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

W. V. Pogosov[+*1)], *M. Combescot*[+ 1)]

[+]*Institut des NanoSciences de Paris, Universite Pierre et Marie Curie, CNRS, Campus Boucicaut, 75015 Paris, France*

[*]*Institute for Theoretical and Applied Electrodynamics RAS, 125412 Moscow, Russia*

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We extend the well-known Cooper's problem beyond one pair and study how this dilute limit is connected to the many-pair BCS condensate. We find that, all over from the dilute to the dense regime of pairs, Pauli blocking induces the same "moth-eaten effect" as the one existing for composite boson excitons. This effect makes the average pair binding energy decrease linearly with pair number, bringing it, in the standard BCS configuration, to half the single-pair value. This proves that, at odds with popular understanding, the BCS gap is far larger than the broken pair energy. The increase comes from Pauli blocking between broken and unbroken pairs. Possible link between our result and the BEC-BCS crossover is also discussed.

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 [1 – 4], 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 (BEC) of molecules built out of two fermion-like atoms and the dense surperfluid state of atom pairs, is a current major question [5, 6]. 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 [7]. At large density, however, excitons suffer a Mott transition to an electron-hole plasma [8] while Cooper pairs evolve toward a Bardeen, Cooper and Schrieffer (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 [9, 10].

In this Letter, we present a conceptually trivial but yet unveiled continuity between the Cooper's one-pair model [11] and the BCS superconductivity [12]. 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 [13] 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 BCS [12], 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 [4] that the single-pair picture has little meaning in the dense BCS regime.

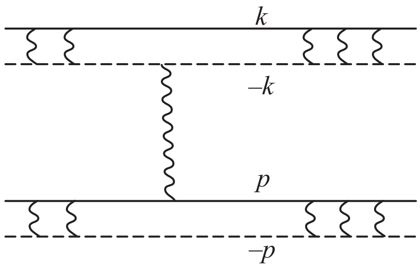
We here overcome this quite old many-body difficulty. To do so, we start with the equations proposed by Richardson [14] for the N-Cooper-pair energy in the canonical ensemble and we manage to solve them analytically for an *arbitrary* number of pairs. This is done by extending the method we used to solve Richardson's equations for just two pairs [15]. 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

[1)]e-mail: Walter.Pogosov@gmail.com,
Monique.Combescot@insp.jussieu.fr

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



Two pairs cannot interact through the BCS potential given in Eq.(2): this would imply $\mathbf{p} = \mathbf{k}$, the 2-free-pair state then reducing to zero due to Pauli blocking

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 the 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 energy 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 [11]. It reads $\mathcal{E}_1 = 2\varepsilon_{F_0} - \epsilon_c$, where ε_{F_0} is the Fermi level of the frozen sea $|F_0\rangle$. In the weak coupling limit, the single pair binding energy reduces to

$$\epsilon_c \simeq 2\Omega e^{-2/\rho_0 V}. \tag{1}$$

ρ_0 is the density of states taken as constant over the potential extension Ω. 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

$$\mathcal{V}_{BCS} = -V \sum_{\mathbf{k},\mathbf{k}'} w_{\mathbf{k}'} w_{\mathbf{k}} a^\dagger_{\mathbf{k}'\uparrow} a^\dagger_{-\mathbf{k}'\downarrow} a_{-\mathbf{k}\downarrow} a_{\mathbf{k}\uparrow} \tag{2}$$

V is the weak potential amplitude ($\rho_0 V \ll 1$) while $w_{\mathbf{k}} = 1$ in the energy layer $\varepsilon_{F_0} < \varepsilon_{\mathbf{k}} < \varepsilon_{F_0} + \Omega$ 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 [14] the *exact* form for the eigenstates of N pairs. Their energies read as $\mathcal{E}_N = R_1 + ... + R_N$ where R_1, ..., R_N are solution of N algebraic equations. For $N = 2$, these equations are

$$1 = V \sum_{\mathbf{p}} \frac{w_{\mathbf{p}}}{2\varepsilon_{\mathbf{p}} - R_1} + \frac{2V}{R_1 - R_2} \tag{3}$$

plus a similar one with 1 changed into 2 – the equations for higher N's reading as Eq.(3) with all possible R differences [16]. Richardson succeeded to recover the BCS result [14] 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 [17]. 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 $z_i = (R_i - \mathcal{E}_1)/\epsilon_c$ and by performing an expansion in $\gamma = 1/N_c$, we found [15] that, for a weak coupling, the two-pair energy reads, at lowest order in γ which turns out to be also an expansion in $1/\rho_0$

$$\mathcal{E}_2 = 2\left[\left(2\varepsilon_{F_0} + \frac{1}{\rho_0}\right) - \epsilon_c\left(1 - \frac{1}{N_\Omega}\right)\right]. \tag{4}$$

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

This result shows that Pauli blocking changes the energy of two single pairs ($2\mathcal{E}_1$) 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 ϵ_c as

$$\epsilon_c = \rho_0 \Omega \left(\frac{2}{\rho_0} e^{-2/\rho_0 V} \right) = N_\Omega \epsilon_V \qquad (5)$$

Eq. (4) then reads

$$\mathcal{E}_2 = 2\left[\left(2\varepsilon_{F_0} + \frac{1}{\rho_0} \right) - (N_\Omega - 1)\,\epsilon_V \right] \qquad (6)$$

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 γ, 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. [15], we first rewrite sums appearing in the Richardson's equations as

$$V \sum_{\mathbf{p}} \frac{w_{\mathbf{p}}}{2\varepsilon_{\mathbf{p}} - R_i} = 1 + \rho_0 V \sum_{m=1}^{\infty} \frac{I_m}{m} z_i^m, \qquad (7)$$

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 γ is such that

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

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

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

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

$$0 \simeq I_1 \left(a_1^2 + ... + a_n^2 \right) + n(n - 1/2). \qquad (10)$$

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

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

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 γ. From it, we get the following expression for the energy of N-pair state

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

The same formula for $\mathcal{E}_N$ can be derived 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 $\varepsilon_{F_0} + (\varepsilon_{F_0} + \frac{1}{\rho_0}) + ... + (\varepsilon_{F_0} + \frac{N-1}{\rho_0})$: This just is the energy of N free 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 $E_{BCS} = \frac{1}{2}\rho_0\Delta^2$ with $\Delta = 2\omega_c e^{-1/\rho_0 V}$. As $2\omega_c = \Omega$ is the potential extension, E_{BCS} also reads

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

$N_\Omega/2$ 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 $N - 1 \simeq N$. 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 μ being, as usual for grand canonical ensemble, afterwards adjusted to get the electron number. Textbook BCS formalism [18] then gives the gap equation as

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

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

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

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

$$\mathcal{E}_N^{cond} = N\,(N_\Omega - N)\,\epsilon_V = N_{occup}N_{empty}\epsilon_V, \qquad (16)$$

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 [4]. This disclosed connection can have hidden experimental consequences in superconductivity because, as revealed from Eq.(12), paired states do have two relevant energy scales: the single pair energy ϵ_c and the excitation gap Δ. These two quantities essentially differ by a factor 2 in the exponent. This factor of 2 however is far from being unimportant because, for $e^{-1/\rho_0 V}$ 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. [4]).

(ii) *BEC-BCS cross-over.* This connection also offers a supplementary route to tackle BEC-BCS cross-over. Indeed, in Eagles's and Leggett's approaches, the pair overlap 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 Ω. (ii) Refs. [1, 2] are based on a BCS wave function ansatz accepted 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 Richardson 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 [4].

(iii) *Excitation gap.* Since the average pair binding energy decreases over the whole density range, the reader most probably stays with one major question: what controls the gap in the excitation spectrum of superconductors? The answer again is Pauli blocking. When a pair is broken, the system not only looses its binding energy, but all the remaining unbroken pairs have their average binding energy decreased: the two free electrons resulting 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 unbroken 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_c, the threshold energy to break a pair achieves the same V and N dependences as Δ. Similar result for the gap change from single-pair to a more cooperative regime was actually found in Refs. [1, 2] within a variational BCS-like approach, this change going along a weak singularity [3].

(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 correlated 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 function ansatz. Schrieffer calls them [4] "superfluid pairs".

These "superfluid pairs" have to be contrasted with what Schrieffer [4] calls "virtual pairs". The latters correspond 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 relevant 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 "virtual 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 [18, 19] to the BCS condensation energy, when writing it as a pair number multiplied 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 Δ, within an irrelevant factor of 2. From it, it is then concluded [20] 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 $N_\Omega/2$ 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 $\epsilon_c/2$ in agreement with Eq. (12).

We wish to stress that, when compared to the understanding based on "virtual pairs", understanding based on"superfluid pairs" provide a natural connection between 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 beyond the one-pair configuration and revealed the simple link which exists between this model and BCS superconductivity. 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 configuration 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 exclusion principle induced by many-body effects between broken and unbroken pairs. Our work evidences that superconductors have a hidden second energy scale – the average pair binding energy – which, in the weak coupling 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 [7].

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