Richardson's exact eigenstate, BCS ansatz and the Pauli exclusion principle

Abstract

I. FORMALISM FOR COMPOSITE BOSONS

A. Free pairs

We consider free pair states with one degree of freedom only, namely

$$\beta_{\mathbf{k}}^\dagger = a_{\mathbf{k}\uparrow}^\dagger a_{-\mathbf{k}\downarrow}^\dagger \tag{1}$$

In BCS superconductivity, these free fermions feel a potential which acts in a potential layer of extension Ω above a frozen Fermi sea $|F_0\rangle$, namely

$$V_{BCS} = -V \sum_{\mathbf{k}'\mathbf{k}} w_{\mathbf{k}} w_{\mathbf{k}'} \beta_{\mathbf{k}'}^\dagger \beta_{\mathbf{k}} \tag{2}$$

with $w_{\mathbf{k}} = 1$ for $\epsilon_{F_0} < \epsilon_{\mathbf{k}} < \epsilon_{F_0} + \Omega$.

The statistical properties of free pair states follow from their composite boson nature. It shows up through

$$\left[\beta_{\mathbf{k}'}^\dagger, \beta_{\mathbf{k}}^\dagger \right] = 0 \tag{3}$$

$$\left[\beta_{\mathbf{k}'}, \beta_{\mathbf{k}}^\dagger \right] = \delta_{\mathbf{k}'\mathbf{k}} - D_{\mathbf{k}'\mathbf{k}} \tag{4}$$

where the operator $D_{\mathbf{k}'\mathbf{k}}$ is equal to

$$D_{\mathbf{k}'\mathbf{k}} = \delta_{\mathbf{k}'\mathbf{k}} \sum_{s=(\uparrow,\downarrow)} a_{\mathbf{k}s}^\dagger a_{\mathbf{k}s} \tag{5}$$

so that, when acting on another free pair, it gives

$$\left[D_{\mathbf{p}\mathbf{k}_1}, \beta_{\mathbf{k}_2}^\dagger \right] = 2\delta_{\mathbf{k}_1\mathbf{p}} \delta_{\mathbf{k}_2\mathbf{p}} \beta_{\mathbf{p}}^\dagger \tag{6}$$

The interaction properties of these free pairs follow from commutations with the system hamiltonian $H = H_0 + V_{BCS}$, the kinetic part reading as $H_0 = \sum_{\mathbf{k}s} \epsilon_{\mathbf{k}} a_{\mathbf{k}s}^\dagger a_{\mathbf{k}s}$. We then find

$$\left[H_0, \beta_{\mathbf{p}}^\dagger \right] = 2\epsilon_{\mathbf{p}} \beta_{\mathbf{p}}^\dagger \tag{7}$$

$$\left[V_{BCS}, \beta_{\mathbf{p}}^\dagger \right] = -V w_{\mathbf{p}} \beta^\dagger + V_{\mathbf{p}}^\dagger \tag{8}$$

where

$$\beta^\dagger = \sum_{\mathbf{p}} w_{\mathbf{p}} \beta_{\mathbf{p}}^\dagger \tag{9}$$

$$V_{\mathbf{p}}^\dagger = -V w_{\mathbf{p}} \beta^\dagger \sum_s a_{\mathbf{p}s}^\dagger a_{\mathbf{p}s} \tag{10}$$

Due to the $w_{\mathbf{p}}$ part of this $V_{\mathbf{p}}^\dagger$ operator, we do have $V_{\mathbf{p}}^\dagger |F_0\rangle = 0$ while

$$\left[V_{\mathbf{p}_2}^\dagger, \beta_{\mathbf{p}_1}^\dagger \right] = 2V \delta_{\mathbf{p}_1\mathbf{p}_2} w_{\mathbf{p}_1} \beta_{\mathbf{p}_1}^\dagger \beta^\dagger \tag{11}$$

B. Correlated pairs

We now consider correlated pairs, i.e., linear combination of free pairs which, unlike excitons, are not one-pair eigenstates of the system hamiltonian. It is convenient to introduce their generalized form defined as

$$C_m^\dagger = \sum (w_\mathbf{k} \varphi_\mathbf{k})^{2m+1} \beta_\mathbf{k}^\dagger \tag{12}$$

with $\varphi_\mathbf{k}$ normalized by

$$\langle F_0 | C_0 C_0^\dagger | F_0 \rangle = \sum w_\mathbf{k} |\varphi_\mathbf{k}|^2 = 1 \tag{13}$$

The commutators between free pairs introduced above lead to

$$[C_{m'}, C_m^\dagger] = I_{1+m+m'} - D_{m'm} \tag{14}$$

$$[D_{m_1', m_1}, C_{m_2}^\dagger] = 2C_{1+m_1+m_1'+m_2}^\dagger \tag{15}$$

$$I_m = \sum |w_\mathbf{k} \varphi_\mathbf{k}|^{2m} \tag{16}$$

with $I_1 = 1$ due to eq. (13).

It is possible to extend the above commutation relations by recursion to N correlated pairs. We find

$$[D_{m0}, C_0^{\dagger N}] = 2N C_0^{\dagger N-1} C_{m+1}^\dagger \tag{17}$$

$$[C_m, C_0^{\dagger N}] = N C_0^{\dagger (N-1)}(I_{1+m} - D_{n0}) - N(N-1) C_{m+1}^\dagger C_0^{\dagger N-2} \tag{18}$$

These N-commutators are necessary to calculate an important quantity for the control of Pauli blocking between correlated pairs, namely the normalization factor,

$$\langle F_0 | C_0^N C_0^{\dagger N} | F_0 \rangle = N! f_N \tag{19}$$

If $C_0^\dagger$ were the creation operator of an elementary boson, i.e., for $[C_0, C_0^\dagger]$ reducing to 1, f_N would reduce to 1 for all N. The f_N factor is the signature of the moth-eaten effect between composite bosons induced by the Pauli exclusion principle. As a result of this effect, f_N is a decreasing function of N. A way to show it is through the recursion relation fulfilled by the f_N's. Since $D_{m'm} | F_0 \rangle = 0$ as readily seen from Eq. (14) acting on $|F_0\rangle$, the above N-commutators give, since $I_1 = 1$

$$\langle F_0 | C_0^N C_0^{\dagger N} | F_0 \rangle = \langle F_0 | C_0^{N-1} [C_0, C_0^{\dagger N}] | F_0 \rangle$$
$$= N \langle F_0 | C_0^{N-1} C_0^{\dagger N-1} | F_0 \rangle - N(N-1) \langle F_0 | C_0^{N-1} C_1^\dagger C_0^{\dagger N-1} | F_0 \rangle \tag{20}$$

3

To calculate the second term, we use $[C_0^{N-1}, C_1^\dagger]$ with $\langle F_0 | C_1^\dagger = 0$ due to the $w_\mathbf{k}$ factor included in $C_1^\dagger$. By repeating the process, we end with the following recursion relation between the f_N's

$$f_N = f_{N-1} - (N-1)I_2 f_{N-2} + (N-1)(N-2)I_3 f_{N-3} - \cdots + (-1)^{N-1} N! I_N f_0 \qquad (21)$$

where $f_0 = 1$.

The above equation is convenient to calculate f_N when the RHS is dominated by its first terms, i.e., when the prefactors $N^p I_{p+1}$ are small. This happens for excitons, and more generally for correlated pairs in the dilute limit. In the dense limit, when Pauli blocking becomes dramatic, the compact form of f_N given by

$$f_N = \frac{\partial^N Z(x)}{\partial x^N}\bigg|_{x=0}$$

$$Z(x) = \prod_\mathbf{k} (1 + x|w_\mathbf{k} \varphi_\mathbf{k}|^2) \qquad (22)$$

turns out to be far more convenient. It is easy to convince ourselves that Eq.(22) leads to Eq.(21).

C. Correlated pairs with a flat distribution

The simplest correlated pair corresponds to replace $\varphi_\mathbf{k}$ by a constant for all $\epsilon_\mathbf{k}$ between ϵ_{F_0} and $\epsilon_{F_0} + \rho_0 N^*$ where ρ_0 is the density of states taken as constant above the frozen sea $|F_0\rangle$, i.e., for $\epsilon_\mathbf{k} > \epsilon_{F_0}$. The N^*'s of physical interest are smaller than the total number of pairs $N_\Omega = \rho_0 \Omega$ feeling the potential, pairs with energy above $\epsilon_{F_0} + \rho_0 N^*$ being anyway cut by the $w_\mathbf{k}$ factor appearing in the definition (12) of $C_m^\dagger$. This amounts to put N^* free pairs $\beta_{\mathbf{k}_1}^\dagger, \cdots, \beta_{\mathbf{k}_{N^*}}^\dagger$ in the sum, all with the same weight $\varphi^* = 1/\sqrt{N^*}$ in order to have $I_1 = 1$. Consequently

$$C_0^\dagger = \frac{1}{\sqrt{N^*}} S_{N^*}^\dagger \qquad (23)$$

where $S_N^\dagger = \sum_{n=1}^N \beta_{\mathbf{k}_n}^\dagger$.

It is clear that due to Pauli blocking, we cannot pile up more correlated pairs than the number of $\mathbf{k}$ states available in the $C_0^\dagger$ sum. Consequently

$$f_N = 0 \quad \text{for} \quad N \geq N^* + 1 \qquad (24)$$

To get f_N when N is exactly equal to the number N^* of $\mathbf{k}$ states, we note that, since $\beta_{\mathbf{k}}^{\dagger 2} = 0$ due to Pauli blocking,

$$(S_{N^*}^{\dagger})^{N^*} = [S_{N^*-1}^{\dagger} + \beta_{\mathbf{k}_{N^*}}^{\dagger}]^{N^*} = (S_{N^*-1}^{\dagger})^{N^*} + N^* \beta_{\mathbf{k}_{N^*}}^{\dagger} (S_{N^*-1}^{\dagger})^{N^*-1} \tag{25}$$

The first term reduces to zero since we cannot pile up more pairs than the available number $N^* - 1$ of $\mathbf{k}$ states in the $S_{N^*-1}^{\dagger}$ sum. By iterating the process, we end with

$$(S_{N^*}^{\dagger})^{N^*} = N^*! \prod_{i=1,\ldots,N^*} \beta_{\mathbf{k}_i}^{+} \tag{26}$$

so that

$$\langle F_0|(S_{N^*})^{N^*}(S_{N^*}^{\dagger})^{N^*}|F_0\rangle = (N^*!)^2 \tag{27}$$

Since this scalar product is nothing but $(N^*)^{N^*}\langle v|C_0^{N^*} C_0^{\dagger N^*}|v\rangle$, we readily find

$$f_{N^*} = N^*!/(N^*)^{N^*} \approx e^{-N^*}\sqrt{2\pi N^*} \tag{28}$$

for N^* large, due to the Stirling formula.

If we now use the same procedure for $N = N^* - 1$, we find

$$\begin{aligned}
\langle F_0|(S_{N^*})^{N^*-1}(S_{N^*}^{\dagger})^{N^*-1}|F_0\rangle =& \langle F_0|(S_{N^*-1})^{N^*-1}(S_{N^*-1}^{\dagger})^{N^*-1}|F_0\rangle \\
& + (N^* - 1)^2 \langle F_0|(S_{N^*-1})^{N^*-2}(S_{N^*-1}^{\dagger})^{N^*-2}|F_0\rangle
\end{aligned} \tag{29}$$

Due to Eq. (27), the first term is just equal to $[(N^* - 1)!]^2$. By iterating the process, the above product ends by being equal to $N^*(N^* - 1)!^2$, which gives $f_{N^*-1} = N^*/(N^*)^{N^*-1}$. This f_{N^*-1} allows to calculate f_{N^*-2} and so on ... We ultimately end with

$$f_N = \frac{N^*!}{(N^* - N)! N^{*N}} = f_{N^*} \frac{(N^*)^{N^*-N}}{(N^* - N)!} \tag{30}$$

It is easy to check that the above f_N fulfills Eq. (21) since for such a flat distribution, I_m reduces to $1/(N^*)^{m-1}$.

D. Correlated pairs with a triangular distribution

We now considered correlated pairs made of the same amount of $\mathbf{k}$ states, namely $\mathbf{k}_1, \ldots, \mathbf{k}_{N^*}$, but with a linearly decreasing weight, taken as

$$\varphi_{\mathbf{k}_n} = \sqrt{\frac{3}{N^*}} \frac{\epsilon_{F_0} + \rho_0^{-1} N^* - \epsilon_{\mathbf{k}_n}}{\rho_0^{-1} N^*} \tag{31}$$

5

which is properly normalized $\sum |\varphi_{\mathbf{k}}|^2 = 1$. Using Eq.(22), we can find

$$f_{N^*} = |\Pi^*|^2 (N^*!) \tag{32}$$

$$\text{where} \quad \Pi^* = \prod_{i=1}^{N^*} \varphi_{k_i}$$

Similarly, we can find

$$f_{N^*-1} = |\Pi^*|^2 ((N^* - 1)!) \sum_i \frac{1}{|\varphi_{\mathbf{k}_i}|^2} \approx |\Pi^*|^2 ((N^* - 1)!) \frac{\pi^2}{6} \frac{N^{*3}}{3} \tag{33}$$

And $\frac{f_{N^*-1}}{f_{N^*}} = N^{*2} \frac{\pi^2}{18}$ instead of order of N^* in the flat case, which suggest that f_n decreases faster in this case, as expected because distribution is more concentrated in low energy and therefore more affected by Pauli blocking.

E. Correlated pairs with a two-step distribution

A third distribution of physical interest is a flat distribution with a tail, namely

$$\varphi_{\mathbf{k}} = \varphi_1 \text{ for } \quad \epsilon_{F_0} < \epsilon_{\mathbf{k}} < \epsilon_{F_0} + \rho_0^{-1} N_1$$
$$\varphi_{\mathbf{k}} = \varphi_2 \text{ for } \quad \epsilon_{F_0} + \rho_0^{-1} N_1 < \epsilon_{\mathbf{k}} < \epsilon_{F_0} + \rho_0^{-1}(N_1 + N_2) \tag{34}$$

with $N_1 + N_2 = N^*$, $\varphi_1 \gg \varphi_2$ and $N_1 \gg N_2$. Such a two-step distribution turns out to be of physical relevance for BCS composite bosons.

The normalized pair creator is

$$C^\dagger = \varphi_1 (\beta_{\mathbf{k}_1}^\dagger + \cdots + \beta_{\mathbf{k}_{N_1}}^\dagger) + \varphi_2 (\Gamma_{\mathbf{k}_1}^\dagger + \cdots + \Gamma_{\mathbf{k}_{N_2}}^\dagger) \tag{35}$$

where $\beta^\dagger$'s are creator for main part, $(\epsilon_{F_0}, \epsilon_{F_0} + \rho_0^{-1} N_1)$, and $\Gamma^\dagger$'s are creator for the tail, $(\epsilon_{F_0} + \rho_0^{-1} N_1, \epsilon_{F_0} + \rho_0^{-1}(N_1 + N_2))$. The m pairs creator would be

$$C^{\dagger m} = \sum_{l=\max\{0, m-N_2\}}^{\min\{N_1, m\}} \varphi_1^l \varphi_2^{m-l} \prod_{t=1}^{l} \beta_{\mathbf{k}_{i_t}}^\dagger \prod_{t'=1}^{m-l} \Gamma_{\mathbf{k}_{j_{t'}}}^\dagger \tag{36}$$

And this gives

$$\langle C^m C^{\dagger m} \rangle = \sum_{l=\max\{0, m-N_2\}}^{\min\{N_1, m\}} |\varphi_1|^{2l} |\varphi_2|^{2(m-l)} \frac{l!(m-l)!}{l!(N_1 - l)!(N_2 - m + l)!} N_1! N_2! \equiv \sum_{l=\max\{0, m-N_2\}}^{\min\{N_1, m\}} S_l \tag{37}$$

Let us look at S_l more carefully

$$\frac{S_l}{S_{l-1}} = \left|\frac{\varphi_1}{\varphi_2}\right|^2 \frac{l(N_1 - l + 1)}{(m - l + 1)(N_2 - m + l)} \tag{38}$$

For l, m in the same order as N_1, $N_1 - l + 1 \sim 1$, $m - l + 1 \sim 1$, $N2 - m + l \sim N_2$, so the above ratio is in the order of $\left|\frac{\varphi_1}{\varphi_2}\right|^2 \frac{N_1}{N_2} \gg 1$ and we can drop every term except the last one. This means that the dominating part in the wave function fills the main part and very little fills the tail.

$$f_m = \begin{cases} |\varphi_1{}^m|^2 \frac{N_1!}{(N_1)!} & m \leq N_1 \\ \left|\varphi_1{}^{N_1}\varphi_2{}^{-(m-N_1)}\right|^2 \frac{N!(m-N_1)!N_1!N_2!}{m!(N_2+N_1-m)!} & m > N_1 \end{cases} \tag{39}$$

II. RICHARDSON'S EXACT EIGENSTATE

Richardson has shown that the *exact* N-pair eigenvalues of the system hamiltonian $H = H_0 + V_{BCS}$ read as $E_N = R_1 + \cdots R_N$, the eigenstates being

$$|\Psi_N\rangle = B^\dagger(R_1) \cdots B^\dagger(R_N)|F_0\rangle \tag{40}$$

$B^\dagger(R)$ turns out to be a simple generalization of the one-pair solution obtained by Cooper, namely

$$B^\dagger(R) = \sum_{\mathbf{k}} \frac{w_{\mathbf{k}}}{2\epsilon_{\mathbf{k}} - R} \beta_{\mathbf{k}}^\dagger \tag{41}$$

while the R_i's are solutions of N coupled equations

$$1 = V \sum \frac{w_{\mathbf{k}}}{2\epsilon_{\mathbf{k}} - R_i} + \sum_{j \neq i} \frac{2V}{R_i - R_j} \qquad \text{for } i = (1, ..., N) \tag{42}$$

We have been able to rederive this exact solution using a coboson approach based on the commutators derived in section I. This approach allowed us to associate the terms $2/(R_i - R_j)$ in these equations, to the Pauli exclusion principle between pairs. Without these terms, the solution of the Richardson's equations would be $R_i = E_1$ where E_1, solution of

$$1 = V \sum \frac{w_{\mathbf{k}}}{2\epsilon_{\mathbf{k}} - E_1} \tag{43}$$

is the single pair binding energy as obtained by Cooper, namely, $E_1 = 2E_{F_0} - \epsilon_c$ with $\epsilon_c \approx 2\Omega e^{-2/\rho_0 V}$ for $\rho_0 V \ll 1$. The fact that E_N differs from the NE_1 comes from the $2/(R_i - R_j)$ terms in the Richardson's equations. (42) which impose all the R_i's to be

7

different, otherwise these terms would diverge. As a direct consequence of all the R_i's being different, the exact eigenstate given in Eq. (40), clearly differs from the commonly accepted idea in BCS superconductivity, that all the pairs are condensed into the same state: this N-pair state is said to read as

$$|\Phi_N\rangle = B^{\dagger N}|F_0\rangle \tag{44}$$

where $B^\dagger$ is an appropriate linear combination of free pairs feeling the attractive BCS potential

$$B^\dagger = \sum_{\mathbf{k}} \phi_{\mathbf{k}} \beta_{\mathbf{k}}^\dagger \tag{45}$$

In the next paragraph, we are going to come back to the origin of this idea.

III. BCS ANSATZ

The BCS ansatz fundamentally corresponds to consider the linear combination of N pair states $|\Phi_N >$ introduced above, and to affect to these states a weight $1/N!$, in order to possibly rewrite this sum in a compact form

$$|\Phi\rangle = \sum_{N=0}^{\infty} \frac{1}{N!} B^{\dagger N}|F_0\rangle = e^{B^\dagger}|F_0\rangle \tag{46}$$

At this stage, the $1/N!$ prefactor appears as a convenient mathematical trick. Since the exponential of a sum is a product of exponentials, this state also reads

$$|\Phi\rangle = \prod_{\mathbf{k}} e^{\phi_{\mathbf{k}} \beta_{\mathbf{k}}^\dagger}|F_0\rangle = \prod_{\mathbf{k}} \sum_{n=0}^{\infty} \frac{1}{n!} (\phi_{\mathbf{k}} \beta_{\mathbf{k}}^\dagger)^n|F_0\rangle \tag{47}$$

By noting that the terms in the sum reduces to zero for $n > 1$ due to Pauli blocking, we end by rewriting $|\Phi\rangle$ as

$$|\Phi\rangle = \prod_{\mathbf{k}} (1 + \phi_{\mathbf{k}} \beta_{\mathbf{k}}^\dagger)|F_0\rangle \tag{48}$$

If we now set

$$\phi_{\mathbf{k}} = v_{\mathbf{k}}/u_{\mathbf{k}} \tag{49}$$

we recover the BCS state

$$|\Psi_{BCS}\rangle = \prod_{\mathbf{k}} (u_{\mathbf{k}} + v_{\mathbf{k}} \beta_{\mathbf{k}}^\dagger)|F_0\rangle \tag{50}$$

within an irrelevant prefactor $U = \prod_{\mathbf{k}} u_{\mathbf{k}}$.

The set of $(u_{\mathbf{k}}, v_{\mathbf{k}})$, which minimizes the mean value of $H - 2\mu\hat{N}$ in the $|\Psi_{BCS}\rangle$ state, with $\hat{N}$ being the *pair* number operator $\sum_{\mathbf{k}} a_{\mathbf{k}s}^{\dagger} a_{\mathbf{k}s}$, is then found to be, for $(u_{\mathbf{k}}, v_{\mathbf{k}})$, normalized by $u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2 = 1$ in order to have $\langle \Psi_{BCS} | \Psi_{BCS} \rangle = 1$,

$$v_{\mathbf{k}}^2 = 1 - u_{\mathbf{k}}^2 = \frac{1}{2}\left(1 - \frac{\xi_{\mathbf{k}}}{\sqrt{\Delta^2 + \xi_{\mathbf{k}}^2}}\right) \tag{51}$$

where we have set $\xi_{\mathbf{k}} = (\epsilon_{\mathbf{k}} - \mu)$, the gap equation reading as

$$1 = \frac{V}{2}\sum \frac{w_{\mathbf{k}}}{\sqrt{\Delta^2 + \xi_{\mathbf{k}}^2}} \approx \frac{V\rho_0}{2}\int_{\epsilon_{F_0}}^{\epsilon_{F_0}+\Omega} \frac{d\epsilon_{\mathbf{k}}}{\sqrt{\Delta^2 + (\epsilon_{\mathbf{k}} - \mu)^2}} \tag{52}$$

For a chemical potential taken in the middle of the potential layer, namely $\mu = \epsilon_{F_0} + \Omega/2$, the quantity Δ, ultimately found to be the superconductor excitation gap, reduces to $\Delta \approx \Omega e^{-1/\rho_0 V}$.

Difference between the $H - 2\mu\hat{N}$ mean value in the normal state, $V = 0$, and in the superconductor state, $V \neq 0$, is then shown to read in the weak coupling limit, $\rho_0 V \ll 1$, as

$$\mathcal{E}^{normal} - \mathcal{E}^{super} \approx \frac{\rho_0}{2}\Delta^2 = \left(\frac{\rho_0 \Omega}{2}\right)(\Omega e^{-2/\rho_0 V}) \tag{53}$$

In order to give a physical meaning to this result, it can be of interest to note that the mean value of the pair number operator $\hat{N}$ in the BCS state given in Eq. (50), reads, since $\langle \Psi_{BCS} | \Psi_{BCS} \rangle = 1$, as

$$\langle \hat{N} \rangle_{BCS} = \langle \Psi_{BCS} | \sum_{\mathbf{k}} a_{\mathbf{k}s}^{\dagger} a_{\mathbf{k}s}^{\dagger} | \Psi_{BCS} \rangle = \sum v_{\mathbf{k}}^2 \tag{54}$$

For a chemical potential set in the middle of the potential layer, $\mu = \epsilon_{F_0} + \Omega/2$, Eq. (54) with $v_{\mathbf{k}}^2$ given by Eq. (51) corresponds to a pair number equal to $N_\Omega/2$ where $N_\Omega = \rho_0 \Omega$ is the total number of states in the potential layer, namely

$$N_\Omega = \sum w_{\mathbf{k}} = \rho_0 \Omega \tag{55}$$

The condensation energy given in Eq. (53) thus corresponds to assign to each of these $N_\Omega/2$ pairs an average binding energy, $\Omega e^{-2/\rho_0 V}$, equal to one half the single pair binding energy ϵ_c found by Cooper.

This understanding fully agrees with the eigenvalue for N pairs deduced from the exact solution of the Richardson's equations that we have shown to read as

$$E_N = R_1 + \cdots + R_N = NE_1 + \frac{N(N-1)}{2}E_{int}$$
$$= 2\left[N\epsilon_{F_0} + \frac{N(N-1)}{2}\frac{1}{\rho_0}\right] - N\epsilon_c(1 - \frac{N-1}{N_\Omega}) \tag{56}$$

The first term just is the energy of N free electron pairs added above $|F_0\rangle$ in a region where the density of state is constant and equal to ρ_0. The second term evidences the average binding energy decrease *induced* by Pauli blocking between pairs. This average binding energy reduces to $\epsilon_c/2$ when $N = N_\Omega/2$. The interaction part, E_{int}, of this N-pair energy actually comes from Pauli blocking only, between free pairs for the first term, between bound pairs for the second term since the very peculiar form of the reduced BCS potential prevents any direct interaction between pairs as in the case of Coulomb interaction between excitons.

The BCS ansatz followed by a mean value minimizeation procedure thus gives the correct ground state energy for N pairs, as obtained from the analyticalresolution of the set of equations derived by Richardson. This ansatz is commonly seen as the grand canonical version of the problem. This understing is based on the idea that the BCS ansatz corresponds to a peaked distribution, the proof of this peaked distribution relying on the fact that $\langle \hat{N}^2 \rangle$ deffers from $(\langle \hat{N} \rangle)^2$ by a quantity small compared to this square mean value. Indeed,

$$\langle (\hat{N} - \bar{N})^2 \rangle = \langle \hat{N}^2 \rangle - (\langle \hat{N} \rangle)^2 = \sum |u_{\mathbf{k}} v_{\mathbf{k}}|^2 = \frac{\rho_0 \Delta}{2} \sinh^{-1} \frac{\Omega}{\Delta} \ll \bar{N} \tag{57}$$

Let us now reconsider this point more carefully from a microscopical point of view, i.e., by directly calculating the distribution of the $|\Phi_N\rangle$ states in $|\Psi_{BCS}\rangle$.

IV. CANONICAL VERSION OF THE BCS ANSATZ

In order to possibly replace calculations in the canonical ensemble, i.e., with a fixed number of particles, by calculations in the grand canonical ensemble, the distribution of the grand canonical state of interest must be very much peaked on the mean value of the particle number operator. In order to check this point in a direct way, for the BCS ansatz, it is convenient to introduce the normalized correlated pair operator associated to BCS pair creation operator $B^\dagger$ defined in Eqs (45,49), namely

$$C^\dagger = \sum \varphi_{\mathbf{k}} \beta_{\mathbf{k}}^\dagger = \alpha^{-1} B^\dagger \tag{58}$$

with α chosen such that

$$\langle F_0 | C C^\dagger | F_0 \rangle = 1 = \alpha^{-2} \sum \phi_{\mathbf{k}}^2 \tag{59}$$

For $\phi_{\mathbf{k}}$ given in Eq. (49) and $(u_{\mathbf{k}}, v_{\mathbf{k}})$ given in Eq. (51), this α constant is found to be read

$$\alpha^2 = \sum \phi_{\mathbf{k}}^2 = N_\Omega \left(1 + \frac{\Omega^2}{6\Delta^2} \right) \approx \frac{N_\Omega}{6} e^{2/\rho_0 V} \tag{60}$$

In terms of this normalized correlated pair operator, the BCS ansatz given in Eq. (46) then looks like a coherent state made of N composite bosons $C^\dagger$

$$|\Phi\rangle = \sum_{N=0}^{\infty} \frac{\alpha^N}{N!} C^{\dagger N} |F_0\rangle \tag{61}$$

The fact that $C^\dagger$ is not an elementary boson operator however plays a major role in this sum, as evidenced below

Using the above equation, it is easy to show that the mean value of any particle-conserving operator A in the BCS state

$$\langle A \rangle = \frac{\langle \Psi_{BCS}|A|\Psi_{BCS}\rangle}{\langle \Psi_{BCS}|\Psi_{BCS}\rangle} = \frac{\langle \Phi|A|\Phi\rangle}{\langle \Phi|\Phi\rangle} = \frac{\left(\frac{\alpha^N}{N!}\right)^2 \langle F_0|C^N A C^{\dagger N}|F_0\rangle}{\sum \left(\frac{\alpha^N}{N!}\right)^2 \langle F_0|C^N C^{\dagger N}|F_0\rangle} \tag{62}$$

expands in terms of the mean value of this A operator in the N-pair state

$$\langle A \rangle_N = \frac{\langle F_0|C^N A C^{\dagger N}|F_0\rangle}{\langle F_0|C^N C^{\dagger N}|F_0\rangle} \tag{63}$$

according to

$$\langle A \rangle = \sum P_N \langle A \rangle_N \tag{64}$$

where P_N is the pair number probability of the BCS state. This distribution reads as

$$P_N = \frac{\left(\frac{\alpha^N}{N!}\right)^2 \langle F_0|C^N C^{\dagger N}|F_0\rangle}{\sum \left(\frac{\alpha^N}{N!}\right)^2 \langle F_0|C^N C^{\dagger N}|F_0\rangle} \tag{65}$$

For a highly peaked probability P_N, calculations of $\langle A \rangle$ and $\langle A \rangle_N$ for N taken at this peaked value, give the same result.

If $C^\dagger$ were an elementary boson-creation operator, i.e., for $[C, C^+] = 1$, the scalar product $\langle F_0|C^N C^{\dagger N}|F_0\rangle$ would reduced to $N!$, the denominator in Eq.(65) would reduce to e^{α^2}, so that P_N would reduce for N large to

$$P_N^{(0)} = \frac{\alpha^{2N}}{N!} e^{-\alpha^2} \approx \left(\frac{\alpha^2}{N}\right)^N e^{N-\alpha^2} \tag{66}$$

This distribution is maximum for $N \approx \alpha^2$. In view of Eq. (60), this pair number is far above the maximum number of pairs feeling the potential: the fact that the $C^\dagger$ operator is not an elementary boson operator does play a key role in the N-pair state distribution of the BCS ansatz.

Indeed, since the operator $C^\dagger$ is a composite boson operator, so that the scalar product of N such composite particles is strongly reduced compared to $N!$ as discussed in section I. We then have

$$\langle F_0 | C^N C^{\dagger N} | F_0 \rangle = N! f_N \tag{67}$$

with f_N far smaller than 1. Using this scalar product, the pair number probability in the BCS ansatz then reads as

$$P_N = \frac{\alpha^{2N} f_N / N!}{\sum \alpha^{2N} f_N / N!} \tag{68}$$

Due to Pauli blocking between pairs, f_N decreases when N increases through a "moth-eaten effect", now standard for composite bosons. This effect turns out to be totally dramatic in the case of composite bosons made of a finite number of pairs as in the case of BCS pairs due to the $w_\mathbf{k}$ cut-off, since the scalar product of N composite bosons must reduce to zero for N larger than this number. This already proves that $f_N = 0$ for N larger than the number of pairs N_Ω feeling the potential. When multiplied by $\alpha^{2N} N!$, this already brings the P_N maximum from α^2 as obtained for the elementary boson distribution $P_N^{(0)}$ down to $N = N_\Omega$. This however is not enough, since for μ taken in the middle of the potential layer, we expect this maximum to occur at $N = N_\Omega/2$.

To understand why P_N is indeed peaked on $N_\Omega/2$, we must consider more carefully the BCS composite boson $C^\dagger$ which enter this distribution. Let us now do it.

V. STUDY OF THE BCS COMPOSITE BOSON

According to section III, the BCS pair creation operator is given by $B^\dagger = \sum \phi_\mathbf{k} \beta_\mathbf{k}^\dagger$ where $\phi_\mathbf{k}$ is given by Eqs. (49,51). For a chemical potential taken in the middle of the potential layer, the $\mathbf{k}$-pair distribution in this composite boson is controlled by the pair wave function

$$\phi_\mathbf{k} = \frac{v_\mathbf{k}}{u_\mathbf{k}} = \sqrt{1 + \frac{\xi_\mathbf{k}^2}{\Delta^2}} - \frac{\xi_\mathbf{k}}{\Delta} \tag{69}$$

This pair wave function should not be mixed with $u_\mathbf{k} v_\mathbf{k}$ as often said, the $u_\mathbf{k} v_\mathbf{k}$ product being actually related to the concept of "virtual pairs".

For $\epsilon_\mathbf{k}$ equal to μ, $\xi_\mathbf{k}$ reduces to 0 so that $\phi_\mathbf{k} = 1$. For $\epsilon_\mathbf{k}$ below μ at the Δ scale, $\phi_\mathbf{k} \approx -2\xi_\mathbf{k}/\Delta = 2(\mu - \epsilon_\mathbf{k})/\Delta$, while far above the chemical potential, $\phi_\mathbf{k} \approx \Delta/2\xi_\mathbf{k}$. The curve $\phi_\mathbf{k}$ in the relevant range $(\epsilon_{F_0}, \epsilon_{F_0} + \Omega)$ is shown in Eq.(1) for a potential μ taken in

the middle of the potential layer, i.e., when $\Delta = \Omega e^{-1/\rho_0 V}$. We see that $\phi_{\mathbf{k}}$ has three quite different scales: $\phi_{\mathbf{k}}$ is essentially 1 very close to the chemical potential at the Δ scale. $\phi_{\mathbf{k}}$ is of the order of $e^{1/\rho_0 V}$ below this potential at the Δ scale while it is of the order of $e^{-1/\rho_0 V}$ above it. This means that the BCS pair operator $B^\dagger$ is essentially made of pair states with energy between $\epsilon_{\mathbf{k}} = \epsilon_{F_0}$ and $\epsilon_{\mathbf{k}} \approx \mu - \Delta/2$, with a small tail up to $\mu + \Delta/2$, the part of the $\phi_{\mathbf{k}}$ wave function above this value, up to the upper limit of the potential layer, being far smaller.
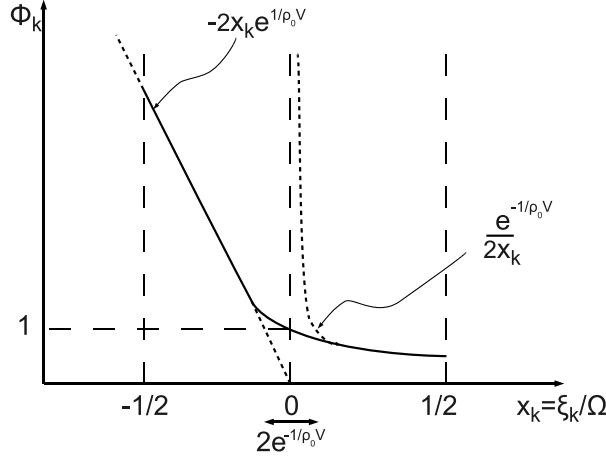

FIG. 1. BCS wave function

In order to make clearer the relative weight of a given $\mathbf{k}$ pair in this distribution, it is convenient to use the normalized BCS pair creation operator defined in Eq. (58) with $\langle F_0 | CC^\dagger | F_0 \rangle = 1$. The wave function then is $\varphi_{\mathbf{k}} = \alpha^{-1} \phi_{\mathbf{k}}$ with $\alpha \approx e^{1/\rho_0 V} \sqrt{N_\Omega/6}$, as given in Eq.(60). This means that the number of pair having a sizeable $\varphi_{\mathbf{k}}$ are essentially between ϵ_{F_0} and $\mu - \Delta/2$, this $\varphi_{\mathbf{k}}$ value being of the order of

$$\varphi_1 \approx \frac{1}{\sqrt{N_\Omega}} \tag{70}$$

where N_Ω is the total number of pair feeling the potential. The $\varphi_{\mathbf{k}}$ distribution has a small tail of the order of

$$\varphi_2 \approx \frac{e^{-1/\rho_0 V}}{\sqrt{N_\Omega}} \tag{71}$$

for pair with energy in the range $\pm\Delta/2$ around the chemical potential. Pairs with higher energy are going to enter with a prefactor $\varphi_3^2 \approx e^{-4/\rho_0 V}/N_\Omega$, since contributions in $e^{4/\rho_0 V}$ are expected to be too small to be relevant; most probably these higer energy pairs play a negligeable role in BCS superconducting.

The above analysis of the $\varphi_{\mathbf{k}}$ wave function controlling the composite boson operator $C^\dagger$ essentially shows that Pauli blocking among these BCS pairs, which mainly affects the ones having a sizeable $\varphi_{\mathbf{k}}$, is going to have a dramatic effect for N close to half filling, not to complete filling-which precisely is the value we want.

Let us now study more in details how the f_N factor of these $C^\dagger$ pairs drops to zero in the Δ layer around the chemical potential μ. For that, we approximate the $\varphi_{\mathbf{k}}$ distribution by a two-step distribution, with a first part equal to φ_1 extending between ϵ_{F_0} and $\mu - \Delta/2$ and a second part equal to φ_2 extending over $\mu \pm \Delta/2$.

The distribution probability of $\mathbf{k}$ pairs in the BCS correlated pair is given by

$$p_{\mathbf{k}} = \langle F_0 | C a_{\mathbf{k}}^\dagger a_{\mathbf{k}} C^\dagger | F_0 \rangle = |\varphi_{\mathbf{k}}|^2 \tag{72}$$