

# Towards a theory of superconductivity based on collective Cooper pairs

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## ABSTRACT

Superconductivity could be seen as a Bose–Einstein condensation (BEC) of Cooper pairs. However, the creation and annihilation operators of Cooper pairs do not satisfy the bosonic commutation relations and then, the mentioned viewpoint has a weakness in its foundation. In this work, we introduce the concept of collective Cooper pairs (CCP) as linear combinations of Cooper pairs and prove their bosonic nature at the dilute limit. This bosonic nature is given rise from their diffuse character on the Cooper pairs, which permits the accumulation of many collective pairs at a single quantum state. Moreover, the superconducting ground state proposed by Bardeen, Cooper and Schrieffer (BCS) can be written in terms of these collective Cooper pairs, which means that the BCS theory is consistent with a possible BEC theory of superconductivity based on collective Cooper pairs. Finally, we calculate the energy spectra and the BEC critical temperature of CCP.

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## 1. Introduction

Superconductivity is one of the most interesting phenomena in physics. Nowadays, there is a consensus that this extraordinary phenomenon is originated from the Cooper pairs (CP). Recently, many experiments have confirmed the existence of a pseudo energy gap at a higher temperature than the superconducting one in cuprate superconductors [1,2]. A possible interpretation of this observation could be the separation of the superconducting transition from the formation of CP, *i.e.*, the superconductivity could be visualized as a Bose–Einstein condensation (BEC) of CP, when their phase coherence is reached. However, CP are not true bosons as stated in the original paper of Bardeen, Cooper and Schrieffer (BCS) [3], since the creation ( $\hat{b}_{\mathbf{k}} \equiv \hat{c}_{\mathbf{k}\uparrow} \hat{c}_{-\mathbf{k}\downarrow}$ ) and annihilation ( $\hat{b}_{\mathbf{k}} \equiv \hat{c}_{-\mathbf{k}\downarrow} \hat{c}_{\mathbf{k}\uparrow}$ ) operators of CP do not satisfy the bosonic commutation relations, because

$$\begin{cases} [\hat{b}_{\mathbf{k}}, \hat{b}_{\mathbf{k}'}^{\dagger}] \equiv \hat{b}_{\mathbf{k}} \hat{b}_{\mathbf{k}'}^{\dagger} - \hat{b}_{\mathbf{k}'}^{\dagger} \hat{b}_{\mathbf{k}} = [\hat{b}_{\mathbf{k}}, \hat{b}_{\mathbf{k}'}] = 0 \\ [\hat{b}_{\mathbf{k}}, \hat{b}_{\mathbf{k}'}] = (1 - \hat{n}_{-\mathbf{k}\downarrow} - \hat{n}_{\mathbf{k}\uparrow}) \delta_{\mathbf{k}, \mathbf{k}'} \end{cases}, \quad (1)$$

where  $\hat{n}_{\mathbf{k}\sigma} = \hat{c}_{\mathbf{k}\sigma}^{\dagger} \hat{c}_{\mathbf{k}\sigma}$  is the number operator of electrons,  $\hat{c}_{\mathbf{k}\sigma}^{\dagger}$  and  $\hat{c}_{\mathbf{k}\sigma}$  are the creation and annihilation operators of a single electron with linear momentum  $\mathbf{k}$  and spin  $\sigma$ , respectively. In addition, from the definition of  $\hat{b}_{\mathbf{k}}^{\dagger}$  and  $\hat{b}_{\mathbf{k}}$ , it is easy to prove that

$$\hat{b}_{\mathbf{k}}^{\dagger} \hat{b}_{\mathbf{k}}^{\dagger} = \hat{b}_{\mathbf{k}} \hat{b}_{\mathbf{k}} = 0, \quad (2)$$

which even emphasizes a fermionic character of CP.

In this article, we demonstrate that the collective Cooper pairs (CCP) defined as linear combinations of CP satisfy the bosonic commutation relations at the dilute limit, as well as that the BCS superconducting ground state can be written in terms of CCP. We further calculate the energy spectra of CCP and the BEC critical temperature.

## 2. Collective Cooper pairs

Let us consider a system with  $M$  possible Cooper pairs and we define  $M$  creation operators of CCP as

$$\hat{a}_{\alpha}^{\dagger} \equiv \sum_{l=1}^M A_{\alpha}(l) \hat{b}_{\mathbf{k}_l}^{\dagger} = \frac{1}{\sqrt{M}} \sum_{l=1}^M \exp\left(\frac{i2\pi l\alpha}{M}\right) \hat{b}_{\mathbf{k}_l}^{\dagger}, \quad (3)$$

where  $\alpha = 0, 1, \dots, M-1$ ,  $A_{\alpha}(l) = \frac{1}{\sqrt{M}} \exp\left(\frac{i2\pi l\alpha}{M}\right)$ , and then

$$\sum_{l=1}^M A_{\alpha}^*(l) A_{\beta}(l) = \frac{1}{M} \sum_{l=1}^M \exp\left[\frac{i2\pi l(\beta - \alpha)}{M}\right] = \delta_{\alpha, \beta}. \quad (4)$$

Hence, the CCP are related to CP by a canonical transformation, and from Eqs. (1) and (4)

$$\begin{aligned} [\hat{a}_{\alpha}, \hat{a}_{\beta}^{\dagger}] &= \sum_{l, l'=1}^M A_{\alpha}^*(l) A_{\beta}(l') [\hat{b}_{\mathbf{k}_l}, \hat{b}_{\mathbf{k}_{l'}}^{\dagger}] \\ &= \sum_{l, l'=1}^M A_{\alpha}^*(l) A_{\beta}(l') (1 - \hat{n}_{-\mathbf{k}_l\downarrow} - \hat{n}_{\mathbf{k}_{l'}\uparrow}) \delta_{ll'} \\ &= \delta_{\alpha, \beta} - \sum_{l=1}^M A_{\alpha}^*(l) A_{\beta}(l) (\hat{n}_{-\mathbf{k}_l\downarrow} + \hat{n}_{\mathbf{k}_l\uparrow}). \end{aligned} \quad (5)$$

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In general, a quantum state with  $N$  CCP can be written as

$$\begin{aligned} |n_0, \dots, n_{M-1}\rangle &\equiv B(n_0, \dots, n_{M-1}) \prod_{v=0}^{M-1} (\hat{a}_v^\dagger)^{n_v} |0\rangle \\ &= B(n_0, \dots, n_{M-1}) \prod_{v=0}^{M-1} \left( \sum_{l=1}^M A_v(l) \hat{b}_{\mathbf{k}_l}^\dagger \right)^{n_v} |0\rangle \\ &= \sum_{l_1=1}^M \dots \sum_{l_N=1}^M C(l_1, \dots, l_N) \hat{b}_{\mathbf{k}_{l_1}}^\dagger \dots \hat{b}_{\mathbf{k}_{l_N}}^\dagger |0\rangle, \end{aligned} \quad (6)$$

where  $B(n_0, \dots, n_{M-1})$  is the normalization factor,

$$\sum_{v=0}^{M-1} n_v = N, \quad (7)$$

and

$$C(l_1, \dots, l_N) = B(n_0, \dots, n_{M-1}) A_0(l_1) \dots A_{M-1}(l_N). \quad (8)$$

From Eq. (6) we find

$$\begin{aligned} \sum_{l=1}^M \hat{n}_{\mathbf{k}_l} |n_0, \dots, n_{M-1}\rangle &= \sum_{l_1=1}^M \dots \sum_{l_N=1}^M C(l_1, \dots, l_N) \sum_{l=1}^M \hat{n}_{\mathbf{k}_l} \hat{b}_{\mathbf{k}_1}^\dagger \dots \hat{b}_{\mathbf{k}_{l_N}}^\dagger |0\rangle \\ &= \sum_{l_1=1}^M \dots \sum_{l_N=1}^M C(l_1, \dots, l_N) \sum_{l=1}^M (\delta_{l,l_1} + \dots + \delta_{l,l_N}) \hat{b}_{\mathbf{k}_1}^\dagger \dots \hat{b}_{\mathbf{k}_{l_N}}^\dagger |0\rangle \\ &= N |n_0, \dots, n_{M-1}\rangle. \end{aligned} \quad (9)$$

By using the inequality  $|\sum_l A_l B_l| \leq \sum_l |A_l| |B_l|$ ,

$$\begin{aligned} &\left| \left\langle \sum_{l=1}^M A_\alpha^*(l) A_\beta(l) (\hat{n}_{-\mathbf{k}_l} + \hat{n}_{\mathbf{k}_l}) \right\rangle \right| \\ &\leq \sum_{l=1}^M |A_\alpha^*(l)| |A_\beta(l)| \langle \hat{n}_{-\mathbf{k}_l} \rangle + \langle \hat{n}_{\mathbf{k}_l} \rangle = \frac{2N}{M}, \end{aligned} \quad (10)$$

where  $\langle \hat{\alpha} \rangle \equiv \langle n_0, \dots, n_{M-1} | \hat{\alpha} | n_0, \dots, n_{M-1} \rangle$ . Hence, at the dilute limit,  $N/M \rightarrow 0$ , Eq. (5) leads to

$$[\hat{a}_\alpha, \hat{a}_\beta^\dagger] = \delta_{\alpha,\beta}. \quad (11)$$

On the other hand, from equation (1) we have

$$[\hat{a}_\alpha^\dagger, \hat{a}_\beta^\dagger] = [\hat{a}_\alpha, \hat{a}_\beta] = 0. \quad (12)$$

Briefly, Eqs. (11) and (12) prove the bosonic nature of CCP at the dilute limit. In addition,

$$B(n_0, \dots, n_{M-1}) = (n_0! \dots n_{M-1}!)^{-1/2}. \quad (13)$$

can be obtained from equations (6), (11) and (12).

### 3. Energy spectrum of CCP

Let us start from the BCS Hamiltonian [3] given by

$$\hat{H} = \sum_{\mathbf{k}, \sigma} \varepsilon(\mathbf{k}) \hat{c}_{\mathbf{k}, \sigma}^\dagger \hat{c}_{\mathbf{k}, \sigma} + \sum_{\mathbf{k} \neq \mathbf{k}'} V_{\mathbf{k}, \mathbf{k}'} \hat{b}_{\mathbf{k}}^\dagger \hat{b}_{\mathbf{k}'}, \quad (14)$$

where  $\varepsilon(\mathbf{k}) = \hbar^2 k^2 / 2m$  is the single electron energy with momentum  $\mathbf{k}$  and

$$V_{\mathbf{k}, \mathbf{k}'} = \begin{cases} -V, & \text{if } |\varepsilon(\mathbf{k}) - E_F| \text{ and } |\varepsilon(\mathbf{k}') - E_F| \leq \hbar\omega_D \\ 0, & \text{otherwise} \end{cases} \quad (15)$$

being  $V > 0$ ,  $E_F$  the Fermi energy, and  $\omega_D$  the Debye frequency. For this case,  $M$  is the number of states with wave vector  $\mathbf{k}$  that satisfy  $|\varepsilon(\mathbf{k}) - E_F| \leq \hbar\omega_D$ . In the strong coupling limit,  $\hbar\omega_D \ll V$ , we can make the approximation of  $\varepsilon(\mathbf{k}) \approx E_F$  and then, Hamiltonian (14) can be

rewritten as

$$\begin{aligned} \hat{H} &= E_F \sum_{\mathbf{k}, \sigma} \hat{c}_{\mathbf{k}, \sigma}^\dagger \hat{c}_{\mathbf{k}, \sigma} - V \sum_{l, l'=1}^M \hat{b}_{\mathbf{k}_l}^\dagger \hat{b}_{\mathbf{k}_{l'}} + V \sum_{l=1}^M \hat{b}_{\mathbf{k}_l}^\dagger \hat{b}_{\mathbf{k}_l} \\ &= E_F \sum_{\mathbf{k}, \sigma} \hat{n}_{\mathbf{k}, \sigma} - MV \hat{a}_0^\dagger \hat{a}_0 + V \sum_{l=1}^M \hat{b}_{\mathbf{k}_l}^\dagger \hat{b}_{\mathbf{k}_l}, \end{aligned} \quad (16)$$

since  $\hat{a}_0^\dagger \equiv \sum_{l=1}^M \hat{b}_{\mathbf{k}_l}^\dagger / \sqrt{M}$ . From Eq. (9),

$$\hat{H} |n_0, \dots, n_{M-1}\rangle = (2NE_F - n_0 MV + NV) |n_0, \dots, n_{M-1}\rangle, \quad (17)$$

and the energy spectrum of  $N$  CCP is given by

$$E(n_0, \dots, n_{M-1}) = 2NE_F + [N - Mn_0]V, \quad (18)$$

which is in agreement with the energy spectrum found by Thouless [4], evaluating for the dilute limit.

Using Eq. (7), Eq. (18) can be rewritten as

$$E(n_0, \dots, n_{M-1}) = \sum_{\alpha=0}^{M-1} n_\alpha E_\alpha. \quad (19)$$

where

$$E_\alpha = \begin{cases} 2E_F - (M-1)V, & \text{if } \alpha = 0 \\ 2E_F + V, & \text{if } \alpha = 1, 2, \dots, (M-1) \end{cases} \quad (20)$$

is the energy spectrum of single CCP. Notice that Eqs. (7) and (19) reveal that the system of  $N$  CCP can be consider as an ideal gas of bosons at dilute limit.

### 4. Bose–Einstein condensation of CCP

Following a standard procedure of the BEC analysis within the grand-canonical ensemble formalism [5], the average number of CCP ( $\langle N \rangle$ ) for  $T > 0$  is, from Eq. (20), given by

$$\langle N \rangle = \sum_{\alpha=0}^{M-1} \frac{1}{e^{\beta(E_\alpha - \mu)} - 1} = \frac{1}{e^{\beta(2E_F - (M-1)V - \mu)} - 1} + \frac{M-1}{e^{\beta(2E_F + V - \mu)} - 1}, \quad (21)$$

where  $\beta = 1/k_B T$  and  $\mu$  is the chemical potential. Since  $M \gg 1$ , the ground state occupation is negligible in comparison with the occupation of excited states for  $\mu < E_0$ , i.e.,

$$\langle N \rangle \approx \frac{M-1}{e^{\beta(2E_F + V - \mu)} - 1}. \quad (22)$$

The BEC occurs when  $\mu = E_0$ , Eq. (22) leads to a critical temperature ( $T_C$ ) given by

$$k_B T_C = \frac{MV}{\ln\left(\frac{M-1}{\langle N \rangle} + 1\right)}. \quad (23)$$

### 5. Comparison with the BCS ground state

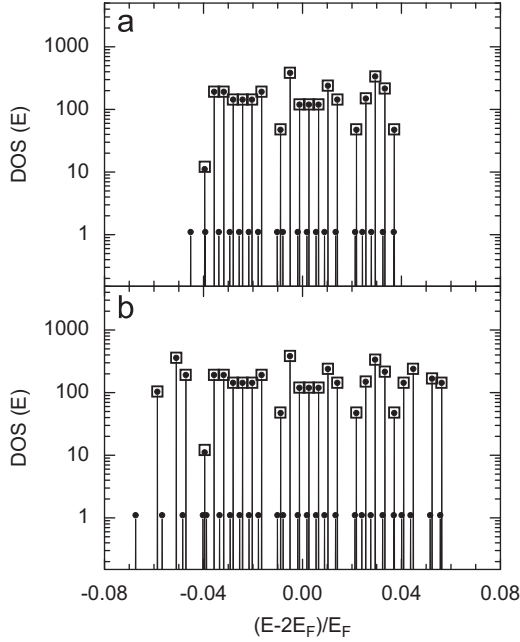
Within the BCS theory, the superconducting ground state can be written as [6],

$$|G\rangle = \prod_{\mathbf{k}} (u_{\mathbf{k}} + v_{\mathbf{k}} \hat{b}_{\mathbf{k}}^\dagger) |0\rangle, \quad (24)$$

where  $|v_{\mathbf{k}}|^2$  and  $|u_{\mathbf{k}}|^2$  are, respectively, the occupied and unoccupied probabilities of the CP ( $\mathbf{k}\uparrow, -\mathbf{k}\downarrow$ ). Expanding Eq. (24) we find that for  $u_{\mathbf{k}} \neq 0$ ,

$$\begin{aligned} |G\rangle &= \left[ \prod_{\mathbf{k}} u_{\mathbf{k}} \right] \left[ 1 + \sum_{\mathbf{k}} \frac{v_{\mathbf{k}}}{u_{\mathbf{k}}} \hat{b}_{\mathbf{k}}^\dagger + \sum_{\mathbf{k}\mathbf{k}'} \frac{v_{\mathbf{k}} v_{\mathbf{k}'}}{u_{\mathbf{k}} u_{\mathbf{k}'}} \hat{b}_{\mathbf{k}}^\dagger \hat{b}_{\mathbf{k}'}^\dagger + \dots \right] |0\rangle \\ &= \left[ \prod_{\mathbf{k}} u_{\mathbf{k}} \right] \sum_{n=0}^M \left( \sum_{\mathbf{k}} \frac{v_{\mathbf{k}}}{u_{\mathbf{k}}} \hat{b}_{\mathbf{k}}^\dagger \right)^n |0\rangle, \end{aligned} \quad (25)$$

where  $M$  is the maximum number of CP.



**Fig. 1.** CCP density of states (DOS) for (a)  $\hbar\omega_D = 0.02E_F$  and (b)  $\hbar\omega_D = 0.03E_F$ , where the energy is discretized by using  $\Delta E = 0.0001E_F$ .

In Eq. (25) each term of the summation corresponds to a state of  $n$  CCP, *i.e.*,

$$|n\rangle \equiv B(n) \left( \sum_{\mathbf{k}} \frac{v_{\mathbf{k}}}{u_{\mathbf{k}}} b_{\mathbf{k}}^\dagger \right)^n |0\rangle, \quad (26)$$

which is same as that of Eq. (6) by making  $n_1 = \dots = n_{M-1} = 0$  and  $v_{\mathbf{k}} = u_{\mathbf{k}} = 1/\sqrt{2}$  for the strong coupling limit [6].

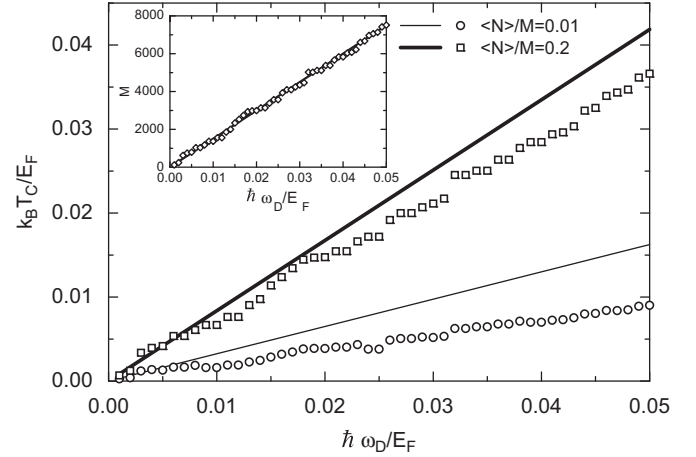
## 6. Beyond the strong coupling limit

In this section, we calculate the energy spectrum of CCP beyond the approximation of  $\varepsilon(\mathbf{k}) \approx E_F$ , by computing numerically the single CCP eigenvalues of Hamiltonian (14) for an interaction  $V = 10^{-5}E_F$ . For a cubic lattice of  $N_S$  sites with one electron per site, the number of  $\mathbf{k}$ -states in the energy band  $\hbar\omega_D$  around  $E_F$  is

$$M = \frac{N_S}{2} \left\{ \left( 1 + \frac{\hbar\omega_D}{E_F} \right)^{3/2} - \left( 1 - \frac{\hbar\omega_D}{E_F} \right)^{3/2} \right\}. \quad (27)$$

The results of energy degeneracy or density of states (DOS) for  $N_S = 10^5$  are illustrated by dots in Fig. 1 for (a)  $\hbar\omega_D = 0.02E_F$  and (b)  $\hbar\omega_D = 0.03E_F$ , in comparison with the corresponding spectra of self-energy  $2\varepsilon(\mathbf{k})$  of CCP (open squares). Observe that the energy band width is almost  $2\hbar\omega_D$ , since  $E$  is the CCP energy. Furthermore, the DOS spectra and the corresponding  $2\varepsilon(\mathbf{k})$  ones are approximately the same, except a lower-energy bonding state appeared for each degenerate energy. This fact is an extension of the energy spectrum at the strong coupling limit given by Eq. (20).

In Fig. 2, the analytical solution (lines) from Eq. (23) and numerical one (open symbols) of  $T_C$  versus  $\hbar\omega_D$  are comparatively plotted for the cases of  $\langle N \rangle / M = 0.01$  and 0.2. Note that the numerical results contain a remarkable fluctuation which is originated from the



**Fig. 2.** A comparison of the BEC critical temperature ( $T_C$ ) obtained with (lines) and without (open symbols) the approximation of  $\varepsilon(\mathbf{k}) \approx E_F$  as a function of the Debye frequency ( $\omega_D$ ). Inset: the number of  $\mathbf{k}$ -states ( $M$ ) in the energy band  $\hbar\omega_D$  around  $E_F$  versus  $\omega_D$ .

fluctuation of  $M$ , as shown the open rhombus in the inset of Fig. 2 which compared with Eq. (27) (line).

## 7. Conclusions

Throughout this article, we have demonstrated that the CCP defined as linear combinations of CP are true bosons at the dilute limit, since their creation and annihilation operators fully satisfy the bosonic commutation relations. This demonstration is an extension of Ref. [7], where only a single kind ( $\alpha$ ) of CCP is considered. Also, we show that the BCS superconducting ground state can be written in terms of CCP, which means that the BCS theory is consistent with a possible BEC theory of superconductivity based on CCP. We further calculate the energy spectrum of CCP with and without the approximation of  $\varepsilon(\mathbf{k}) \approx E_F$  using the BCS Hamiltonian. We can observe from Fig. 1 that the highly-degenerate excited CCP state from the analytical solution (20) is spread to a spectrum of degenerate excited CCP states plus their corresponding bounding state. Hence, a general reduction of  $T_C$  is observed in Fig. 2, as consequence of a diminution of the energy gap defined as  $(E_1 - E_0)$ .

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