ISSN 1054-660X, Laser Physics, 2010, Vol. 20, No. 3, pp. 678–682.

Normal State of Highly Polarized Fermi Gases: The Bound State[1]

R. Combescot*, S. Giraud, and X. Leyronas

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

*e-mail: combesco@lps.ens.fr

Received September 25, 2009; published online February 2, 2010

Abstract—We consider a highly polarized Fermi gas with a single ↓ atom within a Fermi sea of ↑ atoms. We extend a preceding many-body analysis to the case where a bound state is formed between the ↓ atom and an ↑ atom.

DOI: 10.1134/S1054660X10050038

1. INTRODUCTION

The field of ultracold Fermi gases [1] has seen recently a very strong development, in particular to study the case of strongly interacting fermions. In contrast with bosons interesting situations require at least two fermion species, Indeed at very low temperature only *s*-wave scattering is significant, but it is forbidden by Pauli principle for identical fermions. Up to now the two fermion species involved in experiments have been essentially the two hyperfine states corresponding to a same element, for example ^{6}Li. These are very often referred to as ↑ and ↓ atoms, in analogy with electrons in a metal.

An essential feature of scattering between ↑ and ↓ atoms is the frequent occurrence of Feshbach resonances, which allow to control the scattering length a by an homogeneous magnetic field. The one found for ^{6}Li is quite wide in terms of magnetic field range, which is quite convenient. Going through the resonance, where the scattering length diverges, allows to vary a from large negative values to large positive ones. In practice it allows to a large extent to cover the whole range of values from $-\infty$ to $+\infty$ for the parameter $1/k_F a$, where k_F is the common Fermi momentum of the two fermionic species. In particular the BEC–BCS crossover has been studied experimentally in this way for the first time.

We have assumed above the most frequently studied situation where there is the same number of ↑ and ↓ atoms $n_\uparrow = n_\downarrow$. However, in contrast to what happens for electrons in metals, it is easy experimentally to reach situations with a strong imbalance $n_\uparrow \neq n_\downarrow$, between the two atomic populations (which implies a difference between the corresponding chemical potentials $\mu_\uparrow \neq \mu_\downarrow$). These are commonly called polarized gases. These physical systems may be quite stable and very interesting new physics is expected in these situations. They are actually of high interest for physicists interested in quark matter, since similar situations are expected to occur in the superfluid core of neutron stars or in heavy ions collisions. Finally quite interesting physics is also expected when the masses of the fermionic atomic species are not equal $m_\uparrow \neq m_\downarrow$, which is naturally achieved by taking different elements.

Since in the BCS state, ↑ and ↓ atoms form Cooper pairs, it is clear that the most favorable situation for BCS pairing is $n_\uparrow = n_\downarrow$, and accordingly $\mu_\uparrow = \mu_\downarrow$ (in the case of equal masses). Hence increasing $\mu^* = (\mu_\uparrow - \mu_\downarrow)/2$ is detrimental to the BCS state and there is a "critical field" μ_c^* beyond which this state and the corresponding superfluidity disappears. The corresponding critical field is known in superconductivity as the Clogston–Chandrasekhar [2] limit. Experiments on polarized ultracold Fermi gases [3, 4] have indeed observed the existence of this limit. However since experiments deal with trapped gases, the physical system is inhomogeneous which leads to some complications. When $n_\uparrow \neq n_\downarrow$ there is at the center of the trap a superfluid BCS phase in which $n_\uparrow = n_\downarrow$. On the sides of the trap one finds instead a normal phase with a strong polarization $n_\uparrow \neq n_\downarrow$. When the polarization of the gas increases, the size of the superfluid region decreases while the normal phase grows. At some critical population imbalance the superfluid core disappears completely. In the MIT group experiment the critical imbalance $P = (n_\uparrow - n_\downarrow)/(n_\uparrow + n_\downarrow)$ is observed around 0.8, at unitarity where the scattering length a diverges.

These experiments have been very nicely interpreted by Lobo, Recati, Giorgini and Stringari [5] (LRGS) who considered the unitarity case for simplicity. Their approach can be seen as a generalization of the Clogston-Chandrasekhar result to strongly interacting systems. Indeed the Clogston–Chandrasekhar result is merely obtained from a competition

[1] The article is published in the original.

between the energy of the simple BCS phase and the polarization energy of the non-interacting normal metal. Here both the superfluid and the normal state are strongly interacting. At unitarity, for dimensional reasons, the superfluid energy E_S is proportional to the Fermi energy with the result $E_S = 2n_\uparrow\xi(3E_F/5)$ where the coefficient $\xi \simeq 0.42$ has been obtained from Monte Carlo calculations. For the polarized normal state LRGS analysis starts with the extreme situation of a single $\downarrow$ atom in the presence of the Fermi sea of $\uparrow$ (non-interacting) atoms. When this $\downarrow$ atom has zero momentum, its energy is by definition the chemical potential $\mu_\downarrow$, which can be seen as a binding energy of the $\downarrow$ atom in the Fermi sea of $\uparrow$ atoms, the whole object ($\downarrow$ atom plus local modification of the $\uparrow$ Fermi sea around it) being often called "polaron," by analogy with the situation of an electron strongly polarizing the solid around it, when the electron-phonon interaction is large. When the $\downarrow$ atom is moving there is naturally a kinetic energy, with an effective mass m^* associated with it. Hence the energy $e_\downarrow(k)$ of the $\downarrow$ atom is:

$$e_\downarrow(k) = \mu_\downarrow + \frac{k^2}{2m^*}. \quad (1)$$

Then LRGS consider a small Fermi sea of $\downarrow$ atoms. Taking into account the two above contributions together with the energy of the $\uparrow$ Fermi sea, they obtain:

$$\frac{E_N(x)}{n_\uparrow} = \frac{3}{5}E_F\left(1 - \frac{5}{3}\frac{|\mu_\downarrow|}{E_F}x + \frac{m_\uparrow}{m^*}x^{5/3}\right) \quad (2)$$

with $x = n_\downarrow/n_\uparrow$ and where we have omitted an additional interaction term proportional to x^2 they take into account. They have obtained $\mu_\downarrow$ and m^* from Monte Carlo calculations as $|\mu_\downarrow|/E_F \simeq 0.58$ and $m^*/m_\downarrow \simeq 1.04$. The above $E_N(x)$ is similar in shape to a parabola and, when x increases from 0, the energy of the normal state decreases and it is energetically favorable for the system to stay in the polarized normal state. However, for larger x, $E_N(x)$ starts to increase and it is more favorable to switch to the (unpolarized) superfluid state with energy E_S. This corresponds to a first order transition and a phase separation in agreement with experiment. Then, making use of the local density approximation, LRGS have transposed the above discussion, valid for a homogeneous system, to the inhomogeneous situation found in experiments for trapped gases. In this way they have found a critical polarization $P_c = 0.77$ in remarkable agreement with the MIT group results. Furthermore the density distribution of $\uparrow$ and $\downarrow$ atoms, which can be obtained in the same framework, is also in strikingly good agreement with experimental results. The LRGS approach has been more recently generalized out of unitarity by Pilati and Giorgini [6] to provide the phase diagram in the whole BEC–BCS crossover, making use again of Monte Carlo calculations to obtain the unknown parameters coming in the various equation of state.

2. ONE SPIN $\downarrow$ AND N SPINS $\uparrow$: THE POLARON

The above discussion has shown that it is crucial to understand the physics of a single $\downarrow$ atom interacting strongly with the Fermi sea of $\uparrow$ non-interacting atoms. Not only is it by itself a very interesting many-body problem, but it opens the way for an understanding of the whole phase diagram for polarized Fermi gases, as we have seen in the introduction. The first attempt in this direction has been made by Chevy who proposed a simple variational wave function [7]. Then it was shown that a simple T-matrix approach is completely equivalent to this variational approach [8]. A very surprising feature of these works was that, at unitarity, they give for the chemical potential $\mu_\downarrow/E_F = -0.6066$ as well as for the effective mass $m^*/m_\downarrow = 1.17$ results which are very near Monte Carlo results. This is quite unexpected since, at unitarity, we have a very strongly interacting system, while the T-matrix approach as well as the variational wave function seem suitable only for a weakly interacting system. Hence the agreement looked as a kind of coincidence.

Further work by some of us [9] showed that this was not at all the case. We made a systematic approach, starting from the Hamiltonian:

$$H = H_c + V, \quad (3)$$

$$H_c = \sum_{\mathbf{P}} E(\mathbf{P}) b_{\mathbf{P}}^\dagger b_{\mathbf{P}} + \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} c_{\mathbf{k}}^\dagger c_{\mathbf{k}}, \quad (4)$$

$$V = g \sum_{\mathbf{k}\mathbf{k}'\mathbf{P}\mathbf{P}'} \delta_{\mathbf{k}\mathbf{k}'\mathbf{P}\mathbf{P}'} c_{\mathbf{k}}^\dagger c_{\mathbf{k}'} b_{\mathbf{P}}^\dagger b_{\mathbf{P}'}, \quad (5)$$

$$\epsilon_{\mathbf{k}} = \frac{\mathbf{k}^2}{2m_\uparrow}, \quad E(\mathbf{P}) = \frac{\mathbf{P}^2}{2m_\downarrow} \quad (6)$$

and inserted a fully general wave function, corresponding to the full Fermi sea, or the Fermi sea plus any number of particle-hole pairs:

$$|\psi\rangle = \alpha_0 b_0^\dagger|0\rangle + \sum_{\mathbf{k}\mathbf{q}} \alpha_{\mathbf{k}\mathbf{q}} b_{\mathbf{q}-\mathbf{k}}^\dagger c_{\mathbf{k}}^\dagger c_{\mathbf{q}}|0\rangle + \ldots + \frac{1}{(n!)^2} \sum_{\{\mathbf{k}_i\}\{\mathbf{q}_j\}} \alpha_{\{\mathbf{k}_i\}\{\mathbf{q}_j\}} b_{\mathbf{P}}^\dagger \prod_{i=1}^{n} c_{\mathbf{k}_i}^\dagger \prod_{j=1}^{n} c_{\mathbf{q}_j}|0\rangle + \ldots, \quad (7)$$

$$|0\rangle = \prod_{k<k_F} c_{\mathbf{k}}^\dagger|\text{vac}\rangle, \quad (8)$$

where an essential feature is that $\alpha_{\{\mathbf{k}_i\}\{\mathbf{q}_j\}}$ is antisymmetric in exchanges of the particle variables $\mathbf{k}_i$ (corresponding to the operators $c_{\mathbf{k}}$ with $k > k_F$) or of the hole

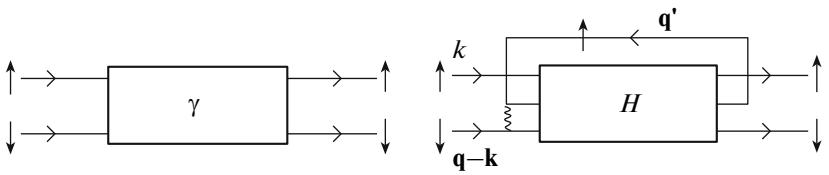

Fig. 1. Diagrams showing the vertex γ and $H_{\mathbf{kqq'}}$.

variables $\mathbf{q}_j$ (corresponding to the operators $c_{\mathbf{q}}$ with $q < k_F$). Inserting this wave function into $H|\psi\rangle = E|\psi\rangle$, we have found that, if the weak dependence of kinetic energies on hole variables q_i is neglected, there is an exact decoupling of the part of the wave function with a given number of particle-hole pairs from all the parts with a larger number of particle-hole pairs. This decoupling is due to a destructive interference resulting from the antisymmetry of $\alpha_{\{\mathbf{k}_i\}\{\mathbf{q}_j\}}$. Naturally the weak dependence on the q_i can not be completely neglected, but our finding implies that there is a very fast convergence toward the exact result when one includes higher and higher number of particle-hole pairs. This explains why the results with a single particle-hole pair is already quite reasonable. We have found that, for any practical purpose, going up to the inclusion of two particle-hole pairs is quite enough.

We have first checked our result on the limiting case $m_\downarrow \longrightarrow \infty$ where the exact result is known [8], because the problem reduces to the one of Fermi sea in the presence of a fixed impurity, which is an exactly solvable one-body problem. At unitarity for example one has merely $\rho \equiv |\mu_\downarrow|/E_F = 0.5$. The result with a single particle-hole pair is 0.465, but we have found 0.498 when we go up to two particle-hole pairs, showing that at this stage the convergence toward the exact result is essentially complete. Similarly we have checked our procedure in one-dimension, where exact results are known, with excellent agreement both for the energy and the effective mass.

Going back to the case of equal masses $m_\downarrow = m_\uparrow$, we have obtained that the above result $\rho = 0.6066$ when a single particle-hole pair is included goes to $\rho = 0.6156$ when we go to two particle-hole pairs. In this case, even more than for the infinite mass case, the convergence is extremely fast. Our result is in particular in excellent agreement with the last diagrammatic Monte Carlo calculations of Prokof'ev and Svistunov [10] who have found $\rho = 0.615$. Hence we have clearly shown that the agreement with Monte Carlo calculations is not coincidental, but has rather a deep and very interesting explanation.

3. ONE SPIN ↓ AND N SPINS ↑: THE BOUND STATE

Up to now the possibility of a bound state between the ↓ atom and a ↑ atom was excluded. In this section we deal with this situation. Such a bound state can merely be seen as a $\uparrow - \downarrow$ molecule dressed by the Fermi sea. It is of obvious physical interest since such a state is a boson and the Bose condensation occurring on the BEC side is a Bose condensation of these bosons. This corresponds to the physical situation investigated by Pilati and Giorgini [6] when they deal with the polarized superfluid.

In this section we will not give technical details. Some of this technical information may be found in [11]. Basically we obtain the energy of the bound state by finding the corresponding pole in the vertex describing the scattering of a ↓ and a ↑ atom. This is just the generalization of what we would do if we were looking at the usual scattering amplitude for a two-body problem in vacuum, where the corresponding vertex would be:

$$T_2^{(0)}(\mathbf{q}, \Omega) = \frac{2\pi}{m_r} \frac{1}{a^{-1} - \sqrt{2m_r(q^2/2M - \Omega)}}, \qquad (9)$$

where m_r is the reduced mass. We would find that the pole with lowest energy corresponds to a total momentum $\mathbf{q} = 0$ and has an energy:

$$\Omega = -\frac{1}{2m_r a^2} = -\epsilon_b, \qquad (10)$$

i.e., the standard binding energy ϵ_b of the two atoms in vacuum.

In the present case we have performed a diagrammatic analysis to obtain the expression of the vertex and its pole. In this analysis we have made an approximation corresponding to the one which has proved in [9] to be of high enough precision. We have restricted ourselves to have at most two explicit bare propagator lines corresponding to ↑-atoms running forward through the diagram. Naturally we have also the propagator line of our single ↓-atom which runs forward throughout the diagram. Again higher level of approximation would give even better precision converging very rapidly toward the exact result. We show in Fig. 1 the basic vertex γ we have to deal with, together with the higher order diagram $H_{\mathbf{kqq'}}$ which comes in our final equation. When we apply our diagrammatic analysis to the previous polaron problem, we are able to rederive the set of equations [9] obtained by the above Hamiltonian approach.

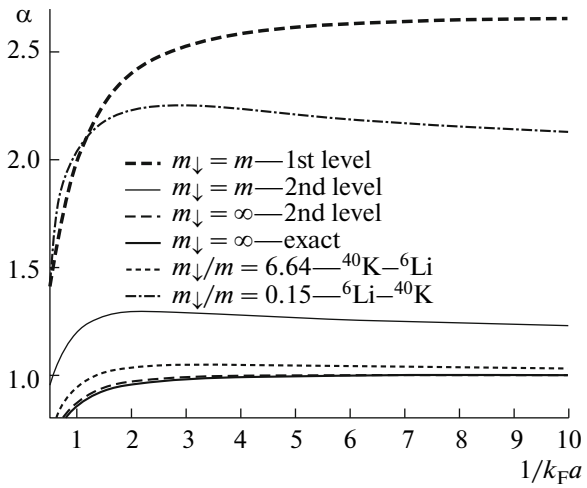

Fig. 2. Reduced chemical potential $\alpha \equiv (3\pi m_r^T/2mE_Fk_Fa)(\epsilon_b + E_F - |\mu_\downarrow|)$ as a function of $1/k_Fa$ for various mass ratios.

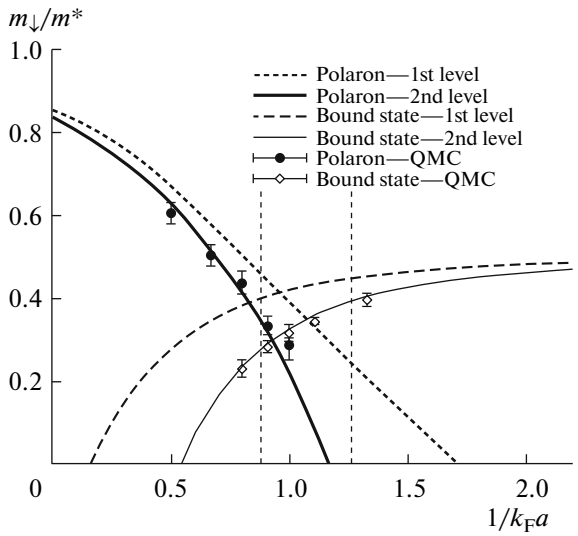

Fig. 3. Reduced inverse effective mass $m_\downarrow/m^*$ of the polaron and of the bound state as a function of $1/k_Fa$, at the first and second level approximations, in the case $m_\downarrow = m$. The dashed lines indicate the location of the appearance of the bound state, both at the first level $1/k_Fa \simeq 1.27$ and the second level $1/k_Fa \simeq 0.88$ approximations.

In this way we have found that the bound state energy is obtained when the following equation for $H_{\mathbf{kqq'}}$ has a solution:

$$[T_2(\mathbf{q}+\mathbf{q'}-\mathbf{k}, \epsilon_{q'}-\epsilon_k)]^{-1} H_{\mathbf{kqq'}} = \sum_{\mathbf{k'}} \frac{H_{\mathbf{k'qq'}}}{\bar{E}^{(2)}_{\mathbf{kk'qq'}}} - \frac{1}{\bar{E}^{(1)}_{\mathbf{kq}}} \sum_{\mathbf{q''}} H_{\mathbf{kqq''}} + \frac{T_2(\mathbf{q},0)}{\bar{E}^{(1)}_{\mathbf{kq}}} \sum_{\mathbf{k'q''}} \frac{H_{\mathbf{k'qq''}}}{\bar{E}^{(1)}_{\mathbf{k'q}}}, \quad (11)$$

where we have again the convention $k > k_F$ and $q < k_F$. Here, $T_2(\mathbf{q}, \Omega)$ is the equivalent of $T_2^{(0)}(\mathbf{q}, \Omega)$, and it is obtained by summing the series of ladder diagrams corresponding to the repeated scattering of $a\downarrow$ and $a\uparrow$ atom. The difference is that it has to be calculated in the presence of the Fermi sea, with chemical potentials $\mu_\uparrow$ and $\mu_\downarrow$. Finally we have $\bar{E}^{(1)}_{\mathbf{kq}} = |\mu_\downarrow| + E_{\mathbf{k}-\mathbf{q}} + \epsilon_{\mathbf{k}} - \mu_\uparrow$ and $\bar{E}^{(2)}_{\mathbf{kk'qq'}} = |\mu_\downarrow| + E_{\mathbf{k}+\mathbf{k'}-\mathbf{q}-\mathbf{q'}} + \epsilon_{\mathbf{k}} + \epsilon_{\mathbf{k'}} - \epsilon_{\mathbf{q'}} - \mu_\uparrow$. If we are looking for the chemical potential $\mu_\downarrow$, we have to set $\mathbf{q} = 0$ for the total momentum $\mathbf{q}$ of the $\downarrow$ and the $\uparrow$ atom. On the other hand the effective mass is obtained from the solution when $\mathbf{q} \neq 0$ and is small.

A very interesting and satisfactory feature of our equation Eq. (11) is found in the BEC strong coupling limit, where $1/k_Fa \longrightarrow +\infty$. This is equivalent to make $k_F \longrightarrow 0$, so if we consider the chemical potential, we have to set $\mathbf{q} = \mathbf{q'} = 0$ and we are left with a single variable $\mathbf{k}$. It can then be shown that our equation reduces to the Skorniakov and Ter-Martirosian equation [12]. This implies that in this limit we find the exact result, which involves the $\uparrow$ atom-bound state scattering length a_3 (whatever the mass ratio), which is precisely obtained from the Skorniakov and Ter-Martirosian equation, and which is given by $a_3 = 1.18a$ in the case of equal masses $m_\downarrow = m_\uparrow \equiv m$.

We display now in Fig. 2 our results for $\mu_\downarrow$. Or rather we plot $\alpha \equiv (3\pi m_r^T/2mE_Fk_Fa)(\epsilon_b + E_F - |\mu_\downarrow|)$ which reduces to a_3/a in the BEC limit and allows to magnify small differences, since we have removed the trivial dominant term, i.e., the binding energy ϵ_b, and the subdominant one E_F, and multiplied by $1/k_Fa$ which magnifies the result in the BEC limit. The first striking result is that α has quite a weak dependence on $1/k_Fa$, starting basically from $1/k_Fa \sim 2$ and is essentially constant, almost equal to its BEC value $a_3/a = 1.18$ in the case of equal masses. This is exactly what is found by QMC calculations [6, 10] in this case of equal masses $m_\downarrow = m$. More precisely we find the actual value of α is slightly higher, the decrease toward the BEC limit being quite slow, behaving as k_Fa. In this case we display also for comparison 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. We consider next the case where the $\downarrow$ atom has an infinite mass $m_\downarrow = \infty$, for which the exact result is known [8] as we have mentioned above. We display both our numerical results and the exact one. This offers a very striking and very direct check of the precision of our results since the difference is barely seen even in our blown up Fig. 2. Another very interesting feature of this limit is that the convergence toward the BEC result $\alpha = 1$ is as $(k_Fa)^2$, 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. Finally the cases of experimental interest $r = 6.64$ and $r = 1/6.64 \simeq 0.15$ for the $^{40}K-^{6}Li$ mixture are also shown.

We consider finally the effective mass to bare mass ratio $m^*/m_\downarrow$. For convenience the inverse of this ratio is plotted in Fig. 3. We show the results both for the polaron and the bound state, to compare them to QMC [10] results. The agreement is perfect within the present precision. It is also remarkable for the location $1/k_F a \simeq 0.88$ of the appearance of the bound state, all the more 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. Note finally that the jump in effective mass from the polaron to the bound state is fairly small. This makes one wonder if they would not be strictly equal in an exact calculation.

4. CONCLUSIONS

In conclusion we have shown that our approach provides an essentially exact analytical theory for these Fermi gases under very high polarization. This is valid for any scattering length, covering the whole extent of the BEC–BCS crossover.

ACKNOWLEDGMENTS

The Laboratoire de Physique Statistique is "Laboratoire associé au Centre National de la Recherche Scientifique et aux Universités Paris 6 et Paris 7."

REFERENCES

1. For a very recent review, see S. Giorgini, L. P. Pitaevskii, and S. Stringari, Rev. Mod. Phys. **80**, 1215 (2008).
2. A. M. Clogston, Phys. Rev. Lett. **9**, 266 (1962); B. S. Chandrasekhar, Appl. Phys. Lett. **1**, 7 (1962).
3. G. B. Partridge, W. Li, R. I. Kamar, Y. A. Liao, and R. G. Hulet, Science **311**, 503 (2006).
4. M. W. Zwierlein, A. Schirotzek, C. H. Schunck, and W. Ketterle, Science **311**, 492 (2006); Y. Shin, M. W. Zwierlein, C. H. Schunck, A. Schirotzek, and W. Ketterle, Phys. Rev. Lett. **97**, 030401 (2006).
5. C. Lobo, A. Recati, S. Giorgini, and S. Stringari, Phys. Rev. Lett. **97**, 200403 (2006).
6. S. Pilati and S. Giorgini, Phys. Rev. Lett. **100**, 030401 (2008).
7. F. Chevy, Phys. Rev. A **74**, 063628 (2006).
8. R. Combescot, A. Recati, C. Lobo, and F. Chevy, Phys. Rev. Lett. **98**, 180402 (2007).
9. R. Combescot and S. Giraud, Phys. Rev. Lett. **101**, 050404 (2008).
10. N. V. Prokof'ev and B. V. Svistunov, Phys. Rev. B **77**, 020408 (2008); Phys. Rev. B **77**, 125101 (2008).
11. R. Combescot, S. Giraud, and X. Leyronas, arXiv:0907.3197.
12. G. V. Skorniakov and K. A. Ter-Martirosian, Zh. Eksp. Teor. Fiz. **31**, 775 (1956) [Sov. Phys. JETP **4**, 648 (1957)].