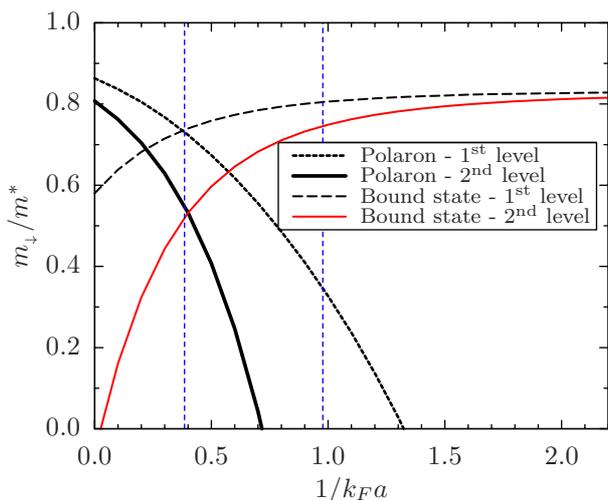


Fig. 4: (Colour on-line) Case $m_\downarrow = 5m$. Reduced inverse effective mass m_\downarrow/m^* of the polaron and of the bound state as a function of $1/k_F a$, at the first- and second-level approximations. The dashed lines indicate the location of the appearance of the bound state, both at the first-level $1/k_F a \simeq 0.98$ and the second-level $1/k_F a \simeq 0.38$ approximations.

more \uparrow -atoms are involved in the dressing of the \downarrow -atom, rather than a single one corresponding to the molecular state as it happens in the BEC limit. The agreement with diagrammatic QMC results [13] is again quite remarkable, both on the polaron side and on the bound-state side. Our results for $m_\downarrow = 5m$ and $m_\downarrow = 0.5m$ are shown respectively in fig. 4 and fig. 5. Note that when the effective mass is calculated beyond the transition from the polaron to the bound state, m_\downarrow/m^* becomes eventually negative, as seen in fig. 3, fig. 4 and fig. 5, which signals an instability. As

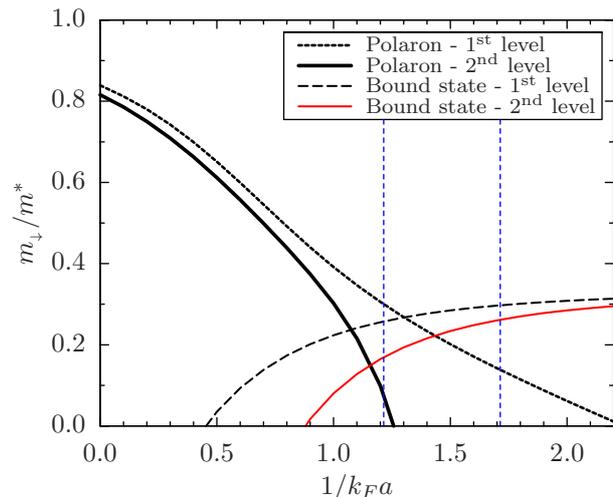


Fig. 5: (Colour on-line) Case $m_\downarrow = 0.5m$. Reduced inverse effective mass m_\downarrow/m^* of the polaron and of the bound state as a function of $1/k_F a$, at the first- and second-level approximations. The dashed lines indicate the location of the appearance of the bound state, both at the first-level $1/k_F a \simeq 1.72$ and the second-level $1/k_F a \simeq 1.22$ approximations.

expected physically the polaron-to-bound-state transition happens before the occurrence of this instability. For $m_\downarrow = \infty$ the bound state appears naturally for $1/k_F a = 0$. On the other hand, when one gets to lighter m_\downarrow , the transition value for $1/k_F a$ goes toward higher and higher values. This evolution is clear from fig. 4, fig. 3 and fig. 5. It is already seen easily at our first-level approximation which although not accurate is nevertheless qualitatively correct.

Conclusion. – In conclusion we have presented a diagrammatic analysis of the many-body problem of a single \downarrow -atom immersed in a Fermi sea of \uparrow -atoms. In this paper we have handled the case where the attractive interaction between the \downarrow -atom and \uparrow -atoms is strong enough to lead to a bound state. However we have indicated that our method allows to recover preceding results regarding the case of a weaker interaction where a polaron is formed without any bound state. Hence our technique provides a unified treatment of the problem across the whole BEC-BCS crossover.

Here we have taken into account at most two particle-hole pairs excitations, but the method could be extended to higher numbers. However comparison with existing Monte Carlo results as well as with known exact results is excellent, and there is presently no need to go to higher order. Hence our equation provide an essentially exact analytical description of the molecular state dressed by a Fermi sea. Consistently, in the BEC limit, our equation reduces exactly to the Skorniakov and Ter-Martirosian equation.

Specifically we have calculated the chemical potential and the effective mass of the \downarrow -atom, not only when the masses of the \uparrow - and \downarrow -atoms are equal, but also when they are different, which is of high interest for experiments

in progress on mixtures of different fermionic gases, for example mixtures of ^6Li and ^{40}K .

Additional remark: After this work was completed and posted as arXiv:0907.3197, we have become aware of independent works addressing the same bound-state problem by Mora and Chevy, arXiv:0908.0608, and by Punk, Dumitrescu and Zwerger, arXiv:0908.1343.

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