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Normal State of Highly Polarized Fermi Gases: Full Many-Body Treatment[1]

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Abstract—We present a full many-body analysis of the problem of a single ↓ atom resonantly interacting with a Fermi sea of ↑ atoms. A series of successive approximations permits us to clarify the quite mysterious agreement between Monte Carlo results and approximate calculations taking only into account single particle-hole excitations. We show that it results from a nearly perfect destructive interference of the contributions of states with more than one particle-hole pair. Our treatment provides, at the same time, an essentially exact solution to this problem.

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1. INTRODUCTION

The study of two-component Fermi gases is an active area of research in the field of ultracold atoms, both experimentally and theoretically [1]. In particular through the existence of Feshbach resonance these systems provide a physical realization of the BEC-BCS crossover, and around the resonance very simple examples of strongly interacting fermionic systems, of high interest for example in condensed matter physics. More recent experimental work has concerned the study of spin polarized configurations with a possibly strong imbalance between the two fermionic populations present in these gases, corresponding for example to the two lowest energy hyperfine states of ^{6}Li or ^{40}K.

One of the major experimental observations has been the occurrence of phase separation [2]. Some of the experiments suggest that, in the unitary limit of strong interactions, there are three phases: an unpolarized superfluid phase, a mixed phase which exhibits a partial polarization, and a fully polarized gas. The analysis of the $T = 0$ phase separation requires the knowledge of the properties of both the superfluid and the partially polarized normal phase [3]. Indeed, if only ↑ atoms with mass $m_\uparrow$ are present, then the energy is that of an ideal Fermi gas $E = 3/5E_FN_\uparrow$, where $N_\uparrow$ is the total number of ↑ atoms and $E_F = (6\pi^2n_\uparrow)^{2/3}/2m_\uparrow$ is the ideal gas Fermi energy (we set $\hbar = 1$ throughout the paper). When we add ↓ atoms with mass $m_\downarrow$, creating a small finite density $n_\downarrow$, they will form a degenerate gas of quasiparticles at zero temperature occupying all the states with momentum up to the Fermi momentum $(6\pi^2n_\downarrow)^{1/3}$. The energy of the system can then be written in a useful form in terms of the concentration $x = n_\downarrow/n_\uparrow$ as

$$\frac{E(x)}{N_\uparrow} = \frac{3}{5}E_F\left(1 - Ax + \frac{m_\uparrow}{m^*}x^{5/3}\right), \qquad (1)$$

where $E_b = 3/5E_FA$ is the binding energy of a single spin-↓ quasiparticle in the presence of a Fermi sea of spin-↑ atoms and m^* is its effective mass.

Hence the problem of a single particle coupled to an ideal Fermi sea is the key one for understanding the phase diagram and one has to know precisely the spin-↓ quasiparticle parameters. At unitarity recent fixed-node Monte Carlo (MC) calculations [4] give A = 0.99(1) and $m^*/m_\downarrow = 1.09(2)$. On the other hand a simple T-matrix analytical calculation, which happens to coincide with a variational calculation [5, 6], gives $E_b = 0.6066E_F$ and $m^*/m_\downarrow = 1.17$ which is remarkably close to the MC result. This closeness has been confirmed recently by diagrammatic MC calculations, leading to $E_b = 0.618E_F$ [7] or $E_b = 0.615R_F$ [8], depending on the specific detailed handling. The very close proximity of the analytical and the MC results, considered to be quite near the exact result, is a major puzzle. Indeed at unitarity the system is strongly interacting, whereas the analytical treatment considers only single particle-hole excitations (of the non-interacting Hamiltonian H_c). This description is only appropriate for a weakly interacting system and should fail to a large extent at unitarity.

We have very recently solved this puzzle and at the same time provided an essentially exact solution to the problem [9]. This has been done by considering states with any number of particle-hole excitations. Here we concentrate on the unitarity case. Indeed in the weak limit $a \longrightarrow 0_-$, an expansion in powers of a should be valid and the lowest order correction should give

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already quite good results. On the other side of unitarity, one can easily see from the details given below that our approximation should improve for increasing $1/a > 0$. Hence unitarity is a kind of worst case for our approach. Generalization away from unitarity is quite obvious.

In Section 2, we present the lowest order solution [6]. This permits us to show the efficiency of the $\mathbf{q}_i$ expansion. Then in Section 3, we describe our full many-body treatment. Section 4 is devoted to a verification of our theoretical scheme in the particular case $m_\downarrow \longrightarrow \infty$ and a presentation of our results for the equal mass situation. Finally, we conclude in Section 5.

2. SINGLE PARTICLE-HOLE EXCITATIONS

The Hamiltonian of our problem is:

$$H = H_c + V, \tag{2}$$

$$H_c = \sum_{\mathbf{P}} E(\mathbf{P}) b^\dagger_{\mathbf{P}} b_{\mathbf{P}} + \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}} c_{\mathbf{k}}, \tag{3}$$

$$V = g \sum_{\mathbf{kk'PP'}} \delta_{\mathbf{kk'PP'}} c^\dagger_{\mathbf{k}} c_{\mathbf{k'}} b^\dagger_{\mathbf{P}} b_{\mathbf{P'}}, \tag{4}$$

where $\epsilon_{\mathbf{k}} = \mathbf{k}^2/2m_\uparrow$, $E(\mathbf{P}) = \mathbf{P}^2/2m_\downarrow$, and $c_{\mathbf{k}}$ and $c^\dagger_{\mathbf{k}}$ are annihilation and creation operators for $\uparrow$-spin atoms while $b_{\mathbf{P}}$ and $b^\dagger_{\mathbf{P}}$ are for the $\downarrow$-spin atom. In the potential energy term V, the short-ranged interaction potential provides an upper cut-off k_c, which we will as usual let go to infinity while the coupling constant g goes to zero, keeping the scattering length finite in the relation $m_r/(2\pi a) = g^{-1} + \sum^{k_c} 2m_r/k^2$, where $m_r = m_\uparrow m_\downarrow/(m_\uparrow + m_\downarrow)$ is the reduced mass. Momentum conservation in the scattering is ensured by the Kronecker symbol $\delta_{\mathbf{kk'PP'}}$. Physically this potential energy term creates (or annihilates) a single particle-hole pair from the Fermi sea, or merely scatters particles or holes, the momentum transfer being taken by the $\downarrow$-spin atom.

The trial wave function $|\psi\rangle$ we consider, for a system of total momentum $\mathbf{p}$, is the following momentum eigenstate:

$$|\psi\rangle = \alpha_0 b^\dagger_{\mathbf{p}}|0\rangle + \sum_{\mathbf{kq}} \alpha_{\mathbf{kq}} b^\dagger_{\mathbf{p}+\mathbf{q}-\mathbf{k}} c^\dagger_{\mathbf{k}} c_{\mathbf{q}}|0\rangle, \tag{5}$$

where $|0\rangle = \prod_{k<k_F} c^\dagger_{\mathbf{k}}|vac\rangle$ is the Fermi sea of $\uparrow$-spins and the sums on q and k are implicitly limited to $q < k_F$ and $k < k_F$. In the first term, the $\uparrow$-spin free Fermi sea is in its ground state and the $\downarrow$-spin atom carries the momentum $\mathbf{p}$, while in the second term it is in excited states corresponding to the creation of a particle-hole pair in the Fermi sea with momentum $\mathbf{k}$ and $\mathbf{q}$, respectively, the $\downarrow$-spin atom carrying the rest of the momentum.

Writing $H|\psi\rangle = E|\psi\rangle$ (where we take as zero for the energy E the energy of the whole Fermi sea, and omit the average potential energy which disappears for $g \longrightarrow 0$) and identifying the coefficients of specific particle-hole states in both terms, we find:

$$-g^{-1} E^{(0)} \alpha_0 = \sum_{\mathbf{kq}} \alpha_{\mathbf{kq}}, \tag{6}$$

$$-g^{-1} E^{(1)}_{\mathbf{kq}} \alpha_{\mathbf{kq}} = \alpha_0 + \sum_{\mathbf{K}} \alpha_{\mathbf{Kq}} - \sum_{\mathbf{Q}} \alpha_{\mathbf{kQ}}, \tag{7}$$

where $E^{(0)} = |E| + E(\mathbf{p})$ and $E^{(1)}_{\mathbf{kq}} = |E| + E(\mathbf{k} - \mathbf{q} - \mathbf{p}) + \epsilon_{\mathbf{k}} - \epsilon_{\mathbf{q}}$. In the second equation the first term comes from the creation of a particle-hole pair in the Fermi sea, the second from the diffusion of the particle and the third from the diffusion of the hole. For $\mathbf{p} = \mathbf{0}$, we have $|E| = -E = E_b$, while the variation of E for small $\mathbf{p}$ gives the effective mass.

At unitarity, for equal masses $m_\uparrow = m_\downarrow = m$, taking the limit $k_c \longrightarrow \infty$, $g \longrightarrow 0$, we obtain [5, 6]:

$$|E| = \sum_{q<k_F} \left[\sum_k \frac{m}{k^2} - \sum_{k>k_F} \frac{1}{E^{(1)}_{\mathbf{kq}}} \right]^{-1}. \tag{8}$$

The exact solution of this equation is $\rho = E_b/E_F = 0.6066$. Setting $\mathbf{q} = \mathbf{0}$ in $E^{(1)}_{\mathbf{kq}}$ leads to the equation $2/3\rho = 1 + \sqrt{\rho/2}\arctan\sqrt{\rho/2}$. The solution $\rho = 0.5347$ is not so far from the actual result, which is already pretty satisfactory for such a crude approximation. However we may quite improve on it by treating $\mathbf{q}$ to lowest significant order instead of neglecting it completely. This means we take for the $\mathbf{k}$ angular average $\langle[|E| + \epsilon_{\mathbf{k}-\mathbf{q}} + \epsilon_{\mathbf{k}} - \epsilon_{\mathbf{q}}]^{-1}\rangle_{\mathbf{k}} \simeq [2\epsilon_k + |E|]^{-1} + q^2k^2/(3m^2) \times [2\epsilon_k + |E|]^{-3}$. This gives at unitarity $\rho = 0.5985$, which is remarkable compared to the exact solution of Eq. (8) and the MC result $(5/3)\rho = 0.99(1)$ [4]. If we do not restrict ourselves to unitarity and let the scattering length vary, the corresponding solution for ρ turns out to be essentially undistinguishable on a graph from the exact numerical solution [6]. Although the situation is somewhat less favorable for unequal masses, this shows very simply and explicitly the validity and efficiency of this $\mathbf{q}_i$ expansion approach. We apply it now to the full many-body problem.

3. FULL MANY-BODY TREATMENT

Following the same idea as in the previous section, we are looking for the ground state as a general superposition of states with any number of particle-hole pairs:

$$|\psi\rangle = \alpha_0 b_{\mathbf{0}}^{\dagger}|0\rangle + \sum_{\mathbf{kq}} \alpha_{\mathbf{kq}} b_{\mathbf{q}-\mathbf{k}}^{\dagger} c_{\mathbf{k}}^{\dagger} c_{\mathbf{q}}|0\rangle + \dots$$
$$+ \frac{1}{(n!)^2} \sum_{\{\mathbf{k}_i\}\{\mathbf{q}_j\}} \alpha_{\mathbf{k}_i\mathbf{q}_j} b_{\mathbf{P}}^{\dagger} \prod_{i=1}^{n} c_{\mathbf{k}_i}^{\dagger} \prod_{j=1}^{n} c_{\mathbf{q}_j}|0\rangle + \dots. \quad (9)$$

In the general term, we have $\mathbf{P} = \sum_j^n \mathbf{q}_j - \sum_i^n \mathbf{k}_i$ for the argument of the creation operator $b_{\mathbf{P}}^{\dagger}$ of the ↓-spin, to ensure that the total momentum of the particles in any term is zero. Here again, we assume implicitly $k_i > k_F$ and $q_j < k_F$.

The coefficients $\alpha_{\mathbf{k}_i\mathbf{q}_j}$ (which is a shorthand for $\alpha_{\{\mathbf{k}_i\}\{\mathbf{q}_j\}}$) are naturally antisymmetric with respect to the exchange of any their arguments $\mathbf{k}_i$ or $\mathbf{q}_j$.

Writing $H|\psi\rangle = E|\psi\rangle$ we obtain for the equations corresponding to the full Fermi sea and the Fermi sea with a single particle-hole pair:

$$-g^{-1}E^{(0)}\alpha_0 = \sum_{\mathbf{kq}} \alpha_{\mathbf{kq}}, \quad (10)$$

$$-g^{-1}E_{\mathbf{kq}}^{(1)}\alpha_{\mathbf{kq}} = \alpha_0 + \sum_{\mathbf{K}} \alpha_{\mathbf{Kq}} - \sum_{\mathbf{Q}} \alpha_{\mathbf{kQ}} - \sum_{\mathbf{KQ}} \alpha_{\mathbf{kKqQ}}, \quad (11)$$

where we have introduced $E_{\mathbf{k}_i\mathbf{q}_j}^{(n)} = |E| + E(\sum_i^n \mathbf{k}_i - \sum_j^n \mathbf{q}_j) + \sum_i^n \epsilon_{\mathbf{k}_i} - \sum_j^n \epsilon_{\mathbf{q}_j}$. The first equation is the same as in the previous section. In the second equation the additional term comes from the annihilation of a particle-hole pair: from two particle-hole pair states, there are four combinations for annihilation of a particle-hole pair (this would be n^2 in the general case). The next equation from two particle-hole pairs states is:

$$-g^{-1}E_{\mathbf{kk'qq'}}^{(2)}\alpha_{\mathbf{kk'qq'}} = -\alpha_{\mathbf{kq}} - \alpha_{\mathbf{k'q'}} + \alpha_{\mathbf{kq'}} + \alpha_{\mathbf{k'q}}$$
$$+ \sum_{\mathbf{K}} \alpha_{\mathbf{Kk'qq'}} + \sum_{\mathbf{K}} \alpha_{\mathbf{kKqq'}} - \sum_{\mathbf{Q}} \alpha_{\mathbf{kk'Qq'}} \quad (12)$$
$$- \sum_{\mathbf{Q}} \alpha_{\mathbf{kk'qQ}} + \sum_{\mathbf{KQ}} \alpha_{\mathbf{Kkk'Qqq'}}.$$

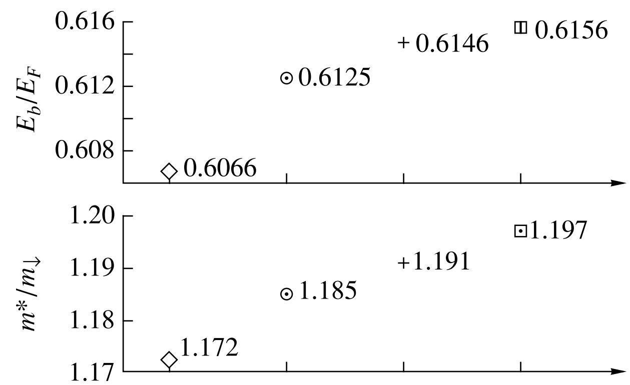
One could write formally the generalization for any order, but we will not do it since this will not be necessary.

In Eq. (11) the second term turns out to give a divergent contribution when $k_c \longrightarrow \infty$ and the limit is finite only after multiplication by g. By comparison the third term, where the summation is on the Fermi sea, displays no divergence and gives a zero contribution after multiplication by g. Hence we omit it from now on. Similarly in Eq. (12) we can omit the two analogous sums over $\mathbf{Q}$.

Now, we can apply the same kind of approximations as we used in the previous section. If we neglect the wave vectors $\mathbf{q}$ and $\mathbf{q}'$ in $E^{(2)}$ and take $E_{\mathbf{kk'qq'}}^{(2)} \simeq E_{\mathbf{kk'00}}^{(2)}$, we can sum Eq. (12) over $\mathbf{q}'$. Because of the antisymmetry of $\alpha_{\mathbf{Kkk'Qqq'}}$ in the exchange of $\mathbf{Q}$ and $\mathbf{q}'$, the last term gives no contribution, making the subspaces with higher number of particle-hole pairs irrelevant for our problem. The precise justification for this approximation is that, k, $k' > k_F$ and q, $q' < k_F$ make indeed in $E_{\mathbf{kk'qq'}}^{(2)}$ the k and k' terms dominant and q and q' ones negligible in a large part of the variables space. Naturally this is an approximation, the interference is not exact but not so far from it. The same argument applied at the level of Eq. (11) allows now to understand the success of the lowest order approach. If we make the approximation $E_{\mathbf{kq}}^{(1)} \simeq E_{\mathbf{k0}}^{(1)}$, the last term is disappearing, which leaves us with a decoupled set of equations for α_0 and $\alpha_{\mathbf{kq}}$, leading to the good approximation discussed in the Section 2.

Conversely we may decide to make the approximation $E_{\mathbf{k}_i\mathbf{q}_j}^{(n)} \simeq E_{\mathbf{k}_i}^{(n)}$ at some higher order n. This provides by the same procedure a decoupling from higher order subspaces resulting in a closed set of n equations to be solved for $|E|$. Hence our analysis leads us to a cascade of successive approximations which converges very rapidly in a controlled way to the exact many-body solution. In practice the convergence is so fast, as shown by the quality of the lowest order results, that we will only need for any practical purpose to implement it to the second order.

In addition to our main scheme of approximations going from one order to the next, we may within a given order introduce an additional graduation of approximations. First, we can as described above make the approximation $E_{\mathbf{kk'qq'}}^{(2)} \simeq E_{\mathbf{kk'00}}^{(2)}$. However, we can easily improve on this handling, if we make only the approximation $E_{\mathbf{kk'qq'}}^{(2)} \simeq E_{\mathbf{kk'q0}}^{(2)}$, which takes better into account the $\mathbf{q}$ dependence. Finally, since we know that the last term in Eq. (12) brings only a small correction, we may just decide to omit it, but treat the rest of the equation exactly without any approximation on $E_{\mathbf{kk'qq'}}^{(2)}$. In this case, since we have restricted the Hilbert space to contain at most two particle-hole pairs, this corresponds to a variational calculation. This is the most precise level of approximation we will implement.



Reduced ↓ atom binding energy E_b and effective mass m^*, in the case of ↑ and ↓ atoms with equal masses, for the approximations of increasing accuracy discussed in the text. E_F is the Fermi energy of the ↑ atoms. Diamond: first order approximation [6]. Circle: second order with **qq**' = **00**. Cross: second order with **qq**' = **q0**. Square: second order with no **q** approximation (variational). For the effective mass we give coherently the last digits of our results to display clearly the trend, but they should not be taken for granted.

4. RESULTS

4.1. Infinite Mass Limit

We have first checked the convergence of our theoretical scheme in the particular case $m_\downarrow \longrightarrow \infty$ where the binding energy is known [6] to be exactly $\rho = 1/2$ at unitarity. This is naturally a very convenient case. However one can easily see that the situation, with respect to the convergence of the $\mathbf{q}_i$ expansion, is slightly less favorable than for the equal mass case. This is apparent in the first order result [6] $\rho = 0.465$ which, while being fairly good, is not so close to 1/2. A convenient feature of this case is that there are no angular integrations to perform in solving the various equations. At second order we find 0.481 when we take **qq**' = **00**. This improves into 0.487 for **qq**' = **q0**. However with no approximation on $E^{(2)}$ (i.e. the variational result) we find $\rho = 0.498$, which shows quite explicitly that essentially, at second order, we have already fully converged toward the exact result.

Another situation where the exact solution is known is the 1D case [6, 11]. Here again we have checked [10] that the second order coincides almost with the exact results, including for the calculation of the effective mass [11].

4.2. Equal Mass Case

We have then proceeded to the same calculations for the equal mass situation (see figure), which is markedly better in terms of convergence than the infinite mass case. For the **qq**' = **00** approximation we find 0.6125, the **qq**' = **q0** result is 0.6146. Finally the variational result is 0.6156. This displays quite clearly the very fast convergence of the $\mathbf{q}_i$ expansion. It is very likely that this last result is essentially exact (say, the exact one is bounded by 0.6158). This is supported by how close our above result for infinite $m_\downarrow$ is from the exact one. More precisely, as seen explicitly from the $m_\downarrow = \infty$ case, each order brings a small correction to the preceding one. Since the second order result brings typically a 10^{-2} correction to the first order one, we expect the third order correction to be at most of order 10^{-4}. Naturally the precision of our result is beyond practical use. We display it only to support our claim that we have a full solution for our problem.

Finally, we have calculated the effective mass, with the same approach applied to a small nonzero momentum for the whole system. This produces only some minor practical complications. We find $m^*/m_\downarrow = 1.20$. Our above precision on the binding energy gives us typically a ±0.02 uncertainty. In agreement with our above findings, this result is fairly close to the first order value 1.17. We see that there is some significant discrepancies with some MC results [3, 4] as well as conclusions from experiments [12]. Though they are not major ones, they may be relevant for the detailed understanding of experiments [13].

5. CONCLUSIONS

We have presented a full many-body analysis of the problem of a single ↓-fermion resonantly interacting with a Fermi gas of ↑-particles. We have obtained an essentially exact solution of this problem and elucidated the quite mysterious agreement between Monte-Carlo results and approximate calculations taking only into account single particle-hole excitations.

It results from a nearly perfect destructive interference of the contributions of states with more than one particle-hole pair. While the ground state of the interacting Hamiltonian H has important weights coming from many particle-hole excitations, we have shown that with respect to the calculation of the energy of the ↓-atom these states give contributions which decrease extremely rapidly with the number of particle-hole excitations. The efficiency of these interferences is directly linked to the key ingredient of our solution, namely the fact that an expansion in powers of the holes wave vectors $\mathbf{q}_i$ turns out, quite surprisingly and unexpectedly, to be an excellent approximation scheme.

To lowest order in this approximation, i.e., when the dependence on the $\mathbf{q}_i$'s is neglected, the interference is perfect and there is a complete decoupling between the states with different number of particle-hole excitations. Improving the approximation by taking more properly into account the $\mathbf{q}_i$ dependence provides a small coupling between these states and a small correction to the energy of the ↓-atom.

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