"Moth-eaten effect" driven by Pauli blocking, revealed for Cooper pairs

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The continuous change from the dilute to the dense regime of correlated fermion pairs still is an open problem. Although this problem initially arose in the context of the microscopic theory of superconductivity, its interest was recently renewed by increasing activity in ultra-cold atomic gases. The so-called BEC-BCS cross-over between the dilute Bose-Einstein condensate of molecules built out of two fermion-like atoms and the dense superfluid state of atom pairs, is a current major question. In the dilute regime, similarities between two-atom molecules and excitons should allow their description through a composite boson many-body formalism similar to the one we developed for excitons. At large density, however, excitons suffer a Mott transition to an electron-hole plasma, while Cooper pairs evolve toward a BCS superconducting condensate. The physics of this BEC-BCS crossover has also been shown to have some relevance for Cooper pairs in high-$T_c$ cuprates.

In this Letter, we present a conceptually trivial but yet unveiled continuity between the Cooper’s one-pair model and the BCS superconductivity. We do it by extending the Cooper’s problem beyond the single pair limit. We start with a "frozen" Fermi sea $|F_0\rangle$ of noninteracting electrons and we increase the number of electron pairs, one by one, within a layer above $|F_0\rangle$ where the BCS potential acts. By using this approach, we can reach the BCS regime continuously starting from the single pair limit.

Although, at the present time, such a pair increase seems hard to experimentally achieve, the present analysis can at least be seen as a gedanken experiment to reveal a possible connection between two famous problems in order to more deeply understand the role of the Pauli exclusion principle in Cooper-paired states. This procedure can also be seen as a simple but well-defined toy model to shed some complementary light on the BEC-BCS crossover problem since, by changing the number of pairs, we do change their overlap.

The extension of the Cooper’s model beyond one pair faces a major many-body problem: the exact handling of the Pauli exclusion principle between a given number of composite particles made of fermion pairs. This can be the reason for this extension not to have been performed yet. As proposed by Bardeen, Cooper and Schrieffer (BCS), the smartest way to circumvent this difficulty is to turn to the grand canonical ensemble because the number of fermion pairs is not fixed anymore. This procedure however masks the existing continuity between the Cooper’s problem and the dense BCS regime. This probably is one of the reasons for Schrieffer’s claim that the single-pair picture has little meaning in the dense BCS regime.

We here overcome this quite old many-body difficulty. To do so, we start with the equations proposed by Richardson for the $N$-Cooper-pair energy in the canonical ensemble and we manage to solve them analytically for an arbitrary number of pairs. This is done by extending the method we used to solve Richardson’s equations for just two pairs. At the present time, our mathematical approach is restricted to the dilute limit on the single pair scale. This is why the dense limit is here addressed by turning to the grand canonical ensemble and by extending the BCS formalism to an arbitrary filling of the potential layer. This allows us to show that the solution of Richardson’s equations we have obtained in the dilute limit, remains valid in the dense regime.

The result we find, proves that the average pair binding energy linearly decreases with pair number over the whole density range. For the standard BCS configuration with a potential extending symmetrically on both sides of the Fermi level $|F\rangle$ for noninteracting electrons - a configuration which just corresponds to fill half the potential layer - this gives an average pair binding energy reduced to half the single pair value.

The present work also makes crystal clear how this happens. Since Pauli blocking is the only way electrons paired by the BCS potential "interact" (see Fig.1), the decrease of the average binding energy we find, results
plainly from the decrease of the number of states available for building paired states within the potential layer. We can visualize this idea by seeing each added new pair as a little moth eating one state, the number of "moth-eaten" states increasing linearly with pair number. This "moth-eaten" effect, which tends to decrease the effect for $N$ as compared to 1, is actually quite standard in the many-body physics of excitons - which also are two-fermion states.

**Ground state energy of $N$ pairs**

As stated above, our work implies handling Pauli blocking between a large number of composite bosons. This is known to be difficult. However, our knowledge on excitons tells us that many important features of this composite boson many-body physics are already seen when going from 1 to 2 pairs: the effect induced by Pauli exclusion principle is already present for two pairs, in this way making the understanding for $N$ pairs far easier. This is why, the 2-Cooper pair problem seeming to us not out of reach, we seriously looked for the ground state of 2 pairs, with the idea to extend the procedure to 3, 4, ..., $N$ pairs.

**(i) One-pair energy.** The energy of an electron pair with opposite spins and zero total momentum, has been calculated by Cooper and Schrieffer. It reads $\epsilon = 2\epsilon_F - \epsilon_c$, where $\epsilon_F$ is the Fermi level of the frozen sea $|F_0\rangle$. In the weak coupling limit, the single pair binding energy reduces to

$$\epsilon_c \simeq 2\rho e^{-2/\rho V}$$

(1)

$\rho_0$ is the density of states taken as constant over the potential extension $\Omega$. Since the purpose of this Letter is to show as simply as possible, the unrevealed consequence of Pauli blocking in BCS superconductivity, we accept, without questioning it, the "reduced" potential used by Bardeen, Cooper, and Schrieffer

$$V_{BCS} = -V \sum_{k,k'} w_k w_{k'} a_{k\uparrow}^\dagger a_{-k'\downarrow}^\dagger a_{-k\downarrow} q_{k\uparrow}$$

(2)

$V$ is the weak potential amplitude ($\rho_0 V \ll 1$) while $w_k = 1$ in the energy layer $\epsilon_F < \epsilon_k < \epsilon_{F_0} + \Omega$ above $|F_0\rangle$. The main advantage of this reduced potential is to be exactly solvable. This allows us to evidence the unrevealed physics induced by Pauli blocking between Cooper pairs in a sharp way.

**(ii) $N$-pair eigenstates.** Forty five years ago, Richardson has derived the exact form for the eigenstates of $N$ pairs. Their energies read as $\epsilon_N = R_1 + \ldots + R_N$ where $R_1, \ldots, R_N$ are solution of $N$ algebraic equations. For $N = 2$, these equations are

$$1 = V \sum_{p} \frac{w_p}{2\epsilon_p - R_1} + \frac{2V}{R_1 - R_2}$$

(3)

plus a similar one with 1 changed into 2 - the equations for higher $N$'s reading as Eq.(3) with all possible $R$ differences. Richardson succeeded to recover the BCS result by solving these equations analytically in the infinite-$N$ limit for a half-filled potential. Today, these equations are currently approached numerically for small superconducting granules with countable number of pairs. However, an analytical solution of these equations for arbitrary $N$ and potential has not been given yet.

**(iii) 2-pair ground state energy.** These equations actually have a small dimensionless parameter which is the inverse of the pair number $N_c = \rho_0 \epsilon_c$ above which pairs start to overlap - this number increasing linearly with sample size. By writing these equations in a dimensional form in terms of $z_i = (R_i - \epsilon_i)/\epsilon_c$ and by performing an expansion in $\gamma = 1/N_c$, we found that, for a weak coupling, the two-pair energy reads, at lowest order in $\gamma$ which turns out to be also an expansion in $1/\rho_0$

$$\epsilon_2 = 2 \left( 2\epsilon_F + \frac{1}{\rho_0} \right) - \epsilon_c \left( 1 - \frac{1}{N\Omega} \right)$$

(4)

$N\Omega = \rho_0 \Omega$ being the number of states in the potential layer.

This result shows that Pauli blocking changes the energy of two single pairs ($\epsilon_2$) in two ways: It increases the free part by $1/\rho_0$ which just is the Fermi level change under a one-electron increase - the extra 2 coming from spin. It also decreases the correlated part, one state being blocked in the 2-pair configuration. A way to better achieve this understanding is to rewrite the single pair binding energy $\epsilon_c$ as

$$\epsilon_c = \rho_0 \Omega \left( \frac{2}{\rho_0} e^{-2/\rho_0 V} \right) = N\Omega \epsilon_V$$

(5)

Eq. (4) then reads

$$\epsilon_2 = 2 \left( 2\epsilon_F + \frac{1}{\rho_0} \right) - (N\Omega - 1) \epsilon_V$$

(6)

Comparison between Eqs.(5) and (6) evidences that the correlation energy of two pairs is controlled by the number of empty states $(N\Omega - 1)$ in the potential layer, i.e., the number of states available to build the paired configuration.

**(iv) $N$-pair energy in the dilute regime.** It is actually possible to solve Richardson’s equations along the same procedure as an expansion in $\gamma$, provided that $N/N_c$ stays small, a restriction which a priori excludes the dense BCS regime, but still corresponds to $N$ arbitrary large since
only $N/N_c$ matters. The detailed derivation of this extension will be presented in the long version of this Letter. Let us here give just a sketch of our procedure.

Following Ref.[13] we first rewrite sums appearing in the Richardson’s equations as

$$V \sum_p \frac{w_p}{2\varepsilon_p - \mu} = 1 + \rho_0 V \sum_{m=1}^{\infty} \frac{I_m}{m^2} e^{-m} \quad (7)$$

where $I_m = 1 - e^{-2m/\rho_0 V}$. It can then be shown that, when the number of pairs is even, $N = 2n$, the solution for the $z_i$’s at the lowest order in $\gamma$ is such that

$$z_1 = -z_{2n} \simeq a_1 \sqrt{\gamma}, \ldots, z_n = -z_{n+1} \simeq a_n \sqrt{\gamma} \quad (8)$$

Substitution of Eq. (8) into the Richardson’s equations leads to $n$ equations for $a_1, \ldots, a_n$ which read like

$$0 \simeq I_1 a_1 + \frac{1}{a_1 - a_2} + \ldots + \frac{1}{a_1 + a_2} + \frac{1}{2a_1} \quad (9)$$

We now multiply Eq. (9) by $a_1$ and add to similar equations for $a_2, \ldots, a_n$. This leads to

$$0 \simeq I_1 (a_1^2 + \ldots + a_n^2) + n(n - 1/2) \quad (10)$$

Next, we turn to the sum of Richardson’s equations, as given by Eq. (7), with two terms kept, namely

$$0 \simeq I_1 \sum_{i=1}^{n} z_i + I_2 \sum_{i=1}^{n} z_i^2 \quad (11)$$

Using Eqs.(10, 11), as well as the definition of $I_1$ and $I_2$, we can find the sum of $z_i$ at lowest order in $\gamma$. From it, we get the following expression for the energy of $N$-pair state

$$\mathcal{E}_N = N \left[ 2 \left( \varepsilon_{F_0} + \frac{N - 1}{2\rho_0} \right) - \varepsilon_c \left( 1 - \frac{N - 1}{N_{\Omega}} \right) \right] \quad (12)$$

The same formula for $\mathcal{E}_N$ can be derived for an odd number of pairs, although the form of $z_i$’s given by Eq. (8) is somewhat more complicated.

Let us now analyze this result. The first term of $\mathcal{E}_N$ is equal to twice the sum $\varepsilon_{F_0} + (\varepsilon_{F_0} + \frac{1}{\rho_0}) + \ldots + (\varepsilon_{F_0} + \frac{N - 1}{\rho_0})$: This just is the energy of $N$ free pairs added to the frozen sea $|F_0\rangle$. The fact that we do recover the exact normal state energy whatever $N$, can be a surprise because Eq.(12) is a priori derived in the small $N/N_c$ limit. This led us to think that, most probably, the second term of $\mathcal{E}_N$ also stays valid for $N$ larger than $N_c$.

(v) Energy in the dense regime. It is first remarkable to note that the above result exactly matches the BCS condensation energy. Indeed, this condensation energy is known to be $E_{BCS} = \frac{1}{2}\rho_0 \Omega^2 \Delta^2$ with $\Delta = 2\omega_c e^{-1/\rho_0 V}$. As $2\omega_c = \Omega$ is the potential extension, $E_{BCS}$ also reads

$$E_{BCS} = \frac{1}{2}\rho_0 \Omega^2 e^{-2/\rho_0 V} = \frac{N_{\Omega} \varepsilon_c}{2} \quad (13)$$

$N_{\Omega}/2$ is the pair number for a potential extending symmetrically on both sides of the Fermi level. The BCS result can thus be understood as all up and down spin electrons pairs in the potential layer form Cooper pairs, their binding energy in this $N$-pair configuration being half the single-pair energy: This is just Eq.(12) extrapolated to half-filling $N = N_{\Omega}/2$ for $N - 1 \approx N$. This shows that the “moth-eaten” effect - derived in the dilute limit - seems to stay valid in the dense BCS regime, where pairs strongly overlap.

One important characteristic of the average binding energy we find in the dilute limit, is its linear decrease with pair number. In order to demonstrate the validity of this result in the dense regime, we consider fillings different from $N_{\Omega}/2$, i.e., a potential extension different from $\mu - \omega_c$ and $\mu + \omega_c$, the chemical potential $\mu$ being, as usual for grand canonical ensemble, afterwards adjusted to get the electron number. Textbook BCS formalism[13] then gives the gap equation as

$$1 = \frac{\rho_0 V}{2} \int_{\mu + \varepsilon_{F_0}}^{\Omega - \varepsilon_{F_0}} \frac{d\xi}{\sqrt{\xi^2 + \Delta^2}} \quad (14)$$

An exact solution exists for $\mu = \varepsilon_{F_0} + \Omega/2$. In the case of asymmetrical potential with boundaries still large enough to have $N \gg \rho_0 \Delta$, we can replace $\sinh^{-1}$ by an exponential. Eq.(14) then gives

$$\Delta \simeq e^{-1/\rho_0 V} 2\sqrt{(\mu - \varepsilon_{F_0}) (\Omega - \mu + \varepsilon_{F_0})} \quad (15)$$

It is possible to show that the condensation energy still reads as $\frac{1}{2}\rho_0 \Omega^2 \Delta^2$, with $\Delta$ now given by Eq.(15). This yields $N_{\varepsilon_c}(1 - N/N_{\Omega})$, which again agrees with Eq.(12).

It can be of interest to note that, by inserting Eq.(5) into Eq.(12), we can rewrite this condensation energy as

$$\mathcal{E}_{N_{cond}} = N (N_{\Omega} - N) \varepsilon_V = N_{\text{occup}} N_{\text{empty}} \varepsilon_V \quad (16)$$

since $N$ is the number of occupied states in the potential layer while $(N_{\Omega} - N)$ is the number of empty states. This $N$ dependence makes the condensation energy maximum when the potential acts symmetrically with respect to the Fermi level which precisely is the BCS configuration. A last - mathematical - result supporting the validity of Eq.(12) at large density, is complete filling. To gain condensation energy, empty states feeling the potential are required. There is none for complete filling. The only possible processes then are electron exchanges. These are forbidden within $\mathcal{V}_{BCS}$. Consequently, condensation energy must then reduce to zero. This again agrees with Eq.(12) for $N = N_{\Omega}$.

Physical consequences of this $N$-pair energy

(i) Continuity between dilute and dense regimes. The above discussion shows that the energy of $N$ Cooper pairs given in Eq.(12), although obtained by solving Richardson’s equations in the dilute limit, remains valid in the dense regime. This supports our understanding, reached from the exciton many-body physics, that, due to Pauli blocking, the average pair binding energy can only decrease when increasing the pair number, whatever the
density. It also reveals a deep connection - missed until to
now - between the Cooper’s picture and the BCS regime, in
spite of the fact that, as often argued, a strong overlap
between pairs in the dense regime should destroy any link
with the Cooper’s model\(^2\). This disclosed connection can
have hidden experimental consequences in superconduct-
ity because, as revealed from Eq. (12), paired states do
have two relevant energy scales: the single pair energy \(\epsilon_e\) and the excitation gap \(\Delta\). These two quantities essen-
tially differ by a factor of 2 in the exponent. This factor
of 2 however is far from being unimportant because, for
\(e^{-1/\rho V}\) very small, it makes the order of magnitude of
these two quantities quite different. Difference between
the two factors has already been noted and discussed in
the literature (see, e.g., p. 169 of Ref.\(^3\)).

(ii) BEC-BCS cross-over. This connection also offers a
supplementary route to tackle BEC-BCS cross-over. In-
deed, in Eagles’ and Leggett’s approaches, the pair over-
lap is increased by decreasing the potential \(V\) while we here increase this overlap by increasing \(N\). These two
procedures however have some important differences: (i)
By acting on \(N\), the Pauli exclusion principle blocks more
and more states while this blocking stays constant when
one changes \(V\) at constant potential extension \(\Omega\). (ii)
Refs.\(^12\) are based on a BCS wave function ansatz ac-
cepted as accurate in the dense and dilute regimes but
more questionable along the crossover\(^2\). In contrast, we
here use the exact wave function obtained by Richard-
son for the ground state energy of \(N\) pairs. In spite of
these differences, the general conclusion of Ref\(^2\) and the
present letter stays the same: ground state pairs in the
dilute and dense regimes are not so much different, a
conclusion at odds with Schrieffer’s claim\(^2\).

(iii) Excitation gap. Since the average pair binding en-
ergy decreases over the whole density range, the reader
most probably stays with one major question: what con-
trols the gap in the excitation spectrum of superconduc-
tors? The answer again is Pauli blocking. When a pair
is broken, the system not only loses its binding energy,
but all the remaining unbroken pairs have their average
binding energy decreased: the two free electrons result-
ing from the Cooper pair broken by a photon, block two
pair states (the photon momentum being small but not
exactly zero). The remaining unbroken pairs feel these
blocked states when trying to construct their correlated
state. The latter effect increases with the number of un-
braken pairs to end in the dense regime, by being far
larger than the broken pair energy.

Preliminary results show strong indications that when
\(N\) becomes larger than \(N_e\), the threshold energy to break
a pair achieves the same value and \(N\) dependences as \(\Delta\).
Similar result for the gap change from single-pair to a
more cooperative regime was actually found in Refs.\(^12\)
within a variational BCS-like approach, this change going
along a weak singularity\(^2\).

(iv) Superfluid and virtual pairs. We here deal with
paired states formed out of all the \(2N\) up and down spin
electrons added in the energy layer where the potential
acts. These electrons feel the potential; they are corre-
lated and form the \(N\) pairs we consider in this Letter.
These pairs are the ones which are "condensed" into the
same quantum-mechanical state in the BCS wave func-
tion ansatz. Schrieffer calls them\(^2\) "superfluid pairs".

These "superfluid pairs" have to be contrasted with what
Schrieffer\(^2\) calls "virtual pairs". The latter corre-
spond to "electrons excited above the Fermi level" \(|F\rangle\)
of the noninteracting electrons. It is of importance to
note that the concept of "virtual pairs" is physically re-
levant in the dense regime only because the Fermi level
\(|F\rangle\) must not be smeared out too much by interactions
in order to keep some physical meaning. As a result,
the understanding of the BCS regime in terms of "vir-
tual pairs" tends to break in an artificial way a possible
continuity with the dilute limit.

These "virtual pairs" are the ones commonly used to
give a qualitative understanding\(^13\) to the BCS condi-
sation energy, when writing it as a pair number multi-
plied by a pair energy. Indeed, their number, deduced
from the width of the BCS distribution change, is of the
order of \(N_\Delta = \rho_0 \Delta\). This gives a pair energy of the order of
\(\Delta\), within an irrelevant factor of 2. From it, it is then
concluded\(^2\) that the "pair energy" must be of the order
of the gap. It is clear that this conclusion fully relies on
what is chosen as pair number. By instead taking the
total number of pairs \(N_{1/2}\) feeling the potential, as we
here do - this number being the natural pair number of
the problem - the same BCS condensation energy gives a
pair energy exactly equal to \(\epsilon_e/2\) in agreement with Eq.
(12).

We wish to stress that, when compared to the under-
standing based on "virtual pairs", understanding based
on "superfluid pairs" provide a natural connection be-
tween the dilute and dense regimes of pairs. Within these
"superfluid pairs", the large value of the excitation gap
is due to many-body effects arising from Pauli blocking
between broken and unbroken pairs, these many-body
effects definitely having some physical relevance.

Conclusion
We have extended the well-known Cooper’s model be-
"ome the one-pair configuration and revealed the simple
link which exists between this model and BCS supercon-
ductivity. We show that the average pair binding energy
linearly decreases with pair number. In agreement with
our understanding of the exciton many-body physics, the
Pauli exclusion principle induces a "moth-eaten effect"
on Cooper pairs, unveiled here for the first time. The
average pair binding energy in the standard BCS con-
figuration is shown to only be half the single pair value,
as a result of their mutual Pauli blocking. This makes
the excitation gap in the dense regime far larger than the
broken pair energy. This increase is due to the Pauli ex-
clusion principle induced by many-body effects between
broken and unbroken pairs. Our work evidences that su-
perconductors have a hidden second energy scale - the
average pair binding energy - which, in the weak cou-
ping limit, is far smaller than the gap. This result should
stimulate new experiments in this very old field. Finally, to precisely understand how the isolated pair and BCS regimes are connected, can be very valuable in a possible approach to the BEC-BCS cross-over within a single composite boson many-body formalism.

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