

Brief Introduction to Superconductivity

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0.1 Preface

Part I

**Conventional
Superconductivity**

Chapter 1

Discovery and first insights

1.1 The lost of the resistivity

In 1908, Onnes found the way to liquify helium and to reach temperatures as low as $4K$. In 1911, he discovered that below a temperature of the order of $4K$, Hg loses the resistivity. His discoveries lead him to realize that he was in the presence of a new state of solid mater. He could establish that when a certain magnetic field than depends on temperature, the critical field, $H_c(T)$, was applied, the normal properties of the metal were recovered. Also a critical current, $j_c(T)$, could have the same effect. He called the new phenomenon, superconductivity.

Superconductivity is a state of metals below a certain critical temperature [1]. Heavily doped semiconductor can become superconducting as Ge or Si. Nor the noble metals (Cu,Ag,Au) neither the alcalins (Li, Na, K, Rb, Cs, Fr) present a superconducting phase transition at least above a few milikelvins. In general, good conductors are not good superconductors (meaning that they do not have high critical temperatures). The number of conducting electrons in a metal is of the order of 10^{22} per cm^3 . In a semiconductor at room temperature these are of the order of 10^{15} and in a heavily doped semiconductor this number (in the same units) is around 10^{18} .

Un superconductor is characterized first by its critical temperature, T_c . For conventional superconductors it is very low. The highest T_c ($\sim 23K$) was found in Nb_3Ge (a compound) which was fabricated for the first time in 1973.

1.2 A superconductor is not a perfect conductor

The first idea that one can have is that a superconductor, a material that losses all its resistivity, is a perfect conductor, that is to say, it is a material with infinite conductivity. By using Ohms law, since the current is finite, the electric field has to be zero. By using Maxwell equations one gets further that the magnetic induction has to be a constant in time.

$$\dot{B} = 0 \quad B = \text{constant} \quad (1.1)$$

This conclusion has very serious implications since it actually means that the superconducting state is not an equilibrium state but it is a metastable state. For such a state the laws of thermodynamics and statistics do not apply. Let's summarize briefly how one can arrive at this conclusion by analyzing two thought experiments.

First experiment (only magnitudes are considered). Let us have a metal that becomes superconductor below T_c , the critical temperature of the superconducting phase transition. The sample is first at a temperature $T = T_1$ which is higher than T_c . At this moment a magnetic field¹, H_1 , is switched on and induces a magnetic induction into the material equal to, say, B_1 , which is different from zero. The sample is in the normal state, since $T_1 > T_c$. We summarize the situation in 1.2.

$$T = T_1 > T_c \quad H = H_1 < H_c(T_2) \quad \implies \quad B(T_1) = B_1 \neq 0 \quad (1.2)$$

At a second step, the sample is cooled down to a temperature $T = T_2 < T_c$ (the sample is in the superconducting state) low enough that the critical field for that temperature is higher than H_1 and therefore the sample remains in the superconducting state. According to Eq. 1.1, the magnetic induction should remain constant in the superconducting state. For that reason $B = B_1$ (**which is different from zero**) at the temperature T_2 where the sample is in the superconducting state. This second step is summarized in 1.3

$$T = T_2 < T_c \quad H = H_1 < H_c(T_2) \quad \implies \quad B = B(T_2) = B_1 \neq 0 \quad (1.3)$$

This concludes the first experiment.

Second experiment. We will do essentially the same but in reverse order. So, we have a metal at a temperature $T = T_1$ which is higher than T_c . But now, no field is applied as shown in 1.4

$$T = T_1 > T_c \quad H = 0 \quad \implies \quad B(T_1) = 0 \quad (1.4)$$

Now let us cool the sample down into the superconducting state to the same temperature $T = T_2 < T_c$. Eq. 1.1 tells us that the magnetic induction remains constant and therefore in this case $B(T_2) = 0$:

$$T = T_2 < T_c \quad H = 0 \quad \implies \quad B(T_2) = \text{const.} = 0 \quad (1.5)$$

Now, as a final step, we switch on the magnetic field to the same value $H_1 < H_c(T_2)$. The sample remains in the superconducting state and again by

¹This magnetic field has a lower intensity than the critical magnetic field at T_2 . The meaning of this condition will be evident in what follows.

1.2. A SUPERCONDUCTOR IS NOT A PERFECT CONDUCTOR⁵

Eq 1.1 the magnetic induction remains constant. Therefore, we finally have the following situation 1.6

$$T = T_2 < T_c \quad H = H_1 < H_c(T_2) \quad \implies \quad B = 0 \quad (1.6)$$

So the conclusion is that **if we assume that a superconductor is a perfect conductor**, we get to a situation where from an identical initial state, *i.e.*, a metal at $T = T_1 > T_c$, which we want to cool into the superconducting state and submit to a magnetic field weaker than the critical one, we end with two different values for the magnetic induction depending on the way we get the sample to the final state. When the final state depends on "the history" the final state is not an equilibrium state but it is rather a metastable state. In 1933, it was discovered that in every situation independently of the history of the sample, the magnetic induction is excluded from the sample in the superconducting state. In that year, Meissner and Ochsenfeld demonstrated that, in any circumstance, the magnetic induction in a superconductor is zero (**The Meissner effect**):

$$B = 0 \quad (1.7)$$

But if a superconductor is not a perfect conductor, what is it then?

Chapter 2

The physics of the Cooper pairs.

I will not mention any of the intermediate efforts made to come to this conclusion. They are indeed very inspiring and interesting but I want to stay on the level of a brief introduction to the main ideas of superconductivity. So I omit them.

2.1 What is superconductivity?

Superconductivity is the physics of the Cooper Pairs. A Cooper pair is a bound state of two electrons. Electrons repel each other in vacuum but under certain circumstances when in a crystal lattice they can attract each other and form a Cooper pair. Electrons have spins. Spin is a number (a quantum number) that characterizes the response of the electrons to a magnetic field and more importantly it characterizes the way in which they behave at very low temperatures, that is to say the statistics. Electrons have spin, $S = 1/2$. They are called fermions. Actually any particle with half integer spin number is called a fermion. A particle with an integer spin (0, 1, 2,...) is called a boson. Fermions and bosons behave differently at low temperatures. Electrons react in two different ways to a magnetic field. In general a fermion reacts in $2S+1$ different ways to a magnetic field. To distinguish them we speak about spin up (or $s = +1/2$) and spin down (or $s = -1/2$) electrons. We call "small s", the projection of the electron spin, S. Electrons at low temperatures behave in such a way that each electronic state (a solution of the Schrödinger Equation, the main equation of Quantum Mechanics), can be occupied by only one electron. This can also be stated as follows: no two electrons are allowed in the same state. This statement is referred to as **The Pauli Principle**. On the contrary, the number of bosons in a particular state is not limited.

2.2 What are the possible states of an electron?

How can we know what are the possible states that a metal electron can occupy? Of interest to us are metals since superconductivity appears in a metallic regime. We will consider crystals. These are periodic arrangements of ions of a certain symmetry (the corners of a cube, for example) with electrons traveling within the space between the ions in all possible directions. The periodic arrangement in real space defines the crystal lattice. A cubic lattice is defined with one single parameter, the length of the side of the cube. Would the lattice be tetragonal, we would need more parameters. Once the lattice is known, a potential with the same symmetry can be defined. This is all that is needed as input to the Schrödinger equation. The problem of solving it is not at all trivial. There are several methods known nowadays to solve this equation. Ready-to-use codes are offered in the literature. The different states that the electrons can be in, given a certain lattice, are obtained as output of these programs. You need an expression for the potential to be inserted into the Schrödinger equation for the element that you want to calculate. You can have the solution for Vanadium, for Niobium, etc... An approximate although very useful method to get the allowed states or the electronic band structure as it is customary to say, is the tight-binding method which is described with the necessary input parameters at the web site of Papaconstantopoulos¹. The states (the band structure) are described in terms of a vector crystal momentum, \mathbf{k} , and an energy, $\epsilon_{\mathbf{k}}$. Each of the electrons existing in the material, say in vanadium, for example, can occupy one state ($\mathbf{k}, \epsilon_{\mathbf{k}}$). The vector crystal momentum, \mathbf{k} , is defined in the reciprocal space. The three-dimensional interval where this vector is defined in such a way that there is no double counting of the allowed electronic states is called the **First Brillouin Zone** (FBZ). Some points of the FBZ are of particular interest because Group Theory applies there. They are called "high-symmetry points". Group theory [?] is a mathematical discipline that teaches us how to take advantage of symmetries to simplify our calculations.

So, in conclusion, the states allowed for the electrons in a particular metal are described by the vector crystal momentum, \mathbf{k} , and the corresponding energy, $\epsilon_{\mathbf{k}}$. These are solutions of the quantum mechanics main equation (the Schrödinger equation) given the corresponding potential. The solutions are given as "electronic band structures". In Fig.2.1, we show a crystal lattice called body centered cubic (bcc). Vanadium is a metal that has this crystal structure. In Fig. ?? its reciprocal lattice and its FBZ are shown for illustration.

To each value of $(\mathbf{k}, \epsilon_{\mathbf{k}})$, we can assign two electrons, since one can have spin up and the other spin down which results in two different states. This difference is not usually taken into account in the electronic band structure when the material is not magnetic. In this case, the same energy is assigned to both electronic states. We say that there are degenerate.

¹www. OJO OJO OJO

2.2. WHAT ARE THE POSSIBLE STATES OF AN ELECTRON?9

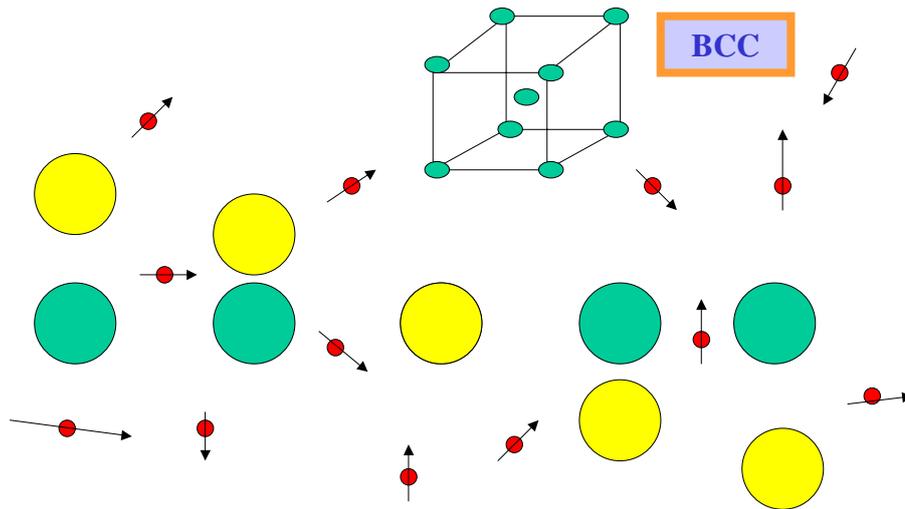


Figure 2.1: In the top of the figure we see a periodical arrangement of atoms called body centered cubic (bcc). Metals like Vanadium (V) or Niobium (Nb) have this structure. The ions are located on the corners of a cube and at the intersection of its main diagonals. Below this cube we see a chain of ions at their equilibrium position (dark circles). As they vibrate (light circles), they built up a wave that travels along the chain while the vibrations occur perpendicular to it (transverse waves: two modes). The ions could vibrate along the chains as well (longitudinal waves: one mode). This modes have momentum and energy are called a vibrational states. The arrows represent the electrons (small circles) that move in all directions in the free space left by the ions.

2.3 The Fermi energy

Imagine a staircase and a finite number of persons (less than the number of steps in the staircase). You want at most one person on each step. Since the staircase has more steps than there is people, some person would be at the highest occupied step. If you wanted a particular person to move one step upstairs keeping the rule that at most one person stands at each step of the staircase, then you would be in trouble. The reason is that the step above every person is occupied and therefore nobody can move. There is one exception though: the person at the highest occupied step. He can move without breaking the rule "at most one person on each step". This makes this position of particular interest since the same thing happens with electrons because they are fermions. If you want to give energy to an electron so that it "jumps" to a higher energetic level, you have to watch out because it is not always possible. But in this case as well, there is a highest occupied energy level, called the **Fermi energy**, ϵ_F . Since the vector crystal momentum is in a three dimensional space, it is enough that two differ in direction only to represent a different state. For that reason these states are drawn in a three dimensional space and the Fermi energy determines actually a surface in the crystal momentum space (which is the reciprocal space to the real one) called the **Fermi surface**. The electrons at the Fermi surface can accept energy from outside (laser light, for example) to jump to a more energetic state as long as it is enough to reach the next energy state (to move to the next step in the stairs you need to climb a minimum height). For that reason these electrons are the most active when the metal interchanges energy with an external source.

The Fermi distribution function, $f(\epsilon, T)$, gives the probability that at a certain temperature T , a state of a fermion with energy, ϵ , is occupied. At $T = 0K$, as we already mention, this function is 1 for energies below ϵ_F , since all the states below the Fermi energy are occupied, and zero above it (all unoccupied). For any temperature, the **Fermi distribution function** is

$$f(\epsilon, T) = \frac{1}{e^{\frac{\epsilon - \epsilon_F}{k_B T}} + 1} \quad (2.1)$$

In the limit $T \rightarrow 0$, for $\epsilon > \epsilon_F$, $f(\epsilon, T)$ (Eq. 2.1) goes to 0 and for $\epsilon < \epsilon_F$, it goes to 1. Notice that when $T > 0K$, a probability tail appears above ϵ_F and therefore the fermions have access to states above this energy. At higher energies this tail converges to the known classical Boltzman distribution function.

2.4 What is a Cooper Pair?

A Cooper pair is a bound state of two electrons with energy at the Fermi surface and spin and vector momentum of opposite sign. Cooper pairs can be formed from electrons having parallel spins (triplet state) but we will be dealing with the

2.5. HOW CAN TWO ELECTRONS FORM A COOPER PAIR? 11

very common case of singlet pairing (antiparalel spins or spin of opposite signs). So, a Cooper pair is a bound state of two electrons, one in the state $(\mathbf{k}, \epsilon_{\mathbf{k}}, \uparrow)$ and the other in the state $(-\mathbf{k}, \epsilon_{\mathbf{k}}, \downarrow)$. Below a certain **critical temperature**, T_c , a phase transition occurs to the electrons that are allowed to travel through the space formed by the regular arrangement of ions. In this new phase, the supeconducting state, they arrange themselves into Cooper pairs. And the consequences of it are tremendous. Several properties change and some of these properties have very interesting technological applications.

2.5 How can two electrons form a Cooper Pair?

This was at the origin Cooper's idea [?]. Cooper considered a non-interacting Fermi gas at $T = 0K$ so that all the states are filled up to the Fermi level. The electron energy is $\epsilon_{\mathbf{k}} = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$, then the Fermi surface will be an sphere of radius $k_F = \frac{\sqrt{2m\epsilon_F}}{\hbar}$. All the states with $k < k_F$ will be occupied. To this Fermi gas two electrons are added. They occupy, obviously, states such that $k > k_F$ (Pauli principle). Then Cooper had assumed that a net attraction, U , of whatever origin exists between the two electrons when their energy does not exceed a certain maximum from the Fermi energy or up to a certain cutoff energy, say ϵ_c . The electron-electron attraction scatters a pair of electrons with momentum $(k, -k)$ to another state $(k', -k')$. U was assumed to be independent of k : $U = U_0$ (weak coupling) within the energy interval $\epsilon_F \pm \epsilon_c$ and zero everywhere else. Cooper showed that even if both electrons have $k > k_F$, they will have a bound state below $2\epsilon_F$. This bound state is called a **Cooper pair**.

2.6 Superconductivity

John Bardeen realized that Cooper's idea might be key to superconductivity. The point is then how the attraction occurs?

It turns out that the critical temperature of a superconductor changes when only the mass of the ion in the lattice is changed while the rest remains exactly the same. How can that be done experimentally? Easily, just by changing an atom by its isotope. And the experiment says that

$$T_c \approx M^{-\frac{1}{2}} \quad (2.2)$$

This is called the "Isotope Effect". What can we learn from this formula? It turns out that the experiment also says that the critical temperature is proportional to typical frequency of oscillation of the ions around their equilibrium positions.

$$T_c \approx \omega \quad (2.3)$$

We can assume that such an ion moves as a small sphere of mass M at the end of a spring characterized by a spring constant K . The model can be solved as a classical harmonic oscillator, that is a system where a force, F , equal to $-Kx$ (it always points against the displacement from the equilibrium position x) is applied to an object of mass M . The mathematical solution of this problem teaches us that the frequency of oscillation of the mass M around its equilibrium position is $\omega_{osc} = \sqrt{\frac{K}{M}}$. We get therefore the appealing result

$$\omega_{osc} \approx M^{-\frac{1}{2}} \quad (2.4)$$

suggesting that superconductivity and the oscillations of the ions in the lattice have something in common.

2.7 Vibrational states and phonons

The ions in the lattice vibrate around their equilibrium position. Due to their mutual interaction they do not vibrate independently. While vibrating around their equilibrium positions, they build up a wave that travels along the lattice (see Fig.1). This is called a **vibrational state of the lattice**. These waves are characterized by a wave momentum, \mathbf{Q} , and an energy $E_{\mathbf{Q}}$. Actually, in general, there are several vibrational states allowed in one crystal. They differ in energy and momentum. When an electron interacts with a lattice, the lattice changes from a vibrational state to another. The electron takes or gives the difference in energy and momentum, between the two vibrational states, since both quantities have to be conserved. The difference in energy and momentum between two vibrational states is called a **phonon**. A phonon has therefore energy, $\varepsilon_{\mathbf{q}}$, and momentum, \mathbf{q} . Since it is not exactly a particle but dynamically (in the sense that it has energy and momentum) it behaves like one, it is called a **quasiparticle**.

And now the question is whether a phonon can supply the attraction to form a Cooper pair. The answer is yes but possibly this could only apply to **conventional superconductors**.

In the Fig.2.2, we see a cartoon representation of this attraction that helps us build up a first image of what a Cooper pair is and how it is formed. An electron (say electron 1) causes through its coulomb attraction that the ions around (the ones forming the lattice) move towards its position slightly. This is called a **polarization**. But then the region around electron 1 would be more positive than it is in equilibrium creating an attraction potentials towards this site. This potential results in an attraction for electron 2 that feels the potential created by electron 1. Since electrons travel in the lattice, electron 1 will not stay a long time at this position but will travel along the lattice creating a polarization wave along its path that will be followed by electron 2. Notice that by polarizing the lattice, electron 1 gives to it some energy and momentum and electron 2 by accelerating itself in the potential that is built during a certain amount of time around position 1, takes back this momentum and this energy

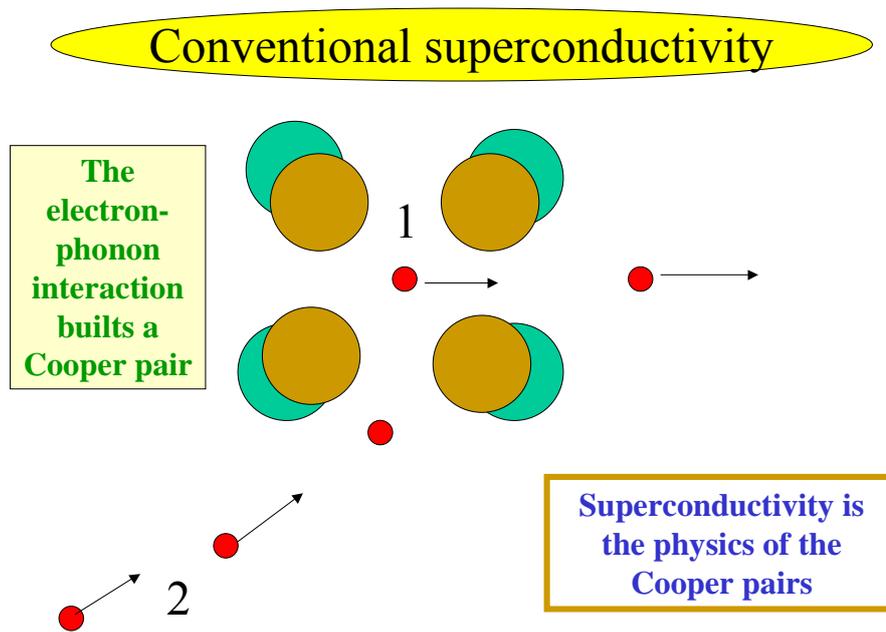


Figure 2.2: The polarization induced by the electron 1 constitutes an attraction potential for the electron 2. This correlation is called a Cooper pair.

Superconductivity is the physics of a system of Cooper Pairs. 

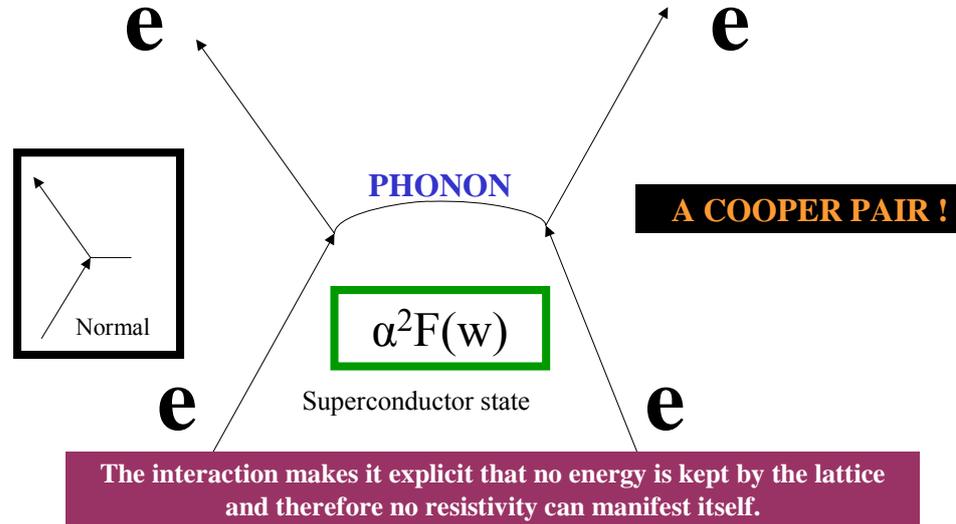


Figure 2.3: This way of representing things will be related to a Feynmann diagram later on (see text for the explanation).

so that the lattice does not retains any. This phenomenon can be conveniently represented by means of Fig. 2.3 as follows.

The lattice interchanges energy and momentum through a phonon. Therefore the polarization referred to in Fig.2.2 can be visualize as a process where a phonon goes in a first step from the electron to the lattice and, immediatelly afterwards, ounce the second electron is attracted, the same phonon (the same energy and momentum) goes back to the second electron. From this point of view, the process takes place without the lattice taking any energy during this particular kind of interaction with the electrons. Actually, the process can be viewed as the interchange of a phonon between two electrons through the lattice. This is what is peculiar to the superconducting state. Refer to Fig.2.3. In the left hand side the situation in the **normal** (non-superconducting, non-magnetic) **state** is illustrated. An electron is represented to interact with the lattice. There are two possibilities to this process. Either the electron "emits" (gives to the lattice) a phonon or "absorbs" one (takes from the lattice a phonon). The lattice and the electron both remain at the end of the process in a different state as they were before. There is no condition imposed to another electron-lattice

interaction to occur next. But in the superconducting state there is such a condition, we say that there is a correlation among the electrons. This is what Fig. 2.3 actually illustrates. An electron interacts with the lattice "emitting" a phonon which is absorbed by the lattice. But another electron (this is the extra-condition) absorbs immediately this phonon back leaving the lattice in its original state. This is the essential feature that is called a Cooper pair.

2.8 Conventional electron-phonon superconductivity

Finally, we arrive at the central point of the problem, that is: how to formulate the physics of the Cooper pairs? We can formulate it by keeping the physics to the simple interaction expressed in Fig.2.2. That is that to formulate the problem as "two electrons in a metal attract each other". We can then become more realistic and say that we want to formulate the problem as "two electrons interchange phonons both belonging to a particular metal with the pairing (extra) condition mentioned above". The first way of looking at the problems leads to a general theory called "BCS theory" and the second to a concrete-system-related theory called "Eliashberg gap Equations". These equations need the exact information on the phonons existing in the superconductor, $F(\omega)$, and the concrete interaction between electrons and the lattice represented by a function $\alpha(\omega)$. There are two electron-lattice interactions in the process. The whole information is condensed into a function called the **Eliashberg function**, $\alpha^2F(\omega)$. This is the process illustrated in Fig. 2.3. In Fig. ?? we show the Eliashberg function for Pb. This function can be calculated theoretically and it is measured in tunnelling experiments.

Chapter 3

BCS theory of superconductivity

BCS theory [15] was at its time a fantastic achievement of Bardeen ¹, Cooper and Schrieffer. The main result of the theory is to establish that the effect of the superconducting phase transition is to arrange the electronic system in such a way that an energy gap is introduced in the electronic band structures in both sides of the Fermi level. The general agreement of BCS theory with much of the experimental results leaves no doubt that the image of a rearrangement of the electrons into Cooper pairs and the existence of the energy gap constitute the main physical basis for a description of the superconducting phase transition.

To express mathematically "two electrons in a metal attract each other", we have to keep in mind that we are addressing to the conduction band of a metal, that is the electrons that move through the free space left by ions that constitute the lattice. Let's assume that they behave like a gas of electrons, a **Fermi gas**. Also, we cannot forget that the Pauli Principle applies (no two electrons in the same state). Since they are described in a the three-dimensional reciprocal space of the vector momentum \mathbf{k} , the most energetic electronic states form a surface in this space, the already mentioned **Fermi Surface**. There is a finite number of electronic states (occupied by definition) at the Fermi surface, say $N(\epsilon_F)$. The occupation probability at $T = 0K$ differs in the superconducting and in the normal state. In the superconducting state the electrons can reach states above the Fermi energy even at $T = 0K$ so that the superconducting distribution function looks rather like the normal state one (Eq. 2.1) but at a temperature of the order of a typical phonon energy, $\hbar\omega_D$, which is also of the order of $K_B T_c$. The difference is illustrated in Fig.3.1

These are the ones that are involved in the interaction that creates the pairs described above. Since in the process an electron absorbs and emits phonons, the Hamiltonian of the non-interacting system should describe the electrons and the phonons that exist in the superconducting metal

¹John Bardeen is the only person to have won twice the Nobel Prize in Physics.

Figure 3.1: The electronic occupation at $T = 0K$ (a) in the normal state and (b) in the superconducting state.

$$H_0 = \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} C_{\mathbf{k}}^{\dagger} C_{\mathbf{k}} + \sum_{\mathbf{q}} \hbar\omega_{\mathbf{q}} a_{\mathbf{q}}^{\dagger} a_{\mathbf{q}} \quad (3.1)$$

The first term refers to electrons. $C_{\mathbf{k}}^{\dagger} C_{\mathbf{k}}$ are creation and annihilation electron operators respectively and combined in this way they constitute the number operator. They are equal to one when the state is occupied in the metal and to zero when it is not. The electronic band structure, $\varepsilon = \varepsilon(\mathbf{k})$, tells us which states are available, the density of states tells us which are occupied at $T = 0K$ and helps us to determine the Fermi energy, and the occupation number (probability) contains the information about which are the occupied states at any temperature. These functions can be determined theoretically and experimentally with a high degree of agreement between the two results. The second term refers to phonons. The operators $a_{\mathbf{q}}^{\dagger} a_{\mathbf{q}}$ are the corresponding ones for phonons. $\hbar\omega_{\mathbf{q}}$ is the energy of the a phonon with momentum \mathbf{q} . So the Hamiltonian in Eq 3.1 represents the energy in the electron and in the phonon system at the outset. Now a further step must be done to describe how the energy goes from one system to the other or, otherwise, the electron-phonon interaction. We can describe the interaction between ions and electrons in a lattice from Fig. 3.2.

The figure describes a lattice where an ion has been displaced from its equilibrium position due to the Coulomb interaction with an electron. The interaction is screened which is a very important fact that will enter in an effective way below. O is the origin of the coordinate system. The crossing points are the equilibrium positions for the ions in the lattice. The ion (i) is displaced

Figure 3.2: The electron-ion interaction

from its equilibrium position l to the position Y_e which is measured from the equilibrium position of the ion, not from the origin. The interacting electron (e^-) is at a distance $|r'|$ from ion, at the point r , from the origin. Therefore, we have $r' = r - l - Y_e$. We can write the interaction Hamiltonian, H_I , as:

$$H_I = \sum_{k, k', l} \langle k | V(r - l - Y_e) | k' \rangle C_k^\dagger C_k \quad (3.2)$$

$$= \sum_{k, k', l} \exp [i(k' - k) \bullet (l - Y_e)] V_{k-k'} C_k^\dagger C_k \quad (3.3)$$

where $V(r)$ is the potential due to a single ion and $V_{k-k'}$ is its Fourier transform. This interaction Hamiltonian contains two parts which are different from the physical point of view. One depends on l which means on the periodicity of the lattice and represents therefore a Bloch term in the Hamiltonian. The interaction Hamiltonian 3.2 describes also the interchange of energy between electrons- and ions through the term that depends on \bar{Y}_e since \bar{Y}_e describes the vibrations of the ions around their equilibrium positions. So, consequently, we divide the interaction Hamiltonian in this two terms:

$$H_I = H_{Bloch} + H_{e-ph} \quad (3.4)$$

Now, the energy due to the discrete character of the lattice is not going to change during an electron-phonon interchange of energy and therefore, for

our purposes it is not of interest and we can drop this term (H_{Bloch}) from our interaction Hamiltonian. What we obtain is the **Fröhlich Hamiltonian**, H_F , where the term H_{e-ph} has been rewritten in a more convenient form for our purposes.

$$H_F = \sum_k \varepsilon_k C_k^\dagger C_k + \sum_q \hbar\omega_q a_q^\dagger a_q + \sum_{k, k', q} M_{kk'} (a_{-q}^\dagger + a_q) C_k^\dagger C_{k'}. \quad (3.5)$$

Here the indices of the fermion operators imply a sum over spins as well and those of the phonon operators imply a sum over the branches. Momentum is conserved during the interaction so that $\mathbf{q} = \mathbf{k} - \mathbf{k}'$ reduced to the FBZ if necessary. This conservation implies that the allowed final states are determined by the existing phonons in the lattice. In the Fröhlich Hamiltonian (Eq. 3.5), the first two terms are known from Eq. 3.1. The third one describes the electron-phonon interaction, that is to say, how the energy goes from one system to the other and back. It tells us that an electron in a state with quantum numbers k' goes to the state k by either emitting (creating) a phonon (therefore transferring energy to the lattice) with quantum numbers $-q$ or absorbing (annihilating) a phonon q from the lattice. The electron-phonon matrix element, $M_{kk'}$ is proportional to the potential matrix element $V_{k-k'}$ as follows:

$$M_{kk'} = i \sqrt{\frac{N\hbar}{2M\omega_q}} |\mathbf{k}' - \mathbf{k}| V_{k-k'} \quad (3.6)$$

with M the ion mass and N the number of ions in the unit lattice [12].

We have now everything that we need to describe the Cooper pairs. We need to describe within this formalism the special double electron-phonon interaction that implies that two electrons interchange a phonon through the lattice (see Fig. 2.3). The appropriate canonical transformation of the Fröhlich Hamiltonian leads to:

$$H' = H_0 + \sum_{\substack{k, k' \\ \mathbf{k}-\mathbf{k}'=\mathbf{q}}} |M_q|^2 \frac{\hbar\omega_q}{(\varepsilon_k - \varepsilon_{k-q})^2 - (\hbar\omega_q)^2} C_{k'+q}^\dagger C_{k-q}^\dagger C_k C_{k'} + \text{tw2eo} \quad (3.7)$$

tw2eo...terms with two electron operators which are the ones that describe the interaction with the lattice of an electron without the pairing condition. These are not important in the superconducting state (the physics of Cooper pairs).

We observed that this four operator term is negligible in the normal state. Also observe that the interaction term between electrons can change sign. If $(\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}-\mathbf{q}})^2 < (\hbar\omega_q)^2$, the interaction term will be negative and the interaction attractive. Otherwise the term is positive and the interaction is repulsive. So we see that the energy of the final and initial states should not be very different from each other to have an attractive interaction. They better be both at the

Fermi surface. We illustrate it in Fig. 3.3. Notice first that the term we are considering describes an electron in state k' that is promoted to the state $k' + q$ by absorbing (emitting) a phonon of energy $\hbar\omega_q$ and momentum \mathbf{q} and, simultaneously, another electron in state k goes to the state $k - q$ by emitting (absorbing) the very same phonon. So it describes the interaction between two electron mediated by the lattice, the transfer of a phonon from one electron to the other by means of the lattice. Further, to describe the attraction of the superconducting state, we need that the two electrons are not promoted too far away from the Fermi Surface. In Fig. 3.3(A), we see the result of this phonon transfer with a final state far away the Fermi surface. In this case the term $(\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}-\mathbf{q}})^2$ will be much larger than $\hbar\omega_q$ and the interaction will be repulsive (Ec. 3.7). If the situation is as it is shown in Fig. 3.3(B), we see that by taking $k' = -k$, both electronic final states end at the Fermi surface and the situation arises where $(\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}-\mathbf{q}})^2 < (\hbar\omega_q)^2$ with an attractive interaction as a result.

It is this effective attractive interaction between two electrons the one that causes the formation of Cooper pairs and therefore the superconducting transition. The important point therefore is the dynamics of these pairs. The BCS model makes an approximation based on the Fröhlich Hamiltonian to construct another one that describes a systems of Cooper pairs alone. The interaction with the lattice of a pair $(\bar{k} \uparrow, -\bar{k} \downarrow)$ ends in a pair-final state $(\bar{k}' \uparrow, -\bar{k}' \downarrow)$, so the dynamics implies always that $(\bar{k} \uparrow, -\bar{k} \downarrow) \implies (\bar{k}' \uparrow, -\bar{k}' \downarrow)$. So, we repeat that the superconducting state is a state where two electrons $(\mathbf{k}, \epsilon_{\mathbf{k}}, \uparrow)$ and $(-\mathbf{k}, \epsilon_{\mathbf{k}}, \downarrow)$ form a pair. The dynamical interactions are taken into account between mates of a pair only. The pair-pair correlation is essentially almost taken into account by the Pauli Principle and it is accounted for by working the simplified problem (formation of pairs) consistently with Fermi statistics [14]. The BCS Hamiltonian is written in the next Eq. 3.8. We will take from now on the origin of the energy at the Fermi level:

$$H_{BCS} = \sum_k \varepsilon_k \left(C_k^\dagger C_k + C_{-k}^\dagger C_{-k} \right) - \sum_{k, k'} V_{kk'} C_{k'}^\dagger C_{-k'}^\dagger C_{-k} C_k \quad (3.8)$$

This Hamiltonian acts on a vector state with only Cooper pair states at $T = 0K$. At $T > 0K$, the correlation weakens because of the thermal energy and some electrons begin to act as if they were independent. This is the basis of the **two fluid model** introduced before. $V_{kk'}$ is the effective attractive interaction. The original BCS paper [?] is very interesting to read. Nevertheless we will not follow them but rather use the Bogoliubov-Valatin transformation to diagonalize the BCS hamiltonian. This transformation was originally used in the Bogoliubov theory of helium [?]. With that purpose, we define two new operators related to the fermion creation and annihilation operators $C_{k'}^\dagger, C_k$ as follows:

$$\begin{aligned} \gamma_k &= u_k C_k - v_k C_{-k}^\dagger \\ \gamma_{-k} &= u_k C_{-k} + v_k C_k^\dagger \end{aligned} \quad (3.9)$$

Figure 3.3: The lattice-mediated interaction between two electrons. When the final state differ in energy less that the phonon energy that is transmited through the lattice, the interaction becomes attractive.

and their conjugates

$$\begin{aligned}\gamma_k^+ &= u_k C_k^+ - v_k C_{-k} \\ \gamma_{-k}^+ &= u_k C_{-k}^+ + v_k C_k\end{aligned}\tag{3.10}$$

The constants u_k and v_k are chosen to be real and positive and to obey the condition

$$u_k^2 + v_k^2 = 1\tag{3.11}$$

Eqs. 3.9, 3.10, and 3.11 constitute the Bogoliubov-Valatin transformation. The operators just defined follow the Fermion anticommutation relations,

$$\{\gamma_k^+, \gamma_k\} = \{\gamma_{-k}^+, \gamma_{-k}\} = \delta_{k,k'} \quad (3.12)$$

and zero otherwise. To rewrite the BCS Hamiltonian, we have to find the inverse transformation:

$$\begin{aligned} C_k &= u_k \gamma_k + v_k \gamma_{-k}^+ \\ C_{-k} &= u_k \gamma_{-k} - v_k \gamma_k^+ \end{aligned} \quad (3.13)$$

and their conjugates

$$\begin{aligned} C_k^+ &= u_k \gamma_k^+ + v_k \gamma_{-k} \\ C_{-k}^+ &= u_k \gamma_{-k}^+ - v_k \gamma_k \end{aligned} \quad (3.14)$$

With Eqs. 3.13 and 3.14, we can express the BCS Hamiltonian 3.8 in terms of the new operators 3.9 and 3.10. The new operators are meant to represent a transformation to a diagonalized Hamiltonian of Cooper pairs. We will proceed as follows. We express the first (H_K) and second term (H_V) of the BCS hamiltonian in the Hilbert space of the new operators. We will set the condition that the off-diagonal terms in H_K and in H_V cancel each other so that we get the diagonalized hamiltonian that we are pursuing. From the condition just mentioned, we deduce the properties of the superconducting state, namely, the main characteristic equations of the superconducting state. We get:

$$H_K = \sum_k \varepsilon_k [2v_k^2 + (u_k^2 - v_k^2)(m_k + m_{-k}) + 2u_k v_k (\gamma_k^+ \gamma_{-k}^+ + \gamma_{-k} \gamma_k)] \quad (3.15)$$

The first term is a constant, the terms with m_k and m_{-k} are diagonal and the third term is off-diagonal. The m_k and m_{-k} are defined as

$$\begin{aligned} m_k &\equiv \gamma_k^+ \gamma_k \\ m_{-k} &\equiv \gamma_{-k}^+ \gamma_{-k}. \end{aligned} \quad (3.16)$$

We get further

$$\begin{aligned} H_V &= - \sum_{kk'} V_{kk'} [u_{k'} v_{k'} u_k v_k (1 - m_{k'} - m_{-k'}) (1 - m_k - m_{-k}) + \\ &\quad + u_{k'} v_{k'} (1 - m_{k'} - m_{-k'}) (u_k^2 - v_k^2) (\gamma_k^+ \gamma_{-k}^+ + \gamma_{-k} \gamma_k)] + 4OT \end{aligned} \quad (3.17)$$

where $4OT$ stands for "fourth order terms". Now, we are left with a system of independent fermions if we assume that the off-diagonal terms in 3.15 cancel exactly those in 3.17. At this point we assume (this can be verified later) that

at the lowest energy state of this system, both m_k and m_{-k} are zero. So to find the Bogoliubov-Valatin transformation that is appropriate to a superconductor in its ground state, we first put in 3.15 and 3.17 $m_k = m_{-k} = 0$. We make further the approximation that the 4OT can be neglected and then assume that the non-diagonal elements cancel. We find

$$2\varepsilon_k u_k v_k - (u_k^2 - v_k^2) \sum_{k'} V_{kk'} u_{k'} v_{k'} = 0 \quad (3.18)$$

To take into account Eq. 3.11, we use a single variable: x , such that $u_k^2 = \frac{1}{2} - x_k$ and $v_k^2 = \frac{1}{2} + x_k$ so that Eq. 3.18 becomes

$$2\varepsilon_k \sqrt{\left(\frac{1}{4} - x_k^2\right)} + 2x_k \sum_{k'} V_{kk'} \sqrt{\left(\frac{1}{4} - x_{k'}^2\right)} = 0 \quad (3.19)$$

We define a quantity, Δ_k , that will be identified with the gap later on:

$$\Delta_k \equiv \sum_{k'} V_{kk'} \sqrt{\left(\frac{1}{4} - x_{k'}^2\right)} \quad (3.20)$$

Eq. 3.19 then leads to

$$x_k = \pm \frac{\varepsilon_k}{2\sqrt{\varepsilon_k^2 + \Delta_k^2}} \quad (3.21)$$

which when substituted in Eq. 3.19 gives the following integral equation for the gap which can be solved in principle once the potential is known:

$$\Delta_k = \frac{1}{2} \sum_{k'} V_{kk'} \frac{\Delta_{k'}}{\sqrt{\varepsilon_{k'}^2 + \Delta_{k'}^2}} \quad (3.22)$$

BCS took the potential as a constant.⁷ Since in the process an electron absorbs a phonon it can reach states above the Fermi energy (see Fig. 3.1). If we adopt for a typical phonon the energy $\varepsilon_{\mathbf{D}} = \hbar\omega_{\mathbf{D}}$ where $\omega_{\mathbf{D}}$ is the so-called **Debye frequency** and $\hbar \approx 6.58 \times 10^{-16}$ eV s is the famous **Planck's constant**, then the electrons involved are in the states with energy in the interval $(\varepsilon_{\mathbf{F}} - \hbar\omega_{\mathbf{D}}, \varepsilon_{\mathbf{F}} + \hbar\omega_{\mathbf{D}})$. So, the attractive potential acts only in this energy interval and we have to consider a gas of otherwise independent electrons submitted to an attraction potential which is different from zero only in the interval just mentioned. Notice that this is a particular potential that does not depend on position but it depends on energy, it is a pseudopotential. The BCS attractive pseudopotential is defined as:

$$\begin{aligned} V_{kk'} &= V_0 \text{ (const) for } \varepsilon_{\mathbf{F}} - \hbar\omega_{\mathbf{D}} < \varepsilon < \varepsilon_{\mathbf{F}} + \hbar\omega_{\mathbf{D}} \\ V_{kk'} &= 0 \text{ for any other value of the electron energy, } \varepsilon. \end{aligned} \quad (3.23)$$

which is illustrated in the next Fig. 3.4 (We write explicitly $\varepsilon_{\mathbf{F}}$ for clearness although we recall that it is the origin).

Figure 3.4: The BCS potential to describe the attraction between electrons.

The BCS approximation for the potential, Eq. 3.23, reduces the gap Δ_k also to a constant. We use $\sum_k \rightarrow \int N(\varepsilon)d\varepsilon$ in Eq. 3.22 and put $N(\varepsilon) \sim N(\varepsilon_F) \equiv N(0)$ since according to Eq. 3.23 the integrand will be different from zero only around the Fermi energy. So, The BCS prediction for the gap energy at the temperature $T = 0K$ is:

$$2\Delta(0) \equiv \Delta_0 = \frac{\hbar\omega_D}{\sinh\left[\frac{1}{N(\varepsilon_F)V_0}\right]} \approx 4\hbar\omega_D \exp\left[-\frac{1}{N(\varepsilon_F)V_0}\right]. \quad (3.24)$$

Summarizing, the correlation between electrons (the attraction) can be broken if a certain amount of energy is given to the superconductor through light (laser), heat (that would rise the temperature above T_c), or another source of energy. The "binding energy" of the two electrons is denoted by 2Δ and Δ is called the **superconducting gap** of the superconductor and it is a function of the temperature, T (see Fig. ??). BCS find a gap in the allowed states about the Fermi energy. Actually, by the time the BCS paper appeared (1957) many experiments indicated a gap of the order of $K_B T_c$. The gap is, in general, a function of \mathbf{k} , so it is anisotropic. This anisotropy has been attributed to non-spherical Fermi surfaces in the real metals and to phonon anisotropy. This anisotropy manifests itself in several experimental results even in very simple weak coupling superconductors as Al [2]. When an appropriate thermodynamic description of a superconductor is obtained with a constant value of the gap, then in the reciprocal space where it is defined it is actually a sphere of constant radius Δ_0 . In this case, we speak about **an "s-wave" superconductor**.

$\Delta(0) \equiv \Delta_0$ and T_c are parameters that characterize a superconductor. An-

other important result of BCS theory is the

$$T_c = 1.14\hbar\omega_D \exp\left[-\frac{1}{N(\epsilon_F)V_0}\right]. \quad (3.25)$$

The formula sometimes is used with another frequency, related or not to the Debye frequency [11], but these are details that belong to an effort to use a BCS-like formula for T_c to reproduce results in stronger coupling superconductors like A15's and others. The idea was to understand which parameters are important to rise the critical temperature of a superconductor. Some limits were cast at about $30K$ but there are superconductors nowadays with $T_c = 138K$ as we shall see below.

Nb	9.2				Nb ₃ Ge	23.3
Pb	7.2				Nb ₃ Ga	20.0
V	5.3				Nb ₃ Al	19.0
Ta	4.5				Nb ₃ Sn	18.1
In	3.4				Nb ₃ Si	17.2
Ti	2.4				V ₃ Ga	16.8
Al	1.2				Ta ₃ Au	16.0

Table I. Critical temperature of some superconductors

On the left hand side of Table I, we show some elements. Nb is the element with the highest critical temperature. On the right hand side we quote the critical temperature for some A15 compounds. The highest critical temperature known before the discovery of the High temperature superconductors, the copper oxides, was for *Nb₃Ge*. The crystal lattice of the A15 compounds is shown in Fig.3.5

Further, if we compare Eq. 3.25 to Eq. 3.24, we get the known **universal BCS relation**:

$$\frac{2\Delta(0)}{K_B T_c} = 3.52. \quad (3.26)$$

The magnitude of the Fermi energy, ϵ_F , is of the order of some units of electron-volts (eV) and the higher phonon energy is usually much less than 50 millielectron-volts (meV) in simple metals. The energy gap at $T = 0K$, $\Delta(0)$, is of the order of meV, in general. The number of states in a Fermi gas, $N(\epsilon)$, at a certain energy, ϵ , can be shown to be proportional to the square root of the energy:

$$N(\epsilon) \sim \sqrt{\epsilon}. \quad (3.27)$$

In the superconducting state we do not expect too much to happen well below the Fermi energy since the electrons that form the Cooper pairs are located in states within a few meV below and above the Fermi energy level as we just mentioned. The modified superconducting density of states, $N_s(\epsilon)$, is:

Figure 3.5: The A15 crystal lattice. It is formed by a body centered cubic (bcc) lattice and three orthogonal chains. In the case of Nb_3Ge , the bcc lattice is formed by Ge ions and the chains are Nb ions.

$$N_s(\varepsilon) = N(\varepsilon_F) \frac{\varepsilon - \varepsilon_F}{\sqrt{(\varepsilon - \varepsilon_F)^2 - \Delta^2}} = N(0) \sqrt{\frac{E}{E^2 - \Delta^2}}. \quad (3.28)$$

In the last Eq. 3.28 the energy E is measured from the Fermi level which is taken as the origin. $N_s(E)$ is shown in Fig. ???. The gap on both sides of the Fermi energy is apparent. The number of states remains the same but they are pushed away by the transition from the energy gap region to the gap edge below and above the Fermi level.

Finally, it is important to quote **the BCS energy of the elementary excitations**:

$$E_k = \sqrt{(\varepsilon - \varepsilon_F)^2 + \Delta^2}. \quad (3.29)$$

where we make it explicit that the electron energy is measured from the Fermi level.

Chapter 4

Characteristics of the superconducting state.

We now list some of the properties of the superconducting state and compare them with the BCS predictions.

4.1 The resistivity

K. Onnes discovered superconductivity when he realized that a phase transition took place in a Hg sample that led to a zero resistivity regime. In the next Fig. 4.1 we illustrate this fact. The resistivity goes to zero (the upper limit set is of the order of $10^{-23}\Omega - cm$) in the superconducting state. A persistent current induced magnetically to a superconducting ring has been found to decay in more than at least 10^5 years but some theoretical estimates give more than 10^{10} years.

4.2 The specific heat

The phase transition from the normal to the superconducting state is a second order phase transition in absence of a magnetic field. That means that the thermodynamic functions, as the total energy, are continuous through the transition but their derivatives are not. The electronic specific heat at constant volume,

$$C_{ev} = \left. \frac{dE}{dT} \right|_v \quad (4.1)$$

has a lambda-shaped discontinuity at T_c . This is shown in Fig. 4.2.

In the normal state the electronic specific heat can be written as

$$C_{en} = \frac{2}{3}\pi^2 N(\varepsilon_F) K_B^2 T \equiv \gamma T. \quad (4.2)$$

Figure 4.1: The resistivity goes to zero at the critical temperature of the phase transition to the superconducting state.

In the **strong coupling limit** $N(\varepsilon_F)$ should be replaced by $N(\varepsilon_F)(1 + \lambda_{e-ph})$ where λ_{e-ph} is the **electron-phonon coupling parameter**. Eq. 4.2 defines the Sommerfeld constant, γ . λ_{e-ph} decreases with temperature and actually goes to zero at high temperatures, This property allows to determine the electron-phonon coupling parameter, λ_{e-ph} , from the knowledge of the Sommerfeld constant at low and high temperatures since $\gamma(0) = (1 + \lambda_{e-ph})\gamma(T)$, for $T \gg 0$. There is also a lattice contribution to the specific heat which does not change with the transition. **Superconductivity is a phase transition that occurs in the electronic system only**. The lattice contributes an approximate $C_{latt} \equiv C_{ph} \sim AT^3$ term.

The BCS expression for the electronic specific heat in the superconducting state is [12]

$$C_{ev} = \sum_{\mathbf{k}} \left(\frac{d\Delta^2}{dT} - \frac{2E^2}{T} \right) \frac{\partial f}{\partial E} \quad (4.3)$$

In Eq. 4.3 the source of the jump is apparent since the derivative of the gap squared is zero above T_c but finite below it. The BCS prediction agrees qualitatively with experiment but important quantitative deviations are measured. The specific heat difference at the transition temperature, $\Delta C \equiv (C_{es} - C_{en})_{T_c}$ is given as

Figure 4.2: The specific heat shows a jump at T_c . At very low temperatures it decreases exponentially in the superconducting state.

$$\Delta C = N(\varepsilon_F) \left[-\frac{d\Delta^2}{dT} - \frac{2E^2}{T} \right]_{T_c} = 9.4N(\varepsilon_F)K_B^2 T_c \quad (4.4)$$

Comparing Eq. 4.2 and Eq. 4.4, we obtain a **second BCS universal ratio**:

$$\frac{\Delta C}{\gamma T_c} = 1.43 \quad (4.5)$$

The parameter γ can be obtained from measurements of the total specific heat in the normal state as a function of temperature $C_{tot}(T) = \gamma T + AT^3$. Constructing a plot $\frac{C_{tot}(T)}{T}$ as a function of T^2 we obtain a straight line with a slope equal to γ . The next Table II compares BCS predictions to experiment [10]

element	$T_c[K]$	$\frac{\Delta C}{\gamma T_c}$	λ_{e-ph}
Al	1.16	1.45	0.38
Zn	0.85	1.27	0.38
Sn	3.72	1.6	0.60
Ta	4.48	1.69	0.65
V	5.30	1.49	0.60
Pb	7.19	2.71	1.12
Hg	4.16	2.37	1.00
Nb	9.22	1.87	0.82

Table II. Comparison between BCS and experiment.

The experimental and theoretical calculations differ somehow in the literature but the previous Table II does give a clear idea of the correct magnitudes. See also [11].

4.3 Coherence effects

The BCS superconducting state is a phase-coherent superposition of occupied one-electron states which can be treated independently in the normal state. This phase coherent superposition can have different effects when calculating matrix elements in perturbation theory [10]. For ultrasonic attenuation calculations, for example, contributions to the transition probability have the same sign and add coherently. For other perturbations, terms in the transition probabilities subtract. This is the case of the nuclear spin lattice relaxation rate. Just below T_c it rises and presents a coherence peak usually called the Hebel-Slichter peak after the people that first observed it in Al [?].

4.4 Ultrasonic attenuation

In the superconducting state, the sound waves are less and less attenuated as the temperature goes to zero. This is due to the fact that the attenuation of the sound (movement of parallel planes perpendicular to the direction of the sound) creates an imbalance between the center of positive and negative charges which results in an internal electric field that accelerates the electrons. These take energy and momentum from the sound wave and eventually the sound wave is attenuated. The electrons give back the energy to the lattice but not in the coherent way to preserve the sound wave. Equilibrium is attained finally and the sample uses the sound energy to rise its temperature. In the superconducting state, the lattice does not like to take energy from the electronic system. So the attenuation mechanism is weakened and the wave is not attenuated. Sound can theoretically persist into a superconductor forever at $T = 0K$. This is illustrated in the next Fig. 4.3.

Figure 4.3: The ultrasonic attenuation.

Chapter 5

The Strong coupling theory

Migdal [16] showed how the strong-coupled electron-phonon interaction can be treated accurately in normal metals. Eliashberg [17] extended the calculation to the superconducting state.

If the electron-phonon interaction is strong (not weak as in BCS) then the quasi-particles have a finite lifetime and are thus damped [3]. As a consequence, Δ_0 decreases. T_c decreases even more. For that reason the ratio $\frac{2\Delta(0)}{K_B T_c}$ increases. Strong coupling theory [4] is based on the Eliashberg gap equations and gives results in very good agreement with experiment. Eliashberg equations are the result of the treatment of the manybody problem of superconductivity in more detail. The problem is stated in the mean field approximation. Eliashberg gap equations are obtained in several books [5, 6, 7]. They are solved numerically since long ago. In ref. [8] these equations are formulated in the imaginary frequency axis and solved. In ref. [13], they are quoted in the real axis. In ref. [9], the influence of spin fluctuations as a disruptive mechanism in conventional superconductors is incorporated into the Eliashberg gap equations and solved. I quote them here written on the real frequency axis .

$$\Delta(\omega) = \frac{1}{Z(\omega)} \int_{\Delta_0}^{\omega_c} d\omega' \operatorname{Re} \left\{ \frac{\Delta(\omega')}{\sqrt{\omega'^2 - \Delta^2(\omega')}} \right\} \{K_+(\omega, \omega') - \mu^*\} \quad (5.1)$$

$$(1 - Z(\omega))\omega = \int_{\Delta_0}^{\omega_c} d\omega' \operatorname{Re} \left\{ \frac{\Delta(\omega')}{\sqrt{\omega'^2 - \Delta^2(\omega')}} \right\} K_-(\omega, \omega') \quad (5.2)$$

$$K_{\pm}(\omega, \omega') = \int_0^{\infty} d\nu \alpha^2 F(\nu) \left\{ \frac{1}{\omega' + \omega + \nu + i\epsilon} \frac{1}{\omega' + \omega + \nu - i\epsilon} \right\} \quad (5.3)$$

Notice that the information on the specific material you are dealing with, enters via the Eliashberg function, $\alpha^2 F(\omega)$, and a parameter μ^* that is actually an electron-electron effective interaction pseudopotential integrated over all its variables. A typical value for this parameter is 0.1 in simple metals and 0.13 for

transition metals and Al5's. Of particular interest is the occupation function (which corresponds to Eq. 2.1 in the normal state) because at $T = 0K$ quasiparticles have access to states above the Fermi energy as it is shown in Fig. ??.

Figure 5.1: We compare here the occupation number (probability) of fermions in the normal state (a) and quasiparticles in the superconducting state. The Fermi energy is denoted by 0 in the graphs.

The functional derivative of the critical temperature, T_c , with respect to the Eliashberg function, $\frac{\delta T_c}{\delta \alpha^2 F(\nu)}$, can also be calculated. This is a very interesting function since it tells us what are the important phonon frequencies to rise T_c . Actually one can calculate the change induced on T_c by a specific change in the Eliashberg function, $\alpha^2 F(\omega)$, as follows:

$$\Delta T_c = \int_0^\infty d\nu \frac{\delta T_c}{\delta \alpha^2 F(\nu)} \Delta \alpha^2 F(\nu). \quad (5.4)$$

A very important characteristic of $\frac{\delta T_c}{\delta \alpha^2 F(\nu)}$ is that it has a maximum at a specific frequency, called **optimal frequency**, ω_{opt} . Moreover, in a graph of $\frac{\delta T_c}{\delta \alpha^2 F(\nu)}$ drawn as a function of $\frac{\omega_{opt}}{K_B T_c}$, a maximum appears in all the curves at a frequency $\frac{\omega_{opt}}{K_B T_c} \sim 7 - 8$. The maximum is universal for all conventional superconductors. Therefore, for a given conventional superconductor, there exists an specific phonon that couples with the electron system in the most efficient way possible and that determines the critical temperature as follows:

$$\hbar \omega_{opt} = G K_B T_c \quad \text{with } G \sim 7 - 8. \quad (5.5)$$

The functional derivative can be used to show, for example, that the highest known conventional electron-phonon superconductor, namely Nb_3Ge is actually optimized for superconductivity and that no higher critical temperature can be obtained by doping or taking the compound off stoichiometry [18]. The essential point is illustrated in Fig. ???. The Eliashberg function (dotted curves) and the functional derivative (dashed curves) for four samples of Nb_3Ge are presented. The samples differ in the concentration of Ge. Stoichiometry is at 25% Ge-content according to the chemical formula and at this Ge content $T_c = 23.2K$. The graph on the up-left, describes a sample with a 16.7% Ge-content and a low $T_c = 7K$. The maximum of the functional derivative (the ideal frequency for superconductivity) in this case is well below the frequency where the Eliashberg function peaks (maximum number of phonons). So we do not expect the critical temperature to be very high. The graph below on the left, belongs to a sample with 21.3% Ge-content and a higher critical temperature $T_c = 13.2K$. The arrow points to the peak that reveals that the chains begin to influence the superconducting behavior of the sample (see Fig. 3.5). Notice also that the maximum in the functional derivative (the optimal frequency) has switched towards higher frequencies. In the upper graph on the right, a sample with a higher Ge-content (22.3%) is studied but still less than 25%. We see that the optimal phonon frequency is displaced towards higher frequencies and that a very pronounced peak appears nearby. So the situation is nearer to ideal (The optimal frequency at the peak of the Eliashberg function). Would the trend follow, one could expect that a higher critical temperature will appear by enhancing the Ge content far away from stoichiometry. But the answer is no. When a sample of Ge content higher than 25% (25.7%) is prepared (lower graph on the right), the peak on the Eliashberg function goes too much towards lower frequencies and the maximum in the functional derivative indicates that one should reverse the trend. To reverse the trend is to go towards stoichiometry, that is to say, there is no way that a Nb_3Ge sample can be manipulated to rise its T_c : the material is optimized for superconductivity!

5.1 Tunneling

Tunneling measurements can yield accurate values for the gap and its temperature dependence. The Eliashberg function can be also obtained as a result of this experiment through an inversion process due to Mc Millan and Rowell [21]. Tunneling is a technique that has been applied to many conventional superconductors and it is now applied to the high- T_c materials. Single particle tunneling in superconductors is known as Giaever tunneling for he was who pioneered this work [19]. When two metals are separated by an insulator, the electrons from one side can tunnel to the other if the insulator is thin enough, of the order of an electron mean free path. In this set up, both sides tend to align their Fermi energies. To enter the second metal, empty states must be available at this site. Tunneling transitions are all horizontal in energy. That means that an electron will tunnel from one energy state on one side to another state of

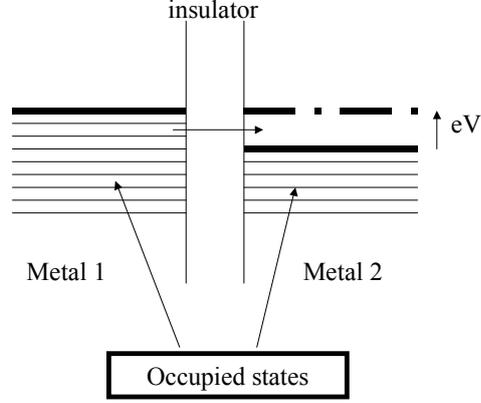


Figure 5.2: The tunnel junction. When a potential is applied, the maximum occupied energy levels on each side move relative to each other. This allows horizontal transitions since it creates empty states on metal 2 at an energy where there are occupied states on metal 1. The electrons can then tunnel from metal 1 to metal 2 (arrow) through the insulator as long as it is thin enough (see text).

the same energy on the other side. The tunneling current at a certain temperature, T , from metal 1 to metal 2 will be, therefore, proportional to the available occupied states in metal 1 times the available unoccupied states in metal 2 at the same energy, ε , at the given temperature. Since both sides align their Fermi energy and the transitions are horizontal, when the voltage, V , is zero, there will be no current. When a voltage is applied in such a way that the electronic states

The current (see Fig. 5.2) from 1 to 2 can be written as:

$$I_{1 \rightarrow 2}(V, T) = I_0 \int_{-\infty}^{\infty} d\varepsilon |T_{12}|^2 N_1(\varepsilon) f(\varepsilon, T) N_2(\varepsilon + eV) [1 - f(\varepsilon + eV, T)]. \quad (5.6)$$

where I_0 is a constant of proportionality and T_{12} is the tunneling matrix element. N_i ($i = 1, 2$) are the electronic density of states of the corresponding metals, e is the electron charge and $f(\varepsilon, T)$ is the Fermi distribution function (see Eq. 2.1). The presentation here is in the so-called semiconductor model. A more detailed many body treatment of tunneling can be seen in many books (see, for example, [5, 7])

We can apply Eq. 5.6 to three different situations, namely, normal-normal, normal-superconductor and superconductor-superconductor tunneling. We will approximate for a normal metal $N_1(\varepsilon)$ and $N_2(\varepsilon + eV)$ by their values at the Fermi level. This approximation is reasonable in this situation.

For **normal-normal tunneling**, we get straightforwardly:

$$\begin{aligned} I_{1 \rightarrow 2}(V, T) &= I_0 |T_{12}|^2 N_1(\varepsilon_F) N_2(\varepsilon_F) \int_{-\infty}^{\infty} d\varepsilon f(\varepsilon, T) [1 - f(\varepsilon + eV, T)] = \\ &= I_0 |T_{12}|^2 N_1(\varepsilon_F) N_2(\varepsilon_F) eV \equiv G_{nn} V. \end{aligned} \quad (5.7)$$

Eq. 5.7 represents the Ohms law and defines the **normal conductance**, G_{nn} .

We can also make use of Eq.5.6 to calculate the **normal-superconductor tunneling** characteristics, $I = I(V, T)$. We emphasize that we are using the semiconductor model of a superconductor. In this case we cannot approximate the superconductor density of states by its value at the Fermi energy in the normal state. The BCS (or the strong coupling density of states) is required. In this case we can have two situations depending on the voltage. The situation for a forward voltage $eV > \Delta$ is shown in Fig 5.3. The electrons in the normal metal can tunnel to the superconductor where they become excited quasiparticles. The arrow indicates the tunneling path and it is drawn horizontally in this case to indicate the conservation of energy.

The situation for reverse bias is illustrated in the Fig. 5.4. In this case, energy must be given to break a pair first. Then, single particle tunneling then takes place as one of the independent electrons reaches the normal metal side as an excited state (thick arrow) and the other becomes a quasiparticle excited state in the superconducting side (vertical thick arrow).

This situation is interesting since it explores the superconducting gap and allows to find its value and its dependence with temperature. In this case we can use again Eq.(5.6) to get:

$$\begin{aligned} I_{s \rightarrow n}(V, T) &= I_0 |T_{ns}|^2 N_n(\varepsilon_F) \int_{-\infty}^{\infty} d\varepsilon N_s(\varepsilon_F) f(\varepsilon, T) [1 - f(\varepsilon + eV, T)] = \\ &\equiv \frac{G_{nn}}{e} \int_{-\infty}^{\infty} d\varepsilon \frac{N_s(\varepsilon)}{N_s(\varepsilon_F)} f(\varepsilon, T) [1 - f(\varepsilon + eV, T)] \end{aligned} \quad (5.8)$$

where the meaning of the sub-indices is obvious.

The single particle tunneling between two superconductor is possible as illustrated in the Fig. 5.5. A Cooper pair breaks giving two independent electrons. One remains in the original superconductor (right hand side in the figure) as an excited quasiparticle and the second tunnels to the other and becomes an excited quasiparticle in the second superconductor. This process conserves energy.

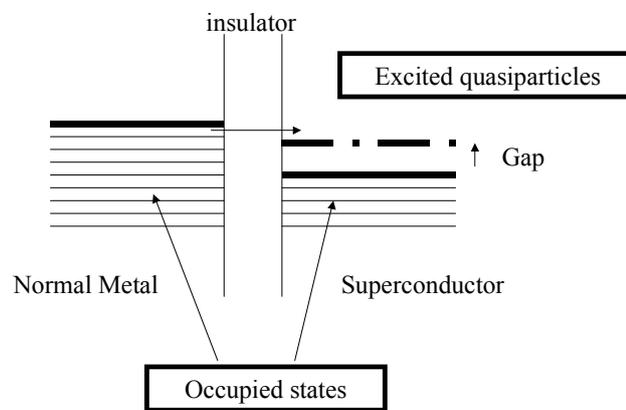


Figure 5.3: At $T = 0K$, in the situation of forward voltage, when $eV > \Delta$, the electrons tunnel horizontally from the normal metal to the superconductor where they become excited quasiparticles.

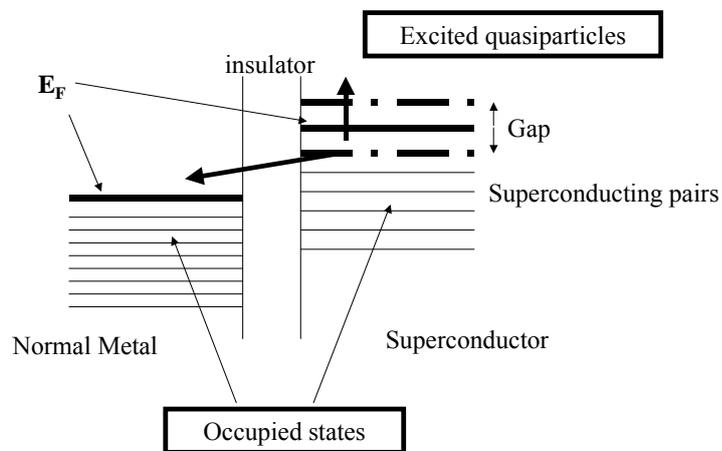


Figure 5.4: At $T = 0K$, in the situation of reverse bias $eV < -\Delta$, the tunneling process takes place by breaking first an electron pair. Then the two independent electrons can behave differently (thick arrows). One can become an excited quasiparticle in the superconductor and the other can tunnel to the normal metal to an excited state. Energy is conserved in this process also.

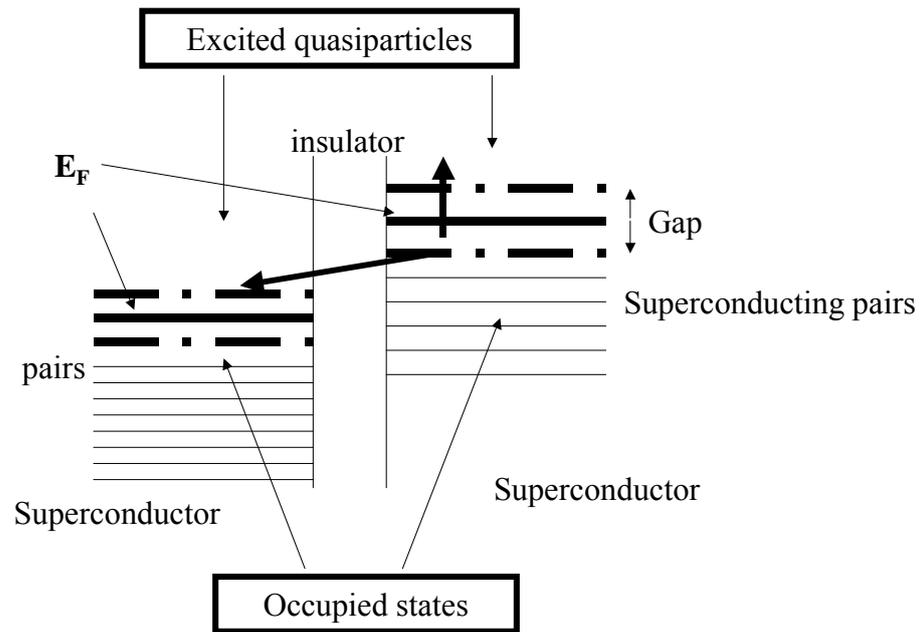


Figure 5.5: Single particle tunneling between two superconductors.

5.1.1 Josephson Effects

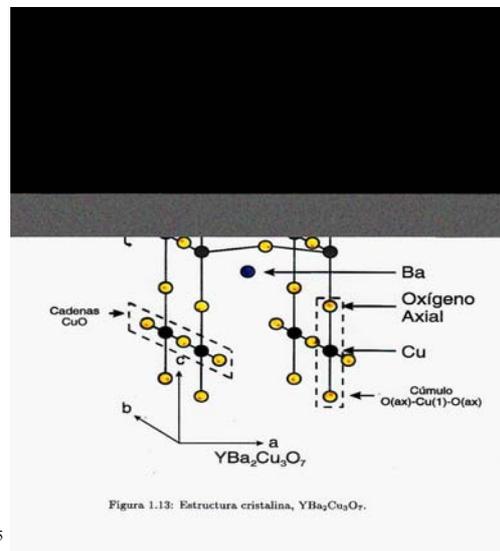
Josephson Effects are actually a special case of tunnelling between two superconductors. Its theoretical importance lies in the OJO FALTA TRADUCIR ESTO this case the particles that tunnel are Cooper pairs. un caso especial de tunelamiento entre dos superconductores, ya que se trata del tunelamiento de pares de Cooper, su importancia teórica es enorme pues estableció experimentalmente, la existencia de los pares de Cooper como "partículas" reales. Josephson en 1962, estableció esta posibilidad, más exactamente, predijo que debería producirse a voltaje cero, una corriente en una muestra superconductor-aislante-superconductor del mismo tipo de las que discutimos arriba con respecto al efecto tunel de una sola partícula (electrones libres). Este efecto se conoce como Efecto Josephson. Tunelan pares de Cooper. La corriente de tunelamiento, por esa razón, lleva el nombre de *corriente Josephson de pares*. El fenómeno resultó tan interesante que Josephson recibió el Premio Nobel por este descubrimiento. Y es que, si se aplica un voltaje a la muestra, el paso de la corriente se acompaña de la emisión de radiación de frecuencia $2eV$. La presencia del "2", delata que la carga de la partícula es $2e$, es decir, que se trata del tunelamiento de un par de Cooper. Existen muchas otras propiedades de estas "junturas Josephson" de gran interés. Existen muchos libros de Superconductividad que las describen. En las referencias puede encontrarse algunos de ellos. Aquí nos contentaremos con señalar su existencia y su importancia.

Part II

**High-Tc superconducting
materials**

Chapter 6

Crystal structures



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Figure 6.1: The perovskite structure of $YBa_2Cu_3O_7$.

Chapter 7

Superconducting properties

7.1 The Coherence lenght

The coherence lenght is one of the important parameters describing a superconductor. It is a measure of the volume where the coherent state takes place. One can also think of it as a measure of the extension of a Cooper pair. One can intuitively think that the bigger this lenght, the weaker the binding between the two electrons that constitute the Cooper pair. So it is not surprising that it relates inversely to the superconducting gap and to critical temperature. Actually, it is given by

$$\xi_0 = \frac{h v_F}{\pi \Delta_0} = \frac{h v_F}{2\pi T_c} \quad (7.1)$$

where $h \equiv 2\pi\hbar$ and v_F is the Fermi velocity. In the next Table III, we compare some values for the conventional metals and the High-Tc uperconductors (HTSC). Using for $T_c = 40K$ (appropriate for $La_{1.8}Sr_{0.2}CuO_4$), we get that the coherence lenght, $\xi_0 \approx 25\text{\AA}$. In convetional superconductors, ξ_0 is of the order of few hundred amstrongs for A15's, up to thouthand amstrongs in materials like Al. So the **small coherence lenght** is a new property worth noticing in HTSC. It is mainly due to the small value of the Fermi velocity although the higher values of the gap and the critical temperature

Quantity	Convnetional metals	HTSC
effective mass, m^* [m_e]	1-15	5
Fermi vector, k_F [cm^{-1}]	10^8	$3.5 \cdot 10^7$
Fermi velocity, v_F [cm/s]	$1-2 \cdot 10^8$	$8 \cdot 10^6$
Fermi energy, ε_F [eV]	5-10	0.1

Table III. Comparison of some typical values for the conventional metals and for the HTSC.

In this table the values quoted for HTSC are those of $La_{1.8}Sr_{0.2}CuO_4$. Notice that the only striking difference is in ε_F .

also contribute to it. The coherence length, ξ_0 , is related to the Ginzburg-Landau coherence length, ξ_{GL} , through the expression

$$\xi_{GL} = \frac{a\xi_0}{[1 - (\frac{T}{T_c})^2]} \quad (7.2)$$

which allows us to calculate the **second critical magnetic field**, H_{c2} , as

$$H_{c2} = \frac{\Phi_0}{2\pi\xi_{GL}^2} \quad (7.3)$$

where Φ_0 is the flux quantum. For $La_{1.8}Sr_{0.2}CuO_4$, we get $H_{c2} \simeq 90T$.

7.2 The coherence length and the scenarios

The small coherence length combined with the existence of different scenarios as in $YBa_2Cu_3O_{7-x}$ (one of the most studied HTSC) rises the question whether a multigap structure arises in this compounds. In $YBa_2Cu_3O_{7-x}$ (see Fig. 6.1) one can distinguish three different scenarios, namely, the CuO_2 planes, the CuO chains and the c -axis. At $x = 0$, the chains are fully formed as it is illustrated in Fig. 6.1. This chains dope with holes the CuO_2 planes. The chains behave like a metallic conductors. Indeed, the conductivity along the chains (b -axis) is more than twice as large as in the a -axis direction perpendicular to the chains [22]. The third scenario, the c -axis, is metallic as well [23, 24]. Nevertheless, the c -axis electrons seem to remain in the normal state below T_c . The small coherence length on the CuO_2 plane, the strong anisotropy in the conductivity, and the interaction between the planes and the chains that supplies holes to the planes, open the possibility that the two scenarios go to the superconducting state at the same critical temperature but with different coherence lengths and values of the superconducting gap. The single critical temperature for both sub-systems could mean that the charge transfer that exists between the chains and the planes can also let transfer Cooper pairs once superconductivity is set in the planes, inducing by this mechanism superconductivity on the chains weakened by the smaller strength of the coupling to the boson that causes the phase transition. This would manifest itself in a smaller gap and therefore, according to Eq. 7.1, in a bigger coherence length. There are several evidences for the existence of two gaps. An example is the temperature dependence of the Knight shift [?] and the Nuclear Magnetic Resonance relaxation time [?] that were both found different in the planes and on the chains. For the ratio $\frac{2\Delta(0)}{k_B T_c}$, Eq. 3.26, we find [?] ~ 5 on the planes (much larger than BCS) and ~ 1.8 (much less than BCS) on the chains [23]. This corresponds to an in-plane gap of $19meV$ and an chain-states gap of $7meV$. Cucolo *et al.* [?] obtained a little smaller values for the ratio in both scenarios (4.1 and 1.5, respectively). Low temperature penetration depth measurement [?] give on the chains $\frac{2\Delta(0)}{k_B T_c} \sim 1.25$. One very interesting point is that when oxygen is removed from $YBa_2Cu_3O_{7-x}$ ($x > 0$), the oxygen is taken from the chains. At $x = 0.5$, a complete chain

alternates with an empty one. The fact that the oxygen is taken from the chains affects the hole content on the planes and the critical temperature of the sample. The maximum critical temperature in this compound ($T_c = 92K$) is found when $x=0.06$ or in $YBa_2Cu_3O_{6.94}$ that is known as the **optimal doping**. For oxygen content less than the optimal we have the **under-doped regime** and for samples with more oxygen content, the **over-doped regime**. The stoichiometric sample is in the over-doped regime. In general, over-doped samples are better understood since the Fermi liquid theory seems to apply with higher accuracy. The fact that oxygen is removed preferentially from the chains has physical consequences. The more obvious is that the gap should weaken quicker on the chains as oxygen is removed from the sample with the consequence that the coherence length will be enhanced (see Eq. 7.1). Since at $x = 0.5$ the oxygen atoms form a perfect chain on half the cases and there is no oxygen on the other half, creates an intermediate quite chaotic situation where some of the remaining oxygen atoms move to the interchain position. This creates a kind of broken chain with Cu atoms at the end. These copper atoms form local magnetic states similar to surface states that act as strong pairing breakers in the chain band. This issue could result in gapless superconductivity. For $YBa_2Cu_3O_7$, the two coherence lengths give $\xi_{0plane} \sim 15\text{\AA}$ and $\xi_{0chains} \sim 40\text{\AA}$.

7.3 The carrier-phonon coupling

In conventional superconductors, a very important parameter is the coupling, λ_{e-ph} , between the electrons and the phonons in conventional superconductivity. Cooper pairs in most of the HTSC are composed by holes on the CuO_2 planes. Nobody knows whether superconductivity is phonon-mediated or not. To be able to judge on that possibility, it is important to know the value of the hole-phonon coupling parameter, λ , in these materials. It has not been easy to measure accurately the phonon spectrum for the HTSC and to identify the different modes [25, 26]. Nevertheless, the hole-phonon coupling parameter can be measured from the knowledge of the high and low temperature Sommerfeld constant since they differ by the factor $(1 + \lambda)$ (see Eq. 4.2 and text around). Estimates of this parameter give for both *LaSrCuO* and *YBaCuO* are $\lambda_{plane} \sim 2 - 2.5$. These values correspond to strong hole-phonon coupling and are much higher than the electron-phonon coupling parameter of a strong coupling conventional superconductor as Pb ($\lambda_{e-ph} \sim 1.4$).

Chapter 8

Models on the mechanism

8.1 The electron-phonon mechanism I

It is obvious to me that the first thing to be absolutely sure of is that the electron-phonon mechanism is unable to explain HTSC. I have the personal feeling that this option was eliminated too quickly at the outset and that recent experiments brouth back this concern into the discussion with renewed strength. I will first reproduce some of the arguments in favor of the phonon-mediated mechanism so that it remains clear to the reader what are the odds and the assets in this direction. I will follow closely ref. [27]. The BCS T_c equation ?? is usually accurate only to about a 15% in reproducing the experimental values. For that reason several efforts were done to improve the original equation keeping its simplicity. One of these efforts tries to incorporate the effect of the Coulomb repulsion. The resulting new T_c equation is

$$T_c = 0.25 \omega_{av} \sqrt{e^{\frac{2}{\lambda_{eff}}} - 1} \quad (8.1)$$

where $\omega_{av} \equiv \sqrt{\langle \omega^2 \rangle}$ with ω the phonon frequency and

$$\lambda_{eff} = \frac{(\lambda - \mu^*)}{1 + 2\mu^* + \lambda\mu^*t(\lambda)} \quad (8.2)$$

where $t(\lambda)$ is a universal simple function of λ that approximately takes the value of about .1.7 at $\lambda = 0$ and decreases very rapidly to a negligible value at $\lambda \sim 10$. Kresin *et al.* [27] use Eqs. 8.1 and 8.2 to show that the phonon-mediated superconductivity can account for the measured critical temperatures in the HTSC. In the case of *LaSrCuO*, they use for ω_{av} 15 meV arguing the existence of low frequency modes in this material. For $\lambda \sim 2.2-2.5$, and $\mu^* \sim 0$. This last value requires an explanation. Kresin *et al.* argue that the existence of an additional attraction caused by electronic exaltations can be presented formally as a diminished or even a negative value in μ^* . Under these condicions one gets $T_c \sim 35 - 40K$ that is a very reasonable value for this compound.

The case of $YBaCuO$ is slightly more difficult to analyze since the existence of several scenarios and two cooper planes do not make things simpler. In this case they use the strong coupling Eliashberg equation valid at T_c adapted to layered systems. Kresin *et al.* consider the two sub-systems, the planes and the chains, as the scenarios of superconductivity. Their model considers further the chains as an intrinsic normal system where superconductivity is induced from the planes. Several parameters characterize this situation. First, the in-plane and in-chain hole-phonon coupling, λ_{plane} , and λ_{chain} , respectively, the coupling constant for the interband transitions between the plane bands and the chain bands, λ_{p-ch} , and a parameter characterizing the tunneling of Cooper pairs from the planes to the chains. The most important parameter is obviously λ_{plane} for which they have used 2.5. With $\mu^* = 0 - 0.1$ they have been able to get $T_c = 80 - 90K$ which is well in the range of the experimental value.

Objections against the electron-phonon mechanism

As it is well known, there is no consensus on the mechanism that would explain the occurrence of the superconducting phase transition at such high energies in the HTSC. The small isotope effect has been the first objection against the electron-phonon mechanism. Eq. ?? tells us how in phonon-mediated superconductivity the critical temperature should change with the mass of the isotope : $T_c \sim M^{-\alpha}$ with $\alpha = 0.5$. In HTSC α is measured to give much lower values. Although at the beginning this result has been taken as a serious argument against the phonon-mediated mechanism, it was realized that the isotope effect in compounds as complex as the perovskite cooper oxydes is much more complex and a sharp conclusion is complicated. Another argument is the evaluation of the hole-phonon coupling parameter. In this new materials it has been evaluated from transport experiments [?]. But these experiments deal with the so-called **transport coupling constant**, λ_{tr} , which is related but different from λ and [?] in a layered structure the difference could be large. An important argument is that the value of the gap obtained on the chains by bcs proximity effect (induced superconductivity) is too small ($\Delta = 0.2meV$) [?] and differs by an order of magnitude from the one assumed by Cucolo *et al.* [?] who reproduced three different experimental results (tunneling, specific heat and ultrasonic attenuation) assuming a three-scenario system to simulate superconducting $YBaCuO$, two superconducting (planes $\Delta = 16meV$, chains $\Delta = 4meV$) and one normal (c-axis $\Delta = 0$). Another argument is s-wave pairing assumed by most phonon mediated mechanism theories which is in conflict with the d-wave character of the pairing found experimentally. Under such perspective and considering the phase diagram of cooper oxydes, it is not surprising that research went on seeking an explanation through mechanisms of magnetic character.

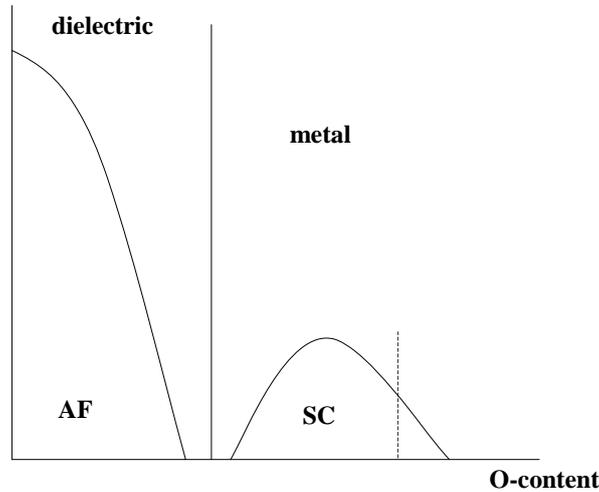


Figure 8.1: A schematic representation of the phase diagram (see text). The vertical axis is the temperature.

8.2 The phase diagram and the symmetry of the pairing

All copper oxides undergo several phase transitions as a function of oxygen content and share **the phase diagram** sketched in Fig. 8.1. In this figure we see that at very low oxygen contents ($YBa_2Cu_3O_6$) and high temperatures, the material is a dielectric. At lower temperatures, below a certain Neel temperature, the material becomes antiferromagnetic. The magnetic moments appear on the Cu atoms on the CuO_2 planes. Still at low temperatures, at higher oxygen contents a spin glass phase takes place. At higher oxygen content, the material becomes metallic and superconductor. The critical temperature rises up to $92K$ for $YBa_2Cu_3O_{6.94}$ which is known as "**the optimal doping**". At stoichiometry ($YBa_2Cu_3O_7$, dotted line on Fig. 8.1), $T_c = 89K$. The crystal structure of $YBa_2Cu_3O_7$ is shown in Fig. 6.1.

An important issue, and one that is closely related to the mechanism of superconductivity in cuprates, is **the symmetry of the superconducting ground state wave function**. Conventional phonon-mediated superconductors have wave functions with **s-symmetry** and therefore have a superconducting gap which is non-zero everywhere on the Fermi surface. Magnetic pairing interactions have higher symmetry wave functions with zeros in the gap. The manifestation of zeros in the gap would be very similar to gapless superconductivity or to the presence of unpaired carriers at very low temperatures which

would occur because of oxygen vacancies in the chain band. Also if the c-axis is metallic and the electron-phonon interaction is not enough to produce pairing, the carriers would stay independent even at low temperatures below T_c . The consensus, nevertheless, is that the new superconductors are **d-wave pairing**. On the plane a representation of this pairing would be

$$\Delta_k = OJO \quad (8.3)$$

8.3 The Hubbard hamiltonian and the spin fluctuation mechanism

Pairing interactions based on repulsive ($U < 0$) single band Hubbard model lead to d-wave pairing. The **Hubbard Hamiltonian** is

$$H = \sum_{i,j,\sigma} (t_{ij} c_{i\sigma}^+ c_{j\sigma} + h.c.) + U \sum_i n_{i\uparrow} n_{i\downarrow}. \quad (8.4)$$

where $t_{i,j}$ is the hopping integral between sites i and j ($-|t|$ is the gain in energy by delocalizing the carriers), $c_{i\sigma}^+$ is the operator that creates an electron with spin σ on site i and the operator $c_{j\sigma}$ annihilates an electron with spin σ at site j . The number operator $n_{i\sigma} = c_{i\sigma}^+ c_{i\sigma}$. U is the interaction energy between two electrons on the same site. It is convenient to describe properties of solids to add a term that describes inter-site interactions. We get the **Extended Hubbard Hamiltonian**

lerolerolero

$$H = \sum_{i,j,\sigma} (t_{ij} c_{i\sigma}^+ c_{j\sigma} + h.c.) + U \sum_i n_{i\uparrow} n_{i\downarrow} + \frac{V}{2} \sum_{\langle i,j \rangle} n_i n_j \quad (8.5)$$

with V the interatomic interaction between two electrons one at site i and one at site j . The symbol $\langle \rangle$ means that we take first nearest neighbors interactions only. $h.c.$ stands for hermitian conjugate. The parameters U and V are phenomenological parameters.

But historically, the idea on the effect of excitations from magnetic degrees of freedom on superconductivity was just the opposite. Indeed, it was realized that it is a breaking mechanism for Cooper pairs. This situation was considered long ago by Berk and Schrieffer [?](Kc5r1:KresiCapVref1) and by Engelsberg [?] who showed that incipient ferromagnetic order could **suppress** phonon-induced s-wave pairing. The generalization of the Eliashberg equations and their solution including the effect of paramagnons was reported by Baquero, Daams and Carbotte [?]. Spin fluctuations have a dramatic effect on superconductivity in Palladium (Pd) where it is totally suppressed by the effect of paramagnons. When hydrogen is added to the sample, Pd-H becomes a superconductor at $T_c = 13K$ as the effect of hydrogen is to weaken the paramagnons and therefore also their effect in breaking Cooper pairs.

Pairing due to magnetic excitations has been first proposed for ${}^3\text{He}$. Anderson and Brinkman [?] proposed that nearly antiferromagnetic spin fluctuations in the p-wave channel can cause the formation of pairs in ${}^3\text{He}$. Further, Scalapino, Low, and Hirsch [?, ?] and Miyake, Schmitt-Rink, and Varma [?] suggested that d-wave pairing due to nearly antiferromagnetic spin fluctuations could cause the formation of Cooper pairs in heavy-fermion materials. When one takes into account these observations and the phase diagram (Fig. 8.1) it is only natural that magnetic mechanisms are considered as an explanation to the HTSC.

8.3.1 A cartoon picture

Let me first introduce a cartoon picture about spin fluctuations to show how the same mechanism can be disruptive and constructive of superconductivity. Refer to Fig. ?? . Let us imagine that we have a crystal field built up by atoms (A) that are localized in the Mendelejev Table just before an atom (B) that crystalizes in an antiferromagnetic phase. The crystal potential around such an ion (A) observed by a conduction d-electron comprises a repulsive part at a small distance away from the ion through which the electrons can tunnel to an attractive part of the potential near the ion. Due to the shape of this potential, a conduction d-electron (**e1**) with spin, say \uparrow , is trapped around **ion 1** during a short relaxation time. During this period of time, the **ion 1** (with the trapped d-electron) builds an antiferromagnetic surrounding since its electron cloud is undistinguishable from the one of atom B which crystalizes as an antiferromagnetic. This clasts a condition on the result of an electron-ion interaction on the neighboring atom. Indeed, if during the relaxation time period, a second electron interacts with **ion2**, it will be trapped only if it has an opposite spin (**e2**) and therefore builds an antiferromagnetic surrounding during the relaxation time period. This is due to the **ion1- ion2 interaction**. Otherwise, if the interacting electron with **ion2** does not have opposite spin, the it will be scattered out (**e3**). After the relaxation time is elapsed both electrons tunnel back to the "free" space between the ions and the whole process begins again. But this time the trapped electron can have a different spin so that at the ion sites the spin fluctuates.

The condition on the interaction of **e2** with **ion2** due to the fact that **e1** is temporary trapped at the **ion1**-site is similar to the attraction that the polarization wave created by an electron exerts on another electron, namely, its Cooper pair mate. This cartoon picture is aimed to make it plausible the idea that spin fluctuations can create under suitable condition Cooper pairs and therefore be responsible for the superconducting phase transition. In what follows we will present a more elaborate formulation of this problem. It is easy to have also from Fig. ?? a cartoon image for the reason why spin fluctuations act as a disruptive mechanism for electron-phonon mediated superconductivity. Given **e1** on **ion1**-site, it is also possible that an electron with the same spin tunnels and gets trapped temporarily at **ion2**-site. But due to the **ion1-ion2** interaction, the minimum energy will be attained when the spin of the trapped electron at

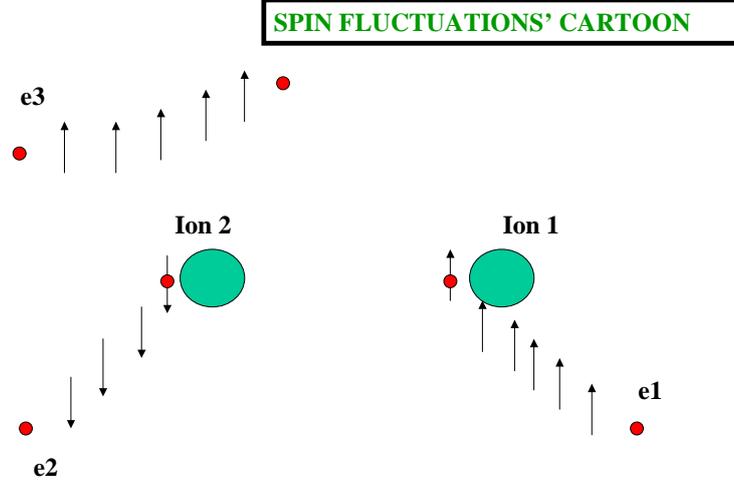


Figure 8.2: The spin fluctuations can act as a disruptive or as an attractive mechanism (see text).

ion2-site is of opposite sign. In that case the trapped electron will switch spin. If it is a mate in a Cooper pair, this switching will kill the pairing condition and the Cooper pair will be destroyed which obviously weakens superconductivity.

8.3.2 Back to the Hubbard Hamiltonian

Let us consider again the Hubbard Hamiltonian 8.4 and use it to describe a one-dimensional chain of N atoms with nearest neighbors interactions t , and an on-site Coulomb repulsion between two carriers of opposite sign U . Let us further consider one electron on each site. If $U = 0$, this situation represents half filling since we can have two electrons of opposite spins on each site. It is easy now to see that if $U \gg t$ and we place electrons of opposite spins on adjacent sites, we have the ground state of an antiferromagnet. And it will be an antimagnetic insulator (see Fig. 8.1) since on moving an electron from one site to the next, the system gains an energy $|t|$ but needs an energy U which is much bigger. The starting question here is how to find the way to describe the transition of the system from an insulator to a conducting state as a function of the carrier concentration for a range of finite values of the parameter, $\eta \equiv \frac{|t|}{U}$. This problem has been solved in one dimension, there is a lot of advance in two dimensions but the problem is not solved yet in three dimensions.

It is appealing to describe LaSrCuO, YBaCuO and other families of HTSC cuprates taking as a starting point the Hubbard Hamiltonian since they all

8.3. *THE HUBBARD HAMILTONIAN AND THE SPIN FLUCTUATION MECHANISM* 59

are antiferromagnetic insulators at the low oxygen concentration of the phase diagram.

Chapter 9

Important recent experiments

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Chapter 10

Appendix: Vortices

10.1 material de trabajo:

R. Baquero *et al.* RMF **35**, 461 (1989)

J.M. Daams *et al.* JLTP (1979)

optical conductivity

SCdivulgacionLIC (power point)

NobelsEscAvVer05 (power point)

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The First Appendix