The Quantum Theory of Superconductivity: An introduction to BCS.

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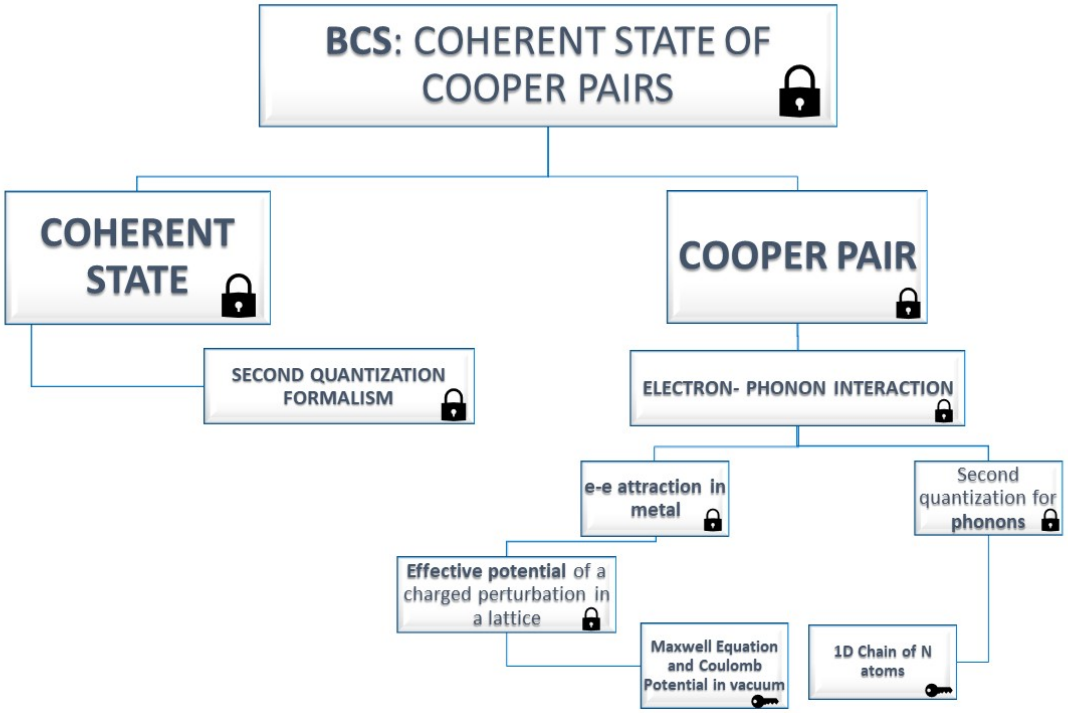
Introduction

In this discussion I'm going to structure a solid guide to face the topic of BCS, the quantum theory that explains low temperature superconductor. This is meant to be an introductory paper, so, we will enters quite deeply in all the fundamental knowledge needed to face the comprehension, but, we will stop once reached the many-body wave function. Our scope is therefore to understand the following sentence:" A low-temperature superconductor is made by a coherent state of Cooper pairs". We will, therefore, focus on the phrase "Coherent State" and "Cooper Pairs", trying to unlocking the meaning behind these. The idea behind the research of meaning for the previous statement is represented in the following scheme.



1 Electrons screening in a solid

1.1 Coulomb Potential: e-e interaction in vacuum

A good starting point for the vast majority of physical theories are by **postulating** Maxwell equations. This very general statement might be confusing, if we are dealing with charges that interact via Coulomb potential, *why we should start with Maxwell?*.
Physics relies on postulates, Coulomb interaction is nothing more than an exchange of photons between two charged particle. So at the end, Coulomb interaction is light or, better, is an exchange of an electromagnetic field (E, B). Therefore, once we have postulated[1] Maxwell, you have Coulomb for free.

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \qquad \nabla \times \mathbf{H} = +\frac{\partial \mathbf{D}}{\partial t} + \mathbf{j} \tag{1}$$

$$\nabla \cdot \mathbf{D} = \rho_l \qquad \nabla \cdot \mathbf{B} = 0 \tag{2}$$

Where obviously **D** and **H** are the associated auxiliary field.

$$\mathbf{D} = \epsilon_0 \mathbf{E} + \mathbf{P} \qquad \mathbf{B} = \mu_0 \mathbf{H} + \mu_0 \mathbf{M}$$

Now, it is often comfortable to work with the four-vector potential $(\mathbf{A}, \phi)$. Where,

$$\nabla \times \mathbf{A} = \mathbf{B}$$
$$-\frac{\partial \mathbf{A}}{\partial t} - \nabla\phi = \mathbf{E}$$

Fixing the Coulomb Gauge, in which $\nabla \cdot \mathbf{A} = 0$ Then we can rewrite the third Maxwell equation as:

$$\nabla \cdot [(-\frac{\partial \mathbf{A}}{\partial t} - \nabla\phi)\epsilon_0 + \mathbf{P}] = \rho_l \tag{3}$$

(3) is an extremely relvant equation that contains all the kind of field generated by a free density charge in a medium characterized by a polarization **P**.
In complete vacuum $\mathbf{P} = 0$, then if we further assume that our world is made by just one electron localized in position $\mathbf{r} = 0$, then equation (3) become:

$$\rho_l = -e\delta(\mathbf{r}) \tag{4}$$

$$-\nabla^2\phi = -\frac{e}{\epsilon_0}\delta(\mathbf{r}) \tag{5}$$

Let's therefore solve (5) and find the field generated by a static electron.
$\phi(\mathbf{r})$ is a 3D spatial function, we can think to decompose it in the 3D Fourier space.
We recall briefly that the Fourier transform is a simple rule that allows an uni-vocal jump from different spaces the coordinate spaces **r** to the reciprocal space, k-space **k**, the latter, in a classical framework, has no particular meaning.
Therefore we can construct this transformation rules as:

$$F(\mathbf{r}) = \frac{1}{(2\pi)^3}\int_{-\infty}^{\infty} \tilde{F}(\mathbf{k}) e^{+i\mathbf{k}\cdot\mathbf{r}} d^3k$$

And its inverse,

$$\tilde{F}(\mathbf{k}) = \int_{-\infty}^{\infty} F(\mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{r}} d^3r$$

[1] I say postulate because I like to think that every time one has to write about physics he must remember which are the things one assumed for true.

Therefore applying this transformation to (5):

$$\nabla^2 \frac{1}{(2\pi)^3} \int_{-\infty}^{\infty} d^3k \tilde{\phi}(\mathbf{k}) e^{+i\mathbf{k}\cdot\mathbf{r}} = \frac{e}{\epsilon_0 (2\pi)^3} \int_{-\infty}^{\infty} d^3k e^{+i\mathbf{k}\cdot\mathbf{r}} \tag{6}$$

$$\tag{7}$$

Where we have used the fact that a delta correspond to a flat function in the k-space. Then,

$$-\int_{-\infty}^{\infty} d^3k k^2 \tilde{\phi}(\mathbf{k}) e^{+i\mathbf{k}\cdot\mathbf{r}} = \frac{e}{\epsilon_0} \int_{-\infty}^{\infty} d^3k e^{+i\mathbf{k}\cdot\mathbf{r}} \tag{8}$$

$$\tag{9}$$

Where r is the modulus of **r**.
It is now easy to show that:

$$\phi(\mathbf{k}) = -\frac{e}{\epsilon_0 k^2} \tag{10}$$

It is less easy to calculate the Fourier inverse, after few calculus[2]

$$\phi(\mathbf{r}) = -\frac{e}{4\pi\epsilon_0} \frac{1}{r} \tag{11}$$

Where r is the modulus of **r**. At this point we are almost close to the Coulomb potential. We can **postulate** that a single classical particle will interact with an electromagnetic field according to its Hamiltonian:

$$H_{electron} = \frac{1}{2m} (\mathbf{p} + e\mathbf{A})^2 - e\phi \tag{12}$$

At this point we have two particles, one that is generating the field, assumed to be static in space, and one that feels the presence of the other thanks to the mediation of the electromagnetic field. The static condition of the former particle brings to $\mathbf{A} = 0$. Therefore, the potential felt by the latter is simply V, that we call **Coulomb potential**.

$$V(r) = \frac{e^2}{4\pi\epsilon_0 r} \tag{13}$$

Where **r** is the position of the "free" particle. In the k-space the Coulomb potential become:

$$V(k) = \frac{e^2}{\epsilon_0 k^2} \tag{14}$$

The static condition on A is mandatory when we want to claim that Coulomb is the only interaction between two charges. However we can easily make the following natural generalization of the Coulomb potential[3] **NOTE**: In the two particle environment k is still a parameter that describe the reciprocal space. However, this time the Fourier transform is defined with $|\mathbf{r}_1 - \mathbf{r}_2|$. Identified the particles positions with $\mathbf{r}_1$ and $\mathbf{r}_2$, we have

$$V(|\mathbf{r}_1 - \mathbf{r}_2|) = \frac{e^2}{4\pi\epsilon_0 |\mathbf{r}_1 - \mathbf{r}_2|} \tag{15}$$

[2]Appendix A

[3]The V Coulomb is NOT the only interaction between two particles, indeed, in principle, one should also add **A**, a electromagnetic field due that takes into account of the reciprocal motion. In general we will consider only the Coulomb potential as the force driving potential.

1.2 Effective potential in a metallic lattice

What if we are in a medium? What will be the interaction between two electrons?
These are a legitimate questions, for sure equation (3) can be used, in principle:

$$\nabla \cdot [(\frac{\partial \mathbf{A}}{\partial t} - \nabla\phi)\epsilon_0 + \mathbf{P}] = \rho_l$$

Where $\nabla \cdot \mathbf{P} = \rho_{fixed}$ are the fixed charge in a solid. So, we can imagine the effective interaction in a lattice as the Coulomb potential generated by an electron surrounded by ions that try to communicate with the second electron.
This picture is nice, but is wrong.
To solve the problem we must reformulate everything. A solid is a locally neutral environment, it means that, if we imagine a metallic lattice, we have localized ions and a sea of electrons around. This means that in equilibrium $\rho_{tot} = 0$. To describe the effective interaction between charges, we can imagine that our localized charged particle is a **perturbation** of the equilibrium condition, ρ_{ext}. But this is not the end, a localized perturbation will induce a reaction of the system made by lattice and electron sea, ρ_{ind}. Therefore defined $\rho = \rho_{ext} + \rho_{ind}$,

$$-\nabla^2\phi(\mathbf{r}) = \frac{1}{\epsilon_0}\rho(\mathbf{r}) \tag{16}$$

For linearity:

$$-\nabla^2\phi_{ext}(\mathbf{r}) = \frac{1}{\epsilon_0}\rho_{ext}(\mathbf{r}) \tag{17}$$

$$-\nabla^2\phi_{ind}(\mathbf{r}) = \frac{1}{\epsilon_0}\rho_{ind}(\mathbf{r}) \tag{18}$$

$$\tag{19}$$

The former term has been already solved, it is the Coulomb scalar field. While for the latter we still have some problems, for sure it must takes into account both the electron sea response and the lattice. What come after is a very strong hypothesis that will reasonably work if the induction is weak.
We can therefore imagine that, in a linear medium, the total scalar potential will be very similar to the external scalar potential. In other terms we feed the medium with a certain real scalar potential, ϕ_{ext}, and the interaction that comes out is a different ϕ. The relation between the two will be given by:

$$\phi(\mathbf{k}) = \frac{1}{\epsilon(\mathbf{k})}\phi_{ext}(\mathbf{k}) \tag{20}$$

Hence, we are fixing a linear relation in the k-space. Moreover, if $\epsilon(\mathbf{k}) > 1 \ \forall k$, then we have an attenuation of the total scalar potential with respect the free charge case. This strong hypothesis leads to an incredibly easy way to derive the total Coulomb potential.

$$-\nabla^2\phi_{ext} = \frac{\rho_{ext}}{\epsilon_0}$$
$$\rho_{ext} = -e\delta(\mathbf{r})$$

Now switching to the Fourier domain, and substituting with (20):

$$k^2\phi(\mathbf{k})\epsilon(\mathbf{k}) = -\frac{e}{\epsilon_0}$$

Therefore:

$$\phi(\mathbf{k}) = -\frac{e}{\epsilon_0\epsilon(\mathbf{k})}\frac{1}{k^2} \tag{21}$$

This is a rather remarkable result. With very general consideration, we have now the total scalar potential that a fixed charge generates inside the lattice, considering already the linear medium response.
Let's consider two example:

i) If $\epsilon(\mathbf{k}) \approx const$ over all the k, we decay in a well known formula often used in many course of electromagnetism.

$$V_{coulmb} = \frac{1}{4\pi\epsilon_0\epsilon_r}\frac{e^2}{r} \tag{22}$$

ii) If $\epsilon(\mathbf{k}) = 1 + \frac{k_0^2}{k^2}$, then exploiting the result of Appendix A we can describe the famous Thomas-Fermi screening.

$$\phi(k) = -\frac{e}{\epsilon_0(k_0^2 + k^2)} \tag{23}$$

$$\phi(r) \propto \frac{1}{r}e^{-k_0 r} \tag{24}$$

1.3 Attractive potential of two electrons in solid

Now we are ready to understand how it is possible to have an attraction of two electrons in a solid, this counter-intuitive condition is the fundamental request that make possible to create a superconductive state where two electron are bonded. We can generalize equation (21) into a more realistic case.

$$\phi(\mathbf{k},\omega) = -\frac{e}{\epsilon_0 \epsilon(\mathbf{k},\omega)}\frac{1}{k^2} \tag{25}$$

(25) is just the consequence of the silliest statement we could have made: charges in a solid can move, so we expect that there will be a time-dependent response from both the lattice and the electron sea. With very easy considerations on the $\epsilon(\mathbf{k},\omega)$ we can build up a reasonable model for the medium response to the localized charge perturbation. We have written:

$$\epsilon\phi = \phi_{ext}$$

Where ϵ is something that takes into account both the bare ions response and the electron sea one. If these two mechanisms are decoupled then, from the linearity:

$$\phi_{tot} = \phi_{ext} + \phi_{bion} + \phi_{ele} \tag{26}$$

We can write, in the k-space:

$$\epsilon_{ele}\phi_{tot} = \phi_{ext} + \phi_{bion} \tag{27}$$

$$\epsilon_{bion}\phi_{tot} = \phi_{ext} + \phi_{electron} \tag{28}$$

These equations can be interpreted in the following way. To focus the idea we take (27), in this case we are looking at the system as if it is made only by the electrons sea and we want to see how an electron see modify an internal scalar potential, to be consistent this internal scalar potential that is modulate by the electron see to create the ϕ_{tot} must contains all the other mechanism. Combining all the equations:

$$(\epsilon_{ele} + \epsilon_{bion} - \epsilon)\phi_{tot} = \phi_{tot}$$

Leading to:

$$\epsilon = \epsilon_{ele} + \epsilon_{bion} - 1 \tag{29}$$

Now we impose two simple model:
i) The electron sea will respond on a perturbation by instantaneously rearranging in a way that the effective field of the electron will be weakened.[4] We can use the Thomas-Fermi screening model:

$$\epsilon_{ele} = 1 + \frac{k_0^2}{k^2} \tag{30}$$

ii) The bare ions are slow objects, and they will react with a certain delay with respect the faster localized electron. A good model to describe the response of a lattice is plasma oscillation.
Therefore given a certain Ω_p, we will have a response of the lattice if the ω, related to the electron velocity, is not too big[5].

$$\epsilon_{bion} = 1 - \frac{\Omega_p^2}{\omega^2} \tag{31}$$

[4] In the case of a localized electron perturbation we can think that the sea electrons will create a static positive charged around by undressing some ions. This lead to a positive screening of the electron potential

[5] If the electron is super-fast with respect the typical lattice oscillation then the bare ions won't see the electron passing, $\epsilon_{bion} \approx 1$

In our model $\epsilon_{bareions}$ do not depends on k, which means we are assuming that the lattice will respond in a spatially localized way to the perturbation. Exploiting the relation found in (29) we can simply achieve:

$$\frac{1}{\epsilon} = \frac{1}{1+\frac{k_0^2}{k^2}} \frac{\omega^2}{\omega^2 - \omega^2(k)} \tag{32}$$

With $\omega(k) = \frac{\Omega_p}{(1+\frac{k_0^2}{k^2})}$. This equation is pretty interesting and can be used in many ways. From (25) with the simple adjustment in the definition of r as $r = |\mathbf{r}_1 - \mathbf{r}_2|$, the instantaneous distance between the two localized particles, and a change in notation to q for the k-space. We can derive the effective Coulomb interaction between electrons in the metal. From:

$$V_{eff}(q,\omega) = \frac{e^2}{\epsilon_0 \epsilon(q,\omega)} \frac{1}{q^2} \tag{33}$$

To:

$$V_{eff}(q,\omega) = \frac{e^2}{\epsilon_0(q^2+k_0^2)}(1 + \frac{\omega^2(q)}{\omega^2 - \omega^2(q)}) \tag{34}$$

We immediately observe that if $\omega < \omega(q)$, so if the two electron relative motion is not too quick with respect the lattice frequency response then $V_{eff} < 0$.
It is possible to have an attractive potential between a pair of electron!
This result obtained in a fully classical environment is wonderful, however we could be still little perplex on the true meaning of the quantities. Forcing a meaning in this classical world is not healthy, however we can anticipate some result. q will be the phonon momentum, given by the difference between the two electrons momentum[6]. While $\hbar\omega$ is the difference in energy between the two electrons.
Now a typical value for $\omega(q)$ is given by the typical lattice oscillation, that depends on the lattice ions mass.

[6] If you think, the concept of k-wave vector for electron has no sense if you regard them as localized object.

2 Second quantization of phonons

We have, thus, understood that it is possible to have a positive attraction between two electrons in a solid, under peculiar condition of the energy. However, we are still far from the BCS. We need the whole quantum mechanics formalism and many of the quantum world idea. Without them is impossible to proceed further. Many time people introduce abruptly the word phonons out of nowhere, this is a very bad attitude. Despite the fact that many people can have an intuitive idea of the world phonons[7] the consequence behind this quasi-particle are extremely profound, therefore they deserve a proper introduction.

2.1 Classical 1D chain of N atoms

The easiest way to show the concept of phonons and to introduce second quantization formalism on a real many body problem is to consider the 1D chain of N identical atoms, of mass m.
Defined x_i the coordinate of the i-th atoms and p_i its momentum, if we assume that there is a perfectly harmonic force, like an ideal spring of constant C, between the two. Then the system Hamiltonian is:

$$\mathcal{H} = \sum_{n=1}^{N} \frac{1}{2m} p_n^2 + \frac{1}{2} C (x_{n+1} - x_n)^2 \tag{35}$$

This is a coupled equation and can be solved in many ways, one remarkable path exploit the Discrete Fourier Transform (DFT), discussed in detail in Appendix B. Since both p_n and x_n are a discrete sequence of number we can use without any worries the discrete Fourier. If we customize the DFT tool by defining $q = \frac{2\pi}{N} k$, where k is an integer number of the generalized DFT.
For x_n, defined $q = \frac{2\pi}{Na} k$, where k is an integer number, a is the distance between nearby atoms.

$$x_n = \frac{1}{\sqrt{N}} \sum_q \tilde{x}_q e^{iqna} \tag{36}$$

$$\tilde{x}_q = \frac{1}{\sqrt{N}} \sum_{n=0}^{N-1} x_n e^{-iqna} \tag{37}$$

With this definition na is the position at equilibrium of the n-th particle.
And for p_n

$$p_n = \frac{1}{\sqrt{N}} \sum_q \tilde{p}_q e^{iqna} \tag{38}$$

$$\tilde{p}_q = \frac{1}{\sqrt{N}} \sum_{n=0}^{N-1} p_n e^{-iqna} \tag{39}$$

What is $\tilde{x}_q$ and what is q? So far it is just legitimated math. It is, however, clear that $\tilde{x}_q$ by construction is associate to a collective way of motion, i.e. it contains all x_n, particle position. While for q, we must look the (36). To vary the value of q correspond to change the wavelength of the waveform associated to the collective way of motion. From now on we will associated to q the word "mode".

2.2 Quantum 1D chain

We don't want to describe a classical chain of N atoms, we want to say something on the quantum mechanical behavior of this many body system. Thus, we only have to use the basic postulate of quantum

[7] Or photons. Here the analogy goes in two sense. Photons are used, as a word, in the same random way as phonons, and, even more deeply, at the end phonons are masked PHOTONS!

mechanics, that create a bridge between $\mathcal{H}$ and $\hat{H}$, via $p_n \leftarrow \hat{p}_n$ and $x_n \leftarrow \hat{x}_n$. This means that our nice discrete Fourier transform has become a relation between operators.

$$\hat{x}_n = \frac{1}{\sqrt{N}} \sum_q \tilde{\hat{x}}_q e^{iqna} \tag{40}$$

$$\tilde{\hat{x}}_q = \frac{1}{\sqrt{N}} \sum_{n=0}^{N-1} \hat{x}_n e^{-iqna} \tag{41}$$

And,

$$\hat{p}_n = \frac{1}{\sqrt{N}} \sum_q \tilde{\hat{p}}_q e^{iqna} \tag{42}$$

$$\tilde{\hat{p}}_q = \frac{1}{\sqrt{N}} \sum_{n=0}^{N-1} \hat{p}_n e^{-iqna} \tag{43}$$

At this point we would like to rewrite the Hamiltonian, $\hat{H}$, as a function of the new q-operators. It is just a matter of taking (40) and (42) and put them in (35).
Let's start with (42):

$$\sum_n \hat{p}_n^2 = \frac{1}{N} \sum_n \sum_q \tilde{\hat{p}}_q e^{iqna} \sum_{q'} \tilde{p}_{q'} e^{iq'na} =$$
$$= \frac{1}{N} \sum_n \sum_q \sum_{q'} \tilde{\hat{p}}_q \tilde{\hat{p}}_{q'} e^{i(q'+q)na}$$

Exploiting the result of orthogonality for the DFT we can delete the $\sum_n$.

$$\sum_n \hat{p}_n^2 = \frac{1}{N} \sum_q \sum_{q'} \delta_{q,-q'} \tilde{\hat{p}}_q \tilde{\hat{p}}_{q'} e^{i(q'+q)na}$$

Finally,

$$\sum_n \hat{p}_n^2 = \sum_q \tilde{\hat{p}}_q \tilde{\hat{p}}_{-q} \tag{44}$$

For (40), remembering that we don't know, yet the commutation rules for $\hat{x}_q$:

$$\sum_n (\hat{x}_{n+1} - \hat{x}_n)^2 = \sum_n \hat{x}_{n+1}^2 + \hat{x}_n^2 - \hat{x}_n \hat{x}_{n+1} - \hat{x}_{n+1} \hat{x}_n =$$
$$= \sum_n (\frac{1}{\sqrt{N}} \sum_q \tilde{\hat{x}}_q e^{iqna})^2 - (\frac{1}{\sqrt{N}} \sum_q \tilde{\hat{x}}_q e^{iq(n+1)a})^2 -$$
$$- \frac{1}{N} \sum_q \tilde{\hat{x}}_q e^{iq(n+1)a} \sum_{q'} \tilde{\hat{x}}_{q'} e^{iq'(n)a} - \frac{1}{N} \sum_q \tilde{\hat{x}}_q e^{iqna} \sum_{q'} \tilde{\hat{x}}_{q'} e^{iq'(n+1)a}$$

With a bit of fatigue we can apply the rules discovered before and find:

$$\sum_n (\hat{x}_{n+1} - \hat{x}_n)^2 = 2 \sum_q \hat{x}_q \hat{x}_{-q} - 2 \hat{x}_q \hat{x}_{-q} \frac{e^{+iqA} + e^{-iqA}}{2}$$

Therefore:

$$\sum_n (\hat{x}_{n+1} - \hat{x}_n)^2 = \sum_q \hat{x}_q \hat{x}_{-q} 4 \sin(\frac{qa}{2}) \tag{45}$$

Surprisingly, this transformation have diagonalized the Hamiltonian $\hat{H}$, neglecting the redundant tildes.

$$\hat{H} = \sum_q \frac{1}{2m}\hat{p}_q\hat{p}_{-q} + \frac{1}{2}m\omega_q^2\hat{x}_q\hat{x}_{-q} \tag{46}$$

Where $\omega_q^2 = \frac{4C}{m}sin^2(\frac{qa}{2})$.
In other terms $\hat{H} = \sum_q \hat{H}_q$,

$$\hat{H}_q = \frac{1}{2m}\hat{p}_q\hat{p}_{-q} + \frac{1}{2}m\omega_q^2\hat{x}_q\hat{x}_{-q} \tag{47}$$

By the definitions of the $\hat{x}_q$ and $\hat{p}_q$ operators

$$\hat{x}_q^\dagger = \hat{x}_{-q}$$
$$\hat{p}_q^\dagger = \hat{p}_{-q}$$

This implies that:

$$\hat{H}_q = \frac{1}{2m}\hat{p}_q\hat{p}_q^\dagger + \frac{1}{2}m\omega_q^2\hat{x}_q\hat{x}_q^\dagger \tag{48}$$

Nice! *So?*

We have started with a many-body problem where the "bodies", the atoms, where coupled in their motion, now we have achieved a new description with different objects that have still an unspecified meaning[8]. However, for sure:
i) The q mode is independent of the others modes, and now the Hamiltonian is given by the sum over all the modes, before was over n.
ii) The meaning of this mode is a certain collective motion of all the particles.

Finally the following commutation relation can be proved, see Appendix C.

$$[\hat{q}_q, \hat{p}_{q'}] = i\hbar\delta_{q,q'} \tag{49}$$
$$[\hat{q}_q, \hat{q}_{q'}] = 0 \tag{50}$$

Completely out of the blue we introduce this operator:

$$\hat{a}_q = \sqrt{\frac{m\omega_q}{2\hbar}}(\hat{x}_q + \frac{i}{m\omega}\hat{p}_q) \tag{51}$$
$$\hat{a}_q^\dagger = \sqrt{\frac{m\omega_q}{2\hbar}}(\hat{x}_{-q} - \frac{i}{m\omega}\hat{p}_{-q}) \tag{52}$$

It is rather easy to prove that:

$$\hat{x}_q = \frac{\hbar}{2m\omega_q}(\hat{a}_q + \hat{a}_{-q}^\dagger)$$
$$\hat{p}_q = \frac{\hbar}{2m\omega_q}(\hat{a}_q - \hat{a}_{-q}^\dagger)$$

This easily bring to:

$$\hat{H} = \sum_q \frac{1}{2}\hbar\omega_q(\hat{a}_q\hat{a}_q^\dagger + \hat{a}_{-q}^\dagger\hat{a}_{-q})$$

By re-indexing, exploiting the silent fact that q is a sum over positive and negative values.

$$\hat{H} = \sum_q \frac{1}{2}\hbar\omega_q(\hat{a}_q\hat{a}_q^\dagger + \hat{a}_q^\dagger\hat{a}_q)$$

[8] Just legal math!

The two proprieties of this new two objects, that we will randomly call the creators and annihilators operators, is here reported:

$$[\hat{a}_q, \hat{a}^\dagger_{q'}] = \delta_{q,q'} \tag{53}$$

$$[\hat{a}^\dagger_q, \hat{a}^\dagger_{q'}] = 0 \tag{54}$$

This commutatators relations[9] that has come out naturally, is so far just a different and interesting way of rewriting the hamiltonian problem.[10]. We have a sum of a certain couple of operator[11], defined for every q-mode of motion of the 1D chain

$$\hat{H} = \sum_q \hbar\omega_q(\frac{1}{2} + \hat{a}^\dagger_q\hat{a}_q) \tag{55}$$

2.3 Phonons

After a very long path that have led to $\{\hat{x}_n, \hat{p}_n\} \rightarrow \{\hat{x}_q, \hat{p}_q\}$, we have this nice reformulation of the Hamiltonian. Now we need a strong imagination: We have decomposed the manybody-Hamiltonian in many many-body Hamiltonians but independent. We should not forget that we are talking about concrete entities! Hamiltonian is the energy operator, so these modes must be something particularly relevant! Now we claim, and later we will prove it, that:

- Each independent q-mode has as a solution, for $\hat{H}_q$, a quantized set of many-body wave-functions, that we define $|n_q\rangle$, each with an energy ϵ_q, the eigenstate

$$\epsilon_q = (\frac{1}{2} + n_q)\hbar\omega_q \tag{56}$$

  With n_q INTEGER!
  Therefore we claim that this n_q is the number of particles in the $q-th$ mode of collective oscillation, for the 1D chain.
- The generic eigenstate of the overall Hamiltonian can be written as the count over the number of excitations, the PHONONS, present in each of the independent q-modes. This is the so called Fock space or occupational number space. $|n_0, n_1, n_2, ..., n_q, ...n_{N-1}\rangle$.

The second quantization formalism has been naturally obtained from this kind of problem. In the vast majority of problems, is not that straightforward, there we will have to invent the proper set of creation and annhiliation operators, fixing, therefore, the Fock space.
If we want to go back to a spatial representation, is not that easy, but in principle can be done. One, however should remember the indistinguishability of the "particle", due to this request the wave-function became quite annoying to be written. At the end of the day, the vast majority of relevant proprieties can be obtained within the Fock space representation.

Let's prove the previous statement and let's wear the hat of the second quantization[12].

We want to prove that the energy eigenstates of a single q-mode exist in a discrete in number, this will justify the label of particle to an excitation:

[9] Proved in Appendix C

[10] Spoiler: We are prooving the existance of quantized excitation of a 1D chain that we will call phonons. These phonon are bosons, like photons... Because they are photons, after all!

[11] That now far relatives of the simple $\hat{x}_n$ and $\hat{p}_n$ operators

[12] It would be nice to jump into a long talk about Fock space, Bosons, Fermions and the profound implications of second quantization. This will be done in a compressed way in the next part. However, we do not have to forget our scope: To understand BCS, some we must faithfully believe that this new way of seeing a chain of N atoms is physically meaningful (Mathematically is ok).

We start by defining $\hat{N}_q = \hat{a}_q^\dagger \hat{a}_q$ as the number operator.
$\hat{N}_q = \hat{N}_q^\dagger$ so it is Hermitian, therefore it must have real eigenvalues. We **define** $|n_q\rangle$ as the eigenstate of $\hat{N}_q$.

$$\hat{N}_q |n_q\rangle = n_q |n_q\rangle \tag{57}$$

A part for $n_q \in \mathbb{R}$, we have no idea what could possibly be the value of the number operator applied of the mode q. We note from (55) that $[\hat{H}_q, \hat{N}_q] = 0$, this implies that $\hat{H}_q$ will share a common eigenstates set, $|n\rangle_q$ with $\hat{N}_q$. Therefore,

$$\hat{H}_q |n_q\rangle = (n_q + \frac{1}{2})\hbar\omega_q |n_q\rangle \tag{58}$$

Let's apply the following trick, if we calculate:

$$\hat{N}_q(\hat{a}_q |n_q\rangle) = (\hat{a}_q^\dagger \hat{a}_q)\hat{a}_q |n_q\rangle$$

We sum and subtract for the same quantity,

$$\hat{N}_q(\hat{a}_q |n_q\rangle) = (\hat{a}_q \hat{a}_q^\dagger + \hat{a}_q^\dagger \hat{a}_q - \hat{a}_q \hat{a}_q^\dagger)\hat{a}_q |n_q\rangle$$

Applying the commutation relation $[\hat{a}_q, \hat{a}_q^\dagger] = 1$

$$\begin{aligned}(\hat{a}_q \hat{a}_q^\dagger + \hat{a}_q^\dagger \hat{a}_q - \hat{a}_q \hat{a}_q^\dagger)\hat{a}_q |n_q\rangle = (\hat{a}_q \hat{a}_q^\dagger - 1)\hat{a}_q |n_q\rangle = \\ = \hat{a}_q \hat{a}_q^\dagger \hat{a}_q |n_q\rangle - \hat{a}_q |n\rangle_q = \hat{a}_q \hat{N}_q |n_q\rangle - \hat{a}_q |n_q\rangle\end{aligned}$$

Finally:

$$\hat{N}_q(\hat{a}_q |n_q\rangle) = (n_q - 1)\hat{a}_q |n_q\rangle \tag{59}$$

We have just proven something very important, $\hat{a}_q |n_q\rangle$, is still an eigenstate of both the Hamiltonian and $\hat{N}_q$, with eigenvalue one unity smaller. Analogously:

$$\hat{N}_q(\hat{a}_q^\dagger |n_q\rangle) = (n_q + 1)\hat{a}_q^\dagger |n_q\rangle \tag{60}$$

At this point we can freely claim that $\hat{a}_q^\dagger$ is creating a **state** in the q-mode with an eigenvalue of one unity bigger, and viceversa for the annihilation operator. If the $\hat{N}_q$ eigenvalue will be discrete in number and integer then the interpretation of "particle" will strongly hold. Before proceeding further let's find the normalization factor for the annihilation and creation operators:

$$\begin{aligned}|\hat{a}_q^\dagger |n_q\rangle = A_q |n_q + 1\rangle \qquad \hat{a}_q^\dagger |n_q\rangle|^2 = |A_q |n_q + 1\rangle|^2 \\ (\hat{a}_q^\dagger |n_q\rangle)^\dagger \hat{a}_q^\dagger |n_q\rangle = |A_q^2| \qquad \langle n_q| \hat{a}_q \hat{a}_q^\dagger |n_q\rangle = |A_q^2| \\ \langle n_q| \hat{a}_q \hat{a}_q^\dagger + \hat{a}_q^\dagger \hat{a}_q - \hat{a}_q^\dagger \hat{a}_q |n_q\rangle = |A_q^2| \\ 1 + n_q = |A_q|^2 \\ |\hat{a}_q |n_q\rangle = B_q |n_q - 1\rangle \qquad \hat{a}_q |n_q\rangle|^2 = |B_q |n_q - 1\rangle|^2 \\ (\hat{a}_q |n_q\rangle)^\dagger \hat{a}_q |n_q\rangle = |B_q^2| \qquad \langle n_q| \hat{a}_q^\dagger \hat{a}_q |n_q\rangle = |B_q^2| \\ n_q = |B_q|^2\end{aligned}$$

Finally,

$$\hat{a}_q^\dagger |n_q\rangle = \sqrt{n_q + 1}\, |n_q + 1\rangle \tag{61}$$

$$\hat{a}_q |n_q\rangle = \sqrt{n_q}\, |n_q - 1\rangle \tag{62}$$

We are almost there, if we impose that for our q-mode Hamiltonian there must be a ground state, below which, if we apply the annihilation operator, there cannot be energy.

$$\hat{a}_q \left|GROUND\right\rangle = 0 \tag{63}$$

This implies:

$$0 = \left|\hat{a}_q \left|GROUND\right\rangle\right|^2 = \left\langle GROUND\right| \hat{a}_q^\dagger \hat{a}_q \left|GROUND\right\rangle \tag{64}$$

But since $N_q = \frac{1}{\hbar\omega_q}\hat{H}_q - \frac{1}{2}$.

$$\left\langle GROUND\right| \frac{1}{\hbar\omega_q}\hat{H} - \frac{1}{2} \left|GROUND\right\rangle = \frac{1}{\hbar\omega_q} E_{ground} - \frac{1}{2} = 0 \tag{65}$$

Therefore,

$$E_{ground} = \frac{1}{2}\hbar\omega_q \tag{66}$$

Which means that our ground state correspond to $n_q = 0$ and every other state are defined with an integer number n_q. We can create any state starting from the ground and adding particles, and there is no upper limit on the number of particle we can create in our system. This justify the label number of particle in the q-mode, and thus, the whole concept of PHONONS!
Thanks to diagonalization of the Hamiltonian over the modes.
The most general state will be: $\phi = |n_1, n_2, n_3, ..., n_q, ..n_N\rangle$ This is an eigenstate of $\hat{H}$ with eigenvalue for energy:

$$E = \sum_q n_q \tag{67}$$

The phonons calculus is very pedagogical and will be used as a comparison with the more general case of N particles We stress one more time that the phonons Hamiltonian is a sum over the possible modes and not over the number of particles, that are in a unspecified number.

3 Second Quantization

We are close to the Cooper pair comprehension. Before, we just need to generalize the result obtained with the phonons to a generic many-body Hamiltonian.
Given a generic single particle operator $\hat{f}$, e.g. the kinetic energy of a single atom $\hat{p}_n$, we know that it will act on a single particle wave-function $|\varphi\rangle$ transforming it in a different object $|\phi\rangle$ that, in general, is no more normalized but still belong to the same space. This means that defined $|\psi_i\rangle$ a complete and orthonormal set in an Hilbert space[13] all single particle function can be described as a superposition of those. The action of $\hat{f}$ on a generic wave-function $|\phi\rangle$ belonging to the Hilbert space can be written as:

$$\hat{f} = \sum_{ij} f_{ij} \left|\psi_i\right\rangle \left\langle\psi_j\right| \tag{68}$$

With $f_{ij} = \langle\psi_i|\hat{f}|\psi_j\rangle$.
The proof is rather easy, once we rembember that $\phi = \sum_i c_i \left|\psi_i\right\rangle$, and $c_i = \langle\psi_i|\phi\rangle$:

$$\begin{aligned}\hat{f}\left|\phi\right\rangle &= \sum_i \langle\psi_i|\hat{f}\phi\rangle \left|\psi_i\right\rangle = \sum_i \langle\psi_i|\hat{f}\sum_j c_j \left|\psi_j\right\rangle\rangle \left|\psi_i\right\rangle \\ &= \sum_i \sum_j \langle\psi_i|\hat{f}\left|\psi_j\right\rangle\rangle \left|\psi_i\right\rangle c_j = \sum_i \sum_j f_{ij} \left|\psi_i\right\rangle \left\langle\psi_j|\phi\right\rangle\end{aligned}$$

In a problem with many identical particles, N, we can define the symmetric single particle many-body operator as:

$$\hat{F} = \sum_a^N \hat{f}_a \tag{69}$$

Note that $\hat{F}$ is an operator that act on a system on N particles. Obviously we expect that the total wave-function will be a many body $\Psi(r_1, r_2, ...r_N)$, with all the difficulties in writing it. The easiest function one can think of is a product among all the single particle wavefunctions. Each single particle wavefunction may be different from the others, but, at the end, they all belongs to the same space, defined with the same orthogonal and complete set $|\psi_i\rangle$ and that describe the single particle operator, $\hat{f}$, in the exact the same way[14]. As before we have defined an Hilbert space that describes all the possible configuration of a single particles, now, we claim that for the problem of N particle, it will exist a peculiar complete set of many-body wave functions that can be used to compose a generic state. This set can be regarded as a simple "count" of how many particles of the system are in which single particle state, described by $|\psi_i\rangle$. We call from now on, in analogy with the phonons, a single particle state as a "mode"[15].

$$|n_1, n_2, n_3, ..., n_M\rangle \tag{70}$$

Where M is the number of modes associated with the choice of the single particle set[16].
This space is called Fock space.
Apparently we have lost the information on the number of particles, we can recover it by imposing $\sum_n n_i = N$. It is rather annoying to always count the number of particle of the system we are describing. One might prefer to simply have a generic description that can suit a generic number of particle. That is the case:
Defined the creator and annihilation operator of a particle in the state $i-th$, with a precise effect on the occupation number that depends on the kind of particle we are describing and a precise relation among them. In the phonon case this abstraction was not necessary, everything come out quite naturally,

[13] It's a functional space where all possible wave-functions exist. If you prefer think to it as a space of peculiar functions that depends on space and time.
[14] This is the point of a symmetric operator.
[15] It will be a mode of the system described by a certain Hamiltonian if it is a eigenstate of the Hamiltonian itself.
[16] This is of course completely arbitrary, we can chose whatever orthonormal basis of the Hilbert Space

like the fact that they are bosons. Moreover, the number of modes was exactly equal to the number of original chain particles, and excitation consideration came out naturally. We **postulate** the many-body single particle operator as:

$$\hat{F}^{(1)} = \sum_{ij} f_{ij}^{(1)} \hat{a}_i^\dagger \hat{a}_j \tag{71}$$

The word postulate is the one that fits better the core of second quantization. We are inventing a different formalism to describe our quantum world. Obviously this new formalism is consistent with the old one,i.e. by starting from (74) and fixed N, we can always recover all the physics that we would have achieved with (69). For a two body operators, that involves an interaction between two particles, like the **Coulomb** potential, a similar argumentation follows.
After one has selected the proper set of single particle modes,ψ_i arbitrarily chosen, one can postulate that the many-body operator that describe all the possible particle-particle interaction can be written as:

$$\hat{F}^{(2)} = \sum_{ij\alpha\beta} f_{\alpha\beta ij}^{(2)} \hat{a}_\alpha^\dagger \hat{a}_\beta^\dagger \hat{a}_i \hat{a}_j \tag{72}$$

Where,

$$f_{ij\alpha\beta} = \langle \psi_\alpha \psi_\beta | \hat{f}^2 | \psi_i \psi_j \rangle \tag{73}$$

All the physics is in the matrix elements of both the single-particle operator and two-particle operator, at this point this can be regarded as a simple number obtained by a "simple" integration of spatial (and temporal) functions with an operator that act on space (and time), it's an expectation value. For instance if we are dealing with energy we can try to find a way to diagonalize the $f_{ij}^{(1)}$ by selecting the proper single function mode.

Now is the right time to divide fermions from bosons. Bosons are subjected to the following rules,

$$\hat{a}_i^\dagger |n_i\rangle = \sqrt{n_i + 1}\, |n_i + 1\rangle \qquad \hat{a}_i |n_i\rangle = \sqrt{n_i}\, |n_i - 1\rangle \tag{74}$$

$$[\hat{a}_q, \hat{a}_{q'}^\dagger] = \delta_{q,q'} \qquad [\hat{a}_q^\dagger, \hat{a}_{q'}^\dagger] = 0 \tag{75}$$

For fermions, due to the particle anti-symmetry to the exchange interaction,

$$\hat{a}_i^\dagger |1\rangle = 0 \qquad \hat{a}_i^\dagger |0\rangle = |1\rangle \tag{76}$$

$$\{\hat{a}_q, \hat{a}_{q'}^\dagger\} = \delta_{q,q'} \qquad \{\hat{a}_q^\dagger, \hat{a}_{q'}^\dagger\} = 0 \tag{77}$$

We are finally ready to describe the Cooper Pair!!

4 Cooper Pair

4.1 Second quantization of electron phonon interaction: effective Hamiltonian

Now, the rule of second quantization should be pretty simple:

- Pick a set of single particle wave-functions.
- Define the state of the system as a collection of occupation number of the single particle states
- Define the associated creation and annihilation operator, with a precise relation with the states, depending on the fact we are talking about fermions or bosons.
- Create a generic operator one-particle many body operator following (71) or two-particle many body operator (72)

In the initial section we have introduced an effective potential for the electron electron interaction in the metallic lattice.

$$V_{eff}(q,\omega) = \frac{e^2}{\epsilon_0(q^2+k_0^2)}(1+\frac{\omega^2(q)}{\omega^2-\omega^2(q)}) \tag{78}$$

Where q is the reciprocal space parameter of the electrons distance[17]. We can say that this V_{eff} is a electron electron interaction mediated by a phonon of momentum q and energy ω. This is not a proof, of course, but know we should accept this statement more easily. Our aim is to describe the external electrons and the lattice environment. The starting point is to define the effective Hamiltonian of the many body system. A reasonable model is:

$$\hat{H}_{eff} = \hat{T}_{kin} + \hat{V}_{crystal-field} + \hat{V}_{e-e-phonon} \tag{79}$$

Now we have to fix a single particle state from which construct the many body Hamiltonian. A choice could be the Bloch states:

$$\psi_{kn\sigma}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}u_{kn}(\mathbf{r})\chi_\sigma \tag{80}$$

Where k is the electron momentum, n is the band index, and χ_σ is the spinor. If we can somehow ignore the crystal field and write down just the kinetic energy term, with eventual correction. Then, another choice could be simply a plane wave:

$$\psi_k = \frac{1}{\sqrt{V}}e^{i\mathbf{k}\cdot\mathbf{r}}\chi_\sigma \tag{81}$$

V will be set to one in all the following discussion.
At this point, we have the modes in which our fermions can be put in. The multi-body state is a collection of $|k\sigma\rangle$, where due to the fermions nature of electron the occupation number can be whether 1 or 0. Therefore, we define $\hat{c}_{k\sigma}$ as the annhiliation operator of an electron in the state characterized by k and spin sigma, up or down, and analogously $\hat{c}^\dagger_{k\sigma}$.

$$\hat{H}_{eff} = \sum_{k\sigma}\epsilon_{k\sigma}\hat{c}^\dagger_{k\sigma}\hat{c}_{k\sigma} + \sum_{k_1\sigma_1,k_2\sigma_2,k_1'\sigma_1',k_2'\sigma_2'} V_{eph}\hat{c}^\dagger_{k_1\sigma_1}\hat{c}^\dagger_{k_2\sigma_2}\hat{c}_{k_1'\sigma_1'}\hat{c}_{k_2'\sigma_2'} \tag{82}$$

Where we are using the fact that the plane wave, free electron model, diagonalize the kinetic energy matrix. In particular,

$$\epsilon_{k\sigma} = \langle\psi_{k\sigma}(\mathbf{1})|\,\hat{H}_{free}\,|\psi_{k\sigma}(\mathbf{2})\rangle \tag{83}$$

$$V^{eff} = \langle\psi_{k_1\sigma_1}(\mathbf{1})\psi_{k_2\sigma_2}(\mathbf{2})|\,\hat{V}_{e-e-phonon}\,|\psi_{k_1'\sigma_1'}(\mathbf{1})\psi_{k_2'\sigma_2'}(\mathbf{2})\rangle \tag{84}$$

Where we have used the bold 1,2 to stress the right particle coordinate to be used once one perform the integrals. Performing (84) with the (78) potential, with the right adjustment it can be proved that the non null condition terms are the one that respect the following $k_1+k_2 = k_1'+k_2'$, momentum conservation. Moreover, associated the phonon momentum with q, we have $q = k_2 - k_1$, we can rewrite the potential as $(k_1+q),(k_2-q),(k1),(k2)$, which means we have only three degree of freedom on the possible particles k state involved in the interaction.

[17] The analogy with the phonons q mode parameter make sense, and holds!

4.2 An unusual couple of electrons

At this point, if we assume that:
i)$|\omega| < \omega_D|$ the energy associated with the electron is below the typical phonon frequency, e.g. take the maximum of the dispersion relation defined in (32). This bring to a negative potential!
ii) The q-dependency of the (34) is neglected.
iii) The spin is conserved in the interaction
Then, $V_{eff}^{k_1,k_2} = -|g_eff|^2$ we have a simplified model for the effective Hamiltonian.

$$\hat{H}_{eff} = \sum_{k\sigma} \epsilon_{k\sigma} \hat{c}^\dagger_{k\sigma} \hat{c}_{k\sigma} - |g_{eff}|^2 \sum_{k_1,k_2,q,\sigma} \hat{c}^\dagger_{k_1+q\sigma} \hat{c}^\dagger_{k_2-q\sigma} \hat{c}_{k_1\sigma} \hat{c}_{k_2\sigma} \tag{85}$$

This is the starting point of BCS, a strongly approximated model that see as the source of formation of stable Cooper pairs an exchange of a phonons that bonds the electrons. Our purpose is to find a ground state for a system of two electrons outside the Fermi sphere.
The last claim perfectly fits with the idea that have originated in section 1 the effective Coulomb interaction. Our two electrons are an external perturbation of a metal, originally at equilibrium.

To have a better understanding of the electron couple we will start with some old fashioned quantum mechanics consideration, after that we will use only occupation number representation of states. A generic two electron wave-function can be reasonably written as:

$$\psi(\mathbf{r}_1, \sigma_1, \mathbf{r}_2, \sigma_2) = e^{i\mathbf{K}_{cm}\cdot\mathbf{R}_{cm}} \varphi(\mathbf{r}_1 - \mathbf{r}_2, \sigma_1, \sigma_2) \tag{86}$$

Where $\mathbf{K}_{cm} = \frac{\mathbf{k}_1+\mathbf{k}_2}{2}$.
Since we are searching the ground state, then we can ask $K_{cm} = 0$. We will prove that this leads to a minimization of the total energy. Consider a two particle Hamiltonian, and the associated eigenvalue problem.

$$(-\frac{\hbar^2}{2m}\nabla_1^2 - \frac{\hbar^2}{2m}\nabla_2^2 + V(r_1 - r_2))\psi(\mathbf{r}_1, \mathbf{r}_2) = E\psi(\mathbf{r}_1, \mathbf{r}_2) \tag{87}$$

Defined $r = |r_1 - r_2|$ and $\mathbf{R} = \mathbf{r}_1 + \mathbf{r}_2$, $\mu = \frac{m}{2}$ reduced mass and M=2m. Then,

$$(-\frac{\hbar^2}{2\mu}\nabla_r^2 - \frac{\hbar^2}{2M}\nabla_R^2 + V(r_1 - r_2))\psi(\mathbf{r}_1, \mathbf{r}_2) = E\psi(\mathbf{r}_1, \mathbf{r}_2) \tag{88}$$

Furthermore by variable separation:

$$\psi(r, \mathbf{R}) = \varphi(r) e^{i\mathbf{K}_{cm}\cdot\mathbf{r}} \tag{89}$$

(88) in (87) leads to[18].

$$(-\frac{\hbar^2}{2\mu}\nabla_r^2 + V(r_1 - r_2))\psi(\mathbf{r}_1, \mathbf{r}_2) = \tilde{E}\psi(\mathbf{r}_1, \mathbf{r}_2) \tag{90}$$

$E = \tilde{E} + \frac{\hbar^2 K_{cm}^2}{2M}$, therefore E is minimized when $K_{cm} = 0$. Which means that $\mathbf{k}_1 = -\mathbf{k}_2 = \mathbf{k}$ Now we have to be more explicit on φ that at this point coincide with ψ, see (86). The main point is that we have to respect the exchange symmetry. Therefore,

$$\psi(\mathbf{r}_1, \sigma_1, \mathbf{r}_2, \sigma_2) = -\psi(\mathbf{r}_2, \sigma_2, \mathbf{r}_1, \sigma_1) \tag{91}$$

One last assumption has to be made on the spin configuration, we can assume, that the we will have anti-parallel spin configuration, this is a not well justified assumption, which means that we can find in

[18] It is essential that V(r) only, there we can use the variable separation.

nature ground state of the effective Hamiltonian in a parallel spin configuration. Now we are ready to write down the possible ground state for (85). Defined:

$$\psi_{k\uparrow}(1) = e^{i\mathbf{k}_1\cdot\mathbf{r}_1}\chi_\uparrow$$
$$\psi_{-k\downarrow}(2) = e^{i\mathbf{k}_2\cdot\mathbf{r}_2}\chi_\downarrow$$

The generic ground state will be a combination of all the possible couple[19] of free electron states, fixing the spin (91):

$$\psi(\mathbf{r}_1,\mathbf{r}_2) = \sum_{\mathbf{k}>\mathbf{k}_f}\varphi_k \begin{vmatrix} \psi_{k\uparrow}(1) & \psi_{k\uparrow}(2) \\ \psi_{-k\downarrow}(1) & \psi_{-k\downarrow}(2) \end{vmatrix} \tag{92}$$

Where φ_k are a set of parameter to be found, that will define our ground state!

In the Fock space representation we could have written everything in a more compact way:

$$|\psi\rangle = \sum_{\mathbf{k}>\mathbf{k}_f}\varphi_k\,|k\uparrow,-k\downarrow\rangle \tag{93}$$

Which means that we are considering all the possible couple of two electrons with opposite momenta, living outside the Fermi sphere, this hypothesis is reflected in a limitation on the sum over k. We impose, now, that we want to satisfy the eigenvalue equation so we impose that (93) is a solution of the $\hat{H}_{eff}$, (85). In the worst case the ground state will exist with an energy greater than the energy of the two independent particles. Let's exploit the Fock space for all the calculus.

$$\hat{H}_{eff}\,|\psi\rangle = E\,|\psi\rangle \tag{94}$$

Let's neglect the sum over the spins[20] and focus only on (93). Solving,

$$\hat{H}_{eff}\,|\psi\rangle = \sum_{k'}\sum_{k}\varphi_k\epsilon_{k'}\hat{c}^\dagger_{k'}\hat{c}_{k'}\,|k\uparrow,-k\downarrow\rangle - |g_{eff}|^2\sum_{k',q}\sum_{k}\varphi_k\hat{c}^\dagger_{k'+q}\hat{c}^\dagger_{-k'-q}\hat{c}_{k'}\hat{c}_{k'}\,|k\uparrow,-k\downarrow\rangle \tag{95}$$

$|k\uparrow,-k\downarrow\rangle$ is a two particle object associated already to the creation and annhiliation operator by construction (82), which means we have zero for all the other states, we can easily achieve:

$$\hat{H}_{eff}\,|\psi\rangle = \sum_{k}2\epsilon_k\varphi_k\,|k\uparrow,-k\downarrow\rangle - |g_{eff}|^2\sum_{k,1}\varphi_k\,|k+q\uparrow,-k-q\downarrow\rangle$$

Where we have used the fact that the kinetic energy $\epsilon_k = \epsilon_{-k}$, $\epsilon_k \propto k^2$. Then, to solve everything, we multiply[21] by $\langle\tilde{k}\uparrow,-\tilde{k}\downarrow|$. If one uses the orthogonality of the basis chosen then,

$$2\epsilon_{\tilde{k}}\varphi_{\tilde{k}} - |g_{eff}|^2\sum_{k}\varphi_k\,\langle\tilde{k}\uparrow,-\tilde{k}\downarrow|k+q\uparrow,-k-q\downarrow\rangle = E\varphi_{\tilde{k}} \tag{96}$$

Minding that,$\langle\tilde{k}\uparrow,-\tilde{k}\downarrow|k+q\uparrow,-k-q\downarrow\rangle = \delta_{\tilde{k},k+q}$ we finally end up with:

$$2\epsilon_{\tilde{k}}\varphi_{\tilde{k}} - |g_{eff}|^2\sum_{k'}\varphi_{k'} = E\varphi_{\tilde{k}} \tag{97}$$

Defined $C = \sum_{k'}\varphi_{k'}$, then we have found that the eigenstate**s** we are looking are defined by this general relation[22]:

$$\varphi_k = -C|g_{eff}|^2\frac{1}{E-2\epsilon_k} \tag{98}$$

[19] k, $-k$
[20] This molteplicity will not be lost but, we will recover it later on.
[21] Or integrate if you wish
[22] We are changing $\tilde{k}$ to k to spare notation.

At this point we ask for self consistency so if our eigenstates satisfies (100), then it must be als true that:

$$\sum_k \varphi_k = -C|g_{eff}|^2 \sum_k \frac{1}{E - 2\epsilon_k} \tag{99}$$

Since the left term is again C, this leads to:

$$1 = -|g_{eff}|^2 \sum_k \frac{1}{E - 2\epsilon_k} \tag{100}$$

To recap, we are searching for an eigenstate, the minimum possibly, made by two electrons that satisfy (94), with total energy that is smaller then the sum of the two kinetic energies. If this is the case, we have stability and we have proved the existence of a strange bonded couple. Let's solve for E, following the here reported steps:

- k must be always bigger than k_f beacause below we have the Fermi sea of electrons.
- Let's make the hypothesis that our energy reference is the Fermi energy $\epsilon_f = 0$ of the metal. So the total kinetic energy for a single electron is re-expressed as $\epsilon_k = \epsilon_f + \hbar\omega$.
- Assume also that the maximum energy is set by $\epsilon_k = \epsilon_f + \hbar\omega_D$, typical phonon frequency. This set the further hypothesis that our electrons, so the state we are evaluating, are very close to the Fermi sphere, energetically speaking. This implies that all the extra kinetic energy of this electrons can be easily interchange by a solid phonon.

(100) is nice but rather hard to solve, it is hard for us to take into account all the mentioned approximation with the 3D k-summation. The k-state are quantized due to boundary condition. In our discussion we wave set V=1, so we will keep that assumption on. The sum over the state on a sphere section with an energy ϵ_f and $\epsilon_f + \hbar\omega_d$ is equivalent to the integration over this region volume, d^3k, divided by the volume of a single state $\Delta k = \frac{V}{(2\pi)^3}$. After few easy steps[23], imposing that the energy $\epsilon_k = \frac{\hbar^2 k^2}{2m} - \epsilon_f$, we end up with:

$$1 = -|g_{eff}|^2 \int_0^{\hbar\omega_D} g(\epsilon) \frac{1}{E - 2\epsilon} d\epsilon \tag{101}$$

Where $g(\epsilon)$ is the energy density of state, per unit volume, V=1. Since we are close to the ϵ_f, $g(\epsilon) \approx g(\epsilon_f)$. This leads to:

$$1 = -|g_{eff}|^2 g(\epsilon_f) \int_0^{\hbar\omega_D} \frac{1}{E - 2\epsilon} d\epsilon$$
$$1 = -|g_{eff}|^2 g(\epsilon_f) \log \frac{E - 2\epsilon}{E}$$

Which leads to:

$$E = \frac{2\hbar\omega_D}{1 - e^{\frac{1}{|g_{eff}|^2 g(\epsilon_f)}}} \tag{102}$$

If we further assume that $|g_{eff}|^2 g(\epsilon_f) << 1$, which correspond to a weak interaction, but not too weak, for this reason it is fundamental the Fermi sea. Then:

$$E = -2\hbar\omega_D e^{-\frac{1}{|g_{eff}|^2 g(\epsilon_f)}} \tag{103}$$

This result is nice and we have succeed in our task. Indeed,

i) It exist a free electron solution for (94)
ii) The energy of this paired electron is lower than the sum of their individual energy, so they are bond and correlated

[23] That you can find in ANY solid state physics book

iii) The energy of this bond is below the Fermi sea! Which means that exist an extra bond state with energy lower than ϵ_f. This may lead us to suspect that the whole system of electrons in the solid is unstable since there is an higher energy configuration.

iv) This interaction is very weak and with a even a small fraction of thermal energy can be destroyed. Indeed, if estimate the Debye temperature $\frac{\hbar\omega_D}{k_b} \approx 100K$, and we give to the exponential an indicicative magnitude of $e^{-\frac{1}{|g_{eff}|^2 g(\epsilon_f)}} \approx \frac{1}{100}$, then the temperature, thermal energy, that allows the stable existence of this object are rather small $T_c \approx 1K$

We call this paired electrons, eigenstate of H_{eff} **Cooper pair**.

5 BCS Theory

Using the result of this Cooper pair problems BCS realized that there could exist an instability of the filled Fermi sea above the Cooper pair level. This could possibly lead to a creation of other Cooper pairs that want to enters in the previously discovered ground state. This of course makes sense only if the Cooper pair state can host more couple, like a Bose-Einstein condensate, where all the particle want to fill the ground state. Moreover, if that is the case, one may wonder which will be the many-body wave-function that best describe the final configuration. Now, after an introduction on the meaning of coherent state we will prove that:

- The many-body Cooper pair state exist and there are no limit on the number of pairs that can be put inside in this low energy state.
- The many-body wavefunction that best describes the eigenstate of the system is a coherent wave-function of Cooper pairs.
- A Cooper pair has a momentum greater than the k_f, but an energy that is lower ϵ_f

The core of BCS, was to invent a reasonable wave-function to be put in (94), an ansatz that worth of Nobel.

5.1 Coherent state

What is a coherent state?
In nature there exist conditions where a lot of particles pile into the same identical single particle state, this peculiar condition exist with some defined proprieties that holds in time and in space, showing a macroscopic behavior. A coherent state is, therefore, a macroscopic manifestation of quantum mechanics, it is a macroscopic object with quantum mechanics proprieties that hold in time. Technically speaking the state that satisfy this description arises as an eigenstate of the annihilation operator. Let's consider a problem with just one possible mode, for simplicity. Then,

$$\hat{a}\,|\alpha\rangle = \alpha\,|\alpha\rangle \tag{104}$$

This leads already to one observation, whatever $|\alpha\rangle$ will be, for sure the number of "particles" are something not well defined! Thanks to the completeness, and orthogonality of the Fock space we can define a generic many-body function as a sum over the possible states[24]:

$$|\alpha\rangle = \sum_n c_n\,|n\rangle \tag{105}$$

Plugging (105) into (104) we have,

$$\begin{aligned}
\sum_n c_n \hat{a}\,|n\rangle &= \sum_n \alpha c_n\,|n\rangle \\
\sum_{n=1} c_n \sqrt{n}\,|n-1\rangle &= \sum_{n=0} \alpha c_n\,|n\rangle \\
\sum_{n=0} c_{n+1} \sqrt{n+1}\,|n\rangle &= \sum_{n=0} \alpha c_n\,|n\rangle
\end{aligned}$$

Therefore,

$$c_{n+1} = \frac{\alpha}{\sqrt{n+1}} c_n \tag{106}$$

This is a recursive problem that has as solution:

$$|\alpha\rangle = c_0(|0\rangle + \frac{\alpha}{\sqrt{1!}}\,|1\rangle + \frac{\alpha^2}{\sqrt{2!}}\,|2\rangle + ...) \tag{107}$$

[24]This state are not random but must be coherent with the definition of the creation and annihilation operator

c_0 can be found imposing a normalization condition on $|\alpha\rangle$.

$$c_0 = e^{-\frac{|\alpha|^2}{2}}$$

At this point we rewrite the eigenstate as:

$$|\alpha\rangle = e^{-\frac{|\alpha|^2}{2}} \sum_n \frac{(\alpha \hat{a}^\dagger)^n}{\sqrt{n!}} |0\rangle \tag{108}$$

This is clear if we look carefully at (107). Just for a matter of notation, in many book the (108) is rewritten in terms of an exponential operator, the meaning of which is simply (108).

$$|\alpha\rangle = e^{-\frac{|\alpha|^2}{2}} e^{\alpha \hat{a}^\dagger} \tag{109}$$

Without entering in too much details; A coherent state have the following proprieties, given $\hat{n}$ the number operator:

1) $\langle \hat{n} \rangle = |\alpha|^2$
2) $\langle \hat{n}^2 \rangle = |\alpha|^4 + |\alpha^2|$
3) $\Delta n = \langle \hat{n}^2 \rangle - \langle \hat{n} \rangle^2 = |\alpha|$
4) In general α, that characterize fundamentally the propriety of our coherent state, is a complex number, $\alpha = |\alpha| e^{i\theta}$

So $\alpha = \sqrt{\langle \hat{n} \rangle} e^{i\theta}$, for a given problem, with a certain number of particle we have a degeneracy of the coherent state with respect the phase. Clearly a coherent state **is NOT** an eigenstate of the energy, if the system is made by only single particle operator. But, in the moment we have an interaction, e.g a two particle operator, it may happen that the coherent state become our eigenstate, which means that the many-body system may have as "stable"[25] state a coherent state.

[25] It will not be 100% stable because a system will collapse in a certain configuration with a certain defined phase. We are not going to discuss this fundamental details concerning phase-symmetry breaking.

5.2 A Coherent state of Cooper Pairs

Schrieffer, the S of the Nobel trio, thought that if a superconductive state exists then it must be made of the Cooper pairs discovered few years before. Moreover he assume that, these state must be written as a coherent state. Our aim is therefore to find a many-body eigenstate for the already written Hamiltonian[26]

$$\hat{H}_{eff} = \sum_{k\sigma} \epsilon_{k\sigma} \hat{c}^{\dagger}_{k\sigma} \hat{c}_{k\sigma} - |g_{eff}|^2 \sum_{k,-k,q,\sigma} \hat{c}^{\dagger}_{k+q\sigma} \hat{c}^{\dagger}_{-k-q\sigma} \hat{c}_{k\sigma} \hat{c}_{-k\sigma} \tag{110}$$

Since the main characters are the Cooper Pair, on good idea might be to define creator and annhiliation operator for this new objects. Therefore,

$$\hat{P}_k = \hat{c}^{\dagger}_{k\uparrow} \hat{c}_{-k\downarrow} \tag{111}$$

Now, let's generalize the definition of coheren state, previously introduced:

$$|\alpha\rangle = const e^{\alpha a^{\dagger}} |0\rangle$$

Now, in analogy we define our Ψ_{BCS} as:

$$|\Psi_{BCS}\rangle = const e^{\sum_k \alpha_k P^{\dagger}_k} |0\rangle \tag{112}$$

We are evaluating, already, the presence of many possible modes, where the particle could be set in. Moreover, the state $|0\rangle$ is the condition where all the particle lies inside the Fermi sphere and no electron are allowed to have a k greater that k_f. If we carefully look at the commutators of P_k operator we may discover some relevant and meaningful proprieties:

i) $[\hat{P}_k, \hat{P}^{\dagger}_k] \neq 1$ which means that Cooper pairs are not really bosons, neither fermions.
ii) $[\hat{P}^{\dagger}_k, \hat{P}^{\dagger}_{k'}] = 0$, which respect, instead, bosons commutation rules.

We stress the fact that $[\hat{P}^{\dagger}_k, \hat{P}^{\dagger}_k] = 0$ because the single electron is still a fermion and therefore we cannot create two particle with the same exact k, we can generalize this fact by saying that $(P^{\dagger}_k)^n = 0 for n > 1$. This implies that:

$$|\Psi_{BCS}\rangle = const e^{(\sum_k \alpha_k P^{\dagger}_k)} |0\rangle = const \prod_k e^{\alpha_k P^{\dagger}_k} |0\rangle = const \prod_k (1 + \alpha_k \hat{P}^{\dagger}_k) |0\rangle$$

We would like to stress the difference between the wave function that we have used to prove the existance of Cooper pairs and this one.

$$|\psi\rangle = \sum_{\mathbf{k}>\mathbf{k}_f} \varphi_k |k\uparrow, -k\downarrow\rangle \tag{113}$$

$$|\Psi_{BCS}\rangle = const \prod_k (1 + \alpha_k \hat{P}^{\dagger}_k) |0\rangle \tag{114}$$

The former is clearly a superposition of two particles state, that sometimes are called Cooper pair, while $|\psi\rangle$ is the Cooper pair state. The latter, instead, is a superposition of an indefinite number of cooper pairs, put in different k states, but still describing a unique many body state. What is left to do is to prove that this many body function can became an eigenstate of $\hat{H}_{eff}$ and minimize the energy. This can be done by putting everything inside the $\hat{H}_{eff}$, and once we have normalized $|\Psi_{BCS}\rangle$, we go for a parameter minimization. This is practically speaking is a variational approach, that leads to correct information about the ground state energy, more then the wavefunction. However, we could guess that

[26] Here, should be clear why a many body formulation is necessary. You don't have to fix the number of particles, and you can use it for one couple as well for N couples of particles.

with this approach we would get pretty close to the right one. So, if it exists a state like (114) leads to a negative energy, like in the cooper pair state, this implies that this configuration can exist. Unfortunately, we will skip the calculations for this minimization, these can be found in any superconductivity book. The main point is, once you have normalized $|\Psi_{BCS}\rangle$

$$|\Psi_{BCS}\rangle = \prod_k (u_k^* + v_k^* \hat{P}_k^\dagger)\,|0\rangle \tag{115}$$

Where $u_k^* = \frac{1}{1+|\alpha_k|}$,$v_k^* = \frac{\alpha_k}{1+|\alpha_k|}$. We can find that:

$$E = \langle \Psi_{BCS}|\hat{H}_{eff}|\Psi_{BCS}\rangle = 2\sum_k \epsilon_k |v_k|^2 - |g_{eff}|^2 \sum_{k,k'} v_k v_{k'}^* u_k u_{k'}^* \tag{116}$$

After the minimization and consideration on the sum of states similar at the one made before for the Cooper state:

$$E_{tot} = -2g(\epsilon_f)(\hbar\omega_D)^2 e^{-\frac{2}{g(\epsilon_f)|g_{eff}|^2}} \tag{117}$$

The stability of this BCS coherent state, depends with a similar law of the Cooper pair one. One final remark is on the band gap Δ that can be found between this nice ground state and the first excited state. Following all the calculus, in can be found that this Δ is exactly the energy of the single Cooper Pair state.

$$\Delta = -2\hbar\omega_D e^{-\frac{1}{g_{\epsilon_f}|g_{eff}|^2}} \tag{118}$$

A Coherent State of Cooper Pairs exists as a ground state of the many-body problem.

6 Conclusion

So that's it!
We have now, almost, understood all the basic block that leads to a more easy way to approach the topic on superconductivity. We are still far from the proof of all the proprieties of a superconductor, but at least we have made sense of the main character of the discussion. One important message that I want you to leave with message: Physics is easy, once you have understood the starting point of the discussion, what are the postulates and what are the models. Of course the hiking is long, but at the end the view is breathtaking, and the path doesn't look so hard. What is less easy is the Math that one has to face if we wants to claim something practical, and to find reasonable model to build a physical description of something.

From my point of view I'm still far from the comprehension of superconductivity, but at least, now, I know where to start if ever I would like to follow more advanced discussion.

The full comprehension of the superconductivity as a phenomena in general has not been achieved completely yet. Indeed, there is an almost accurate comprehension of the low temperature superconductor, thanks to BCS, but there is a lack of fundamental comprehension on the high temperature superconductor, a good theoretical description is still missing at the moment.

A Appendices

A.1 Appendix A: Potential in k-space

Consider then a $V(k) = \frac{1}{k^2+a^2}$, with a generic parameter. Then,

$$I(a, \mathbf{r}) = \int_{-\infty}^{+\infty} \frac{1}{(2\pi)^3} \frac{1}{k^2 + a^2} e^{+i\mathbf{k}\cdot\mathbf{r}} d^3k \tag{119}$$

In spherical coordinates $d^3k = k^2 sin\theta d\theta d\varphi$.

$$I(a, \mathbf{r}) = \frac{2\pi}{(2\pi)^3} \int_0^{\pi} d\theta \int_0^{+\infty} dk\, k^2 \frac{\sin(\theta)}{k^2 + a^2} e^{ikr\cos(\theta)} \tag{120}$$

$$\tag{121}$$

Few simple calculus leads to:

$$I(a, \mathbf{r}) = \frac{1}{2\pi} \frac{1}{r} \int_{-\infty}^{\infty} dk \frac{k}{k^2 + a^2} \sin(kr) \tag{122}$$

Here the trick: $I(a, \mathbf{r})$ is the immaginary part of the generalized:

$$\hat{I}(a, \mathbf{r}) = \frac{1}{2\pi} \frac{1}{r} \int_{-\infty}^{\infty} dk \frac{k}{k^2 + a^2} e^{ikr} \tag{123}$$

This one can be solved with the residual, observing that the singularity is in $+ia$, we can invent a path around, legitimized by the decay of e^{ikr} in the imaginary plane of k.
This leads to:

$$\hat{I} = 2\pi i Res[\frac{ia}{(ia)^2 + a^2} e^{(} - ar))] = i\frac{1}{2\pi} \frac{1}{r} e^{-ar}\pi \tag{124}$$

This is a purely imaginary number, therefore:

$$I(a, \mathbf{r}) = \frac{1}{4\pi r} e^{-ar} \tag{125}$$

A.2 Appendix B: Discrete Fourier Transform

Consider a sequence of N complex number a_n. We define for them the discrete Fourier transform as the following operation.

$$\tilde{a}_k = \frac{1}{\sqrt{N}} \sum_{n=0}^{N-1} a_n e^{-ikn\frac{2\pi}{N}} \tag{126}$$

And its inverse rule:

$$a_n = \frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} \tilde{a}_k e^{+ikn\frac{2\pi}{N}} \tag{127}$$

Let's prove that this definition is self consistent, i.e. we want to see if applying in circle the two transformation we recover the a_n. Note that k and n are just integer numbers.

$$\begin{aligned} a_n =& \frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} (\frac{1}{\sqrt{N}} \sum_{n'=0}^{N} a_{n'} e^{-ikn'\frac{2\pi}{N}}) e^{+ikn\frac{2\pi}{N}} = \\ =& \frac{1}{N} \sum_{k=0}^{N-1} \sum_{n'=0}^{N-1} a_{n'} e^{-ik(n'-n)\frac{2\pi}{N}} \end{aligned}$$

This object can be divided in two terms n=n' and otherwise. If n=n' the exponential is equal to one for every k. Otherwise we have a geometric series $\sum_{n=0}^{N-1} x^n = \frac{1-x^N}{1-x}$ with $x < 1$ Therefore:

$$a_n = a_n + \frac{1}{N} \sum_{n'=0, n' \neq n}^{N-1} a_{n'} \frac{1 - e^{-i2\pi(n-n')}}{1 - e^{-i(n'-n)\frac{2\pi}{N}}}$$

But $e^{-i2\pi(n-n')} = 1$ then, we the self consistency is proved. We have proved that the DFT behave properly and also we have proved a sort of orthogonality.

$$\delta_{nn'} = \sum_{k=0}^{N-1} e^{-ik(n'-n)\frac{2\pi}{N}} \tag{128}$$

It can be proved that one can define a re-centered DFT by changing the sum on k. However, we must be careful to choose integer numbers. so if N is odd $k = [-\frac{N-1}{2}, \frac{N-1}{2}]$, while for N even $k = [-\frac{N}{2} + 1, \frac{N}{2}]$. Provided this then we write, take N odd:

$$\tilde{a}_k = \frac{1}{\sqrt{N}} \sum_{n=0}^{N-1} a_n e^{-ikn\frac{2\pi}{N}} \tag{129}$$

And its inverse rule:

$$a_n = \frac{1}{\sqrt{N}} \sum_{k=-\frac{N-1}{2}}^{\frac{N-1}{2}} \tilde{a}_k e^{+ikn\frac{2\pi}{N}} \tag{130}$$

This different notation have different advantages, for example with real numbers.

A.3 Appendix C: Commutation relation for phonons

Let's prove some commutation relation. We will start from $[\hat{x}_q, \hat{p}_{q'}]$:

$$[\hat{x}_q, \hat{p}_{q'}] = \hat{x}_q\hat{p}_{q'} - \hat{p}_{q'}\hat{x}_q = \\ = \frac{1}{N}\sum_{nn'} \hat{x}_n\hat{p}_{n'}e^{-iqna}e^{-iq'n'a} - \frac{1}{N}\sum_{nn'} \hat{x}_{n'}\hat{p}_n e^{-iqna}e^{-iq'n'a}$$

From the original meaning of the space and momentum operator, basic quantum mechanics, we know $[\hat{p}_n, \hat{x}_{n'}] = -i\hbar\delta_{nn'}$:

$$[\hat{x}_q, \hat{p}_{q'}] = \frac{1}{N}\sum_{n}(\hat{x}_n\hat{p}_n - \hat{x}_n\hat{p}_n)e^{-iqna}e^{-iq'na}$$

$$[\hat{x}_q, \hat{p}_{q'}] = \frac{i\hbar}{N}\sum_{n}(\hat{x}_n\hat{p}_n - \hat{x}_n\hat{p}_n)e^{-i(q+q')na}$$

From the usual DFT orthogonality:

$$[\hat{x}_q, \hat{p}_q] = i\hbar\delta_{k,-k'} \tag{131}$$

(...)