Mémoire

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Faculté : Faculté des Sciences
Diplôme : Master en sciences physiques, à finalité approfondie
Année académique : 2022-2023
URI/URL : http://hdl.handle.net/2268.2/18462

FACULTY OF SCIENCES
DEPARTMENT OF PHYSICS

Superconductivity in open quantum systems

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A thesis submitted for the degree of
Master in physics

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Acknowledgments

I would like to express my deepest gratitude to Dr. François Damanet for his supervision of this thesis. He has always been available to answer all my questions and gave me many good advice for the writing of this thesis.

I would like to sincerely thank the members of my reading committee, Prof. Stéphane Dorbolo, Prof. John Martin and Prof Alejandro Silhanek. I appreciate that you accepted this role and I hope you will find pleasure in your reading.

Finally, I would like to thank my friends and family for the support during all these years.

Contents

Introduction

When he discovered superconductivity in 1911 [1], Kamerlingh Onnes probably did not foresee the impact of this discovery. And yet here we are, more than a hundred years later, and superconductors are still a hot topic in scientific research and they regularly make their way to mainstream news as we can see with the very recent announcement and controversy about the LK-99 [2]. From the 4.2 Kelvin superconductivity of the mercury to a critical temperature of 138 K at ambient pressure for the cuprate $Hg_{12}Tl_3Ba_{30}Ca30Cu_{45}O_{127}$ [3] and of 250 K at a pressure of 170 GPa for LaH_{10} [4] many superconducting materials have been discovered during all those years (see Fig. 1) for a timeline of the discoveries). But the holy grail, a room-temperature, atmospheric pressure, superconductor, still eludes all the researchers of the discipline.
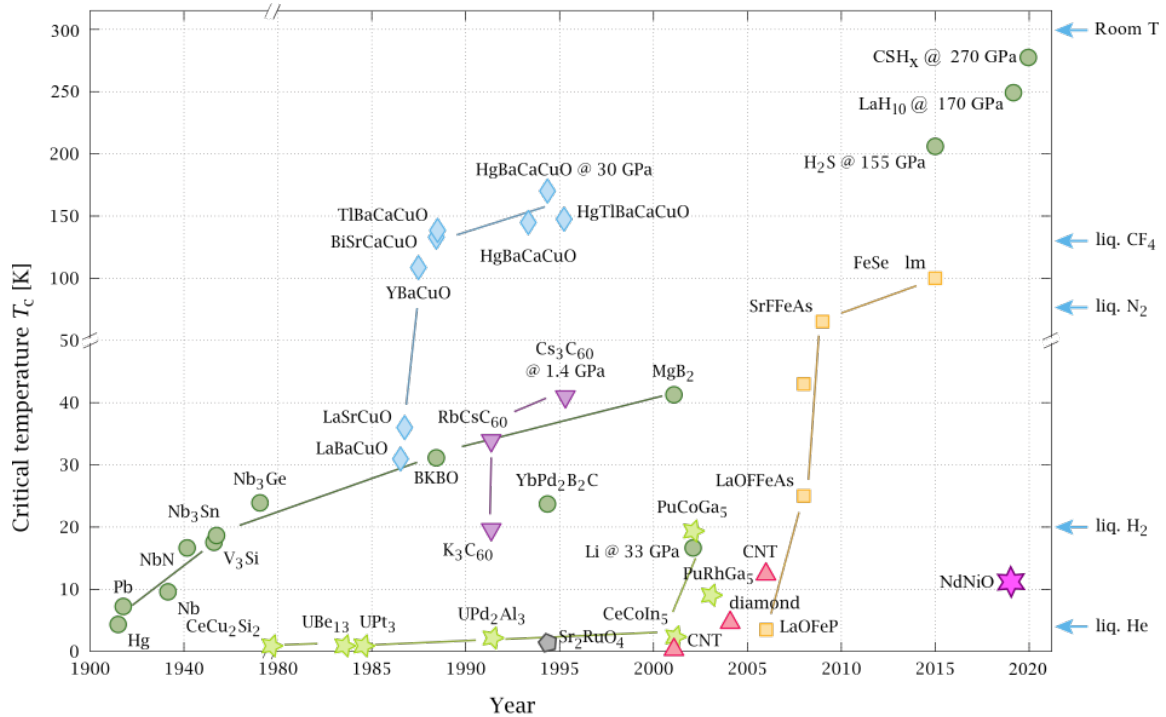
Figure 1: Timeline of the discovery of all the superconducting materials with their critical temperature and, if not atmospheric, the pressure at which the superconductivity is obtained. The colored shapes represent different classes of superconductors. Figure taken from the Wikipedia page on superconductivity [5]

Nevertheless, superconductors have found their way to practical applications. We can indeed find them in different technological applications. Superconducting electromagnets are used in magnetic resonance imaging (MRI) [6] and nuclear magnetic resonance (NMR) [7] but also in particles accelerators like the large hadron collider (LHC) [8]. Superconductors are at the basis of ultrasensitive measurement devices like bolometers [9, 10], magnetometers [11] or photon detector [12]. And

obviously, superconductivity has found is way to quantum computing with superconducting qubits [13, 14]. Future applications for superconductors are expected and even already being tested like electromagnets for nuclear fusion reactor [15], maglev trains [16] or superconducting power lines [17]. But technological applications would greatly benefit from that holy grail that is room-temperature superconductors. Such a discovery would indeed allow for applications outside of the industrial and research worlds, as it would make it possible to avoid the use of expensive and cumbersome cryogenic systems.

The goal of this thesis is to explore ways of enhancing the critical temperature of superconductors. The general idea is to push a superconductor out-of-equilibrium by coupling it to fermionic reservoirs, which requires to treat the superconducting system with the tools of open quantum system. Exploiting the interaction of a quantum system with an environment has already been used with success for the preparation of entangled states [18, 19] or to improve quantum algorithm [20] or quantum communication protocol [21] for examples. Enhancement of superconductivity has been performed by using electromagnetic fields leading to light-induced superconductivity [22] or to Eliashberg effect [23] but a systematic, full-quantum, theoretical way of treating superconducting system in interaction with some environment is yet to be developed. This thesis constitutes a new contribution along these lines. Using the simplest models for both the superconductor and its environment, we will derive the equation governing the dynamic of the superconductor coupled to fermionic reservoirs and study how such a coupling affect its properties.

Chapter 1 will be dedicated to define the essential tools we will be using all along the thesis. Indeed, this work will require to use of second quantization formalism which makes use of what is called creation and annihilation operators. We will be defining those operators and give their most basic properties so that the reader will be able to follow the developments in the subsequent chapters.

In chapter 2 we will present the BCS theory of superconductivity. This theory is the first microscopic theory explaining the origin of standard superconductivity (meaning not what is called high-temperature superconductivity). BCS explains superconductivity by the pairing of opposite spin and momentum electrons mediated by interaction with the phonons. At the end of the chapter, we will also talk about the standard algorithm used to solve numerically superconducting systems, the self consistent Hartree-Fock-Bogoliubov (HFB) algorithm. We will be implementing the HFB algorithm ourselves and using it to verify some theoretical properties previously given.

Chapter 3 will be used to discuss the theory of open quantum systems. Once we consider a quantum system to be in interaction with some environment (for example an atom irradiated by a laser) then its time evolution is no longer only unitary (like when it obeys the Schrodinger equation) but has also a non-unitary (irreversible) evolution. We will begin the chapter by defining and give some properties of the density operator, a more general way to describe a quantum state than the ket vector. After that we will explain how to derive a Markovian master equation, that is the dynamical equation of the open quantum system when the interaction with the system is weak. We will then apply that derivation to a fermionic 4-level system and numerically solve the master equation in a few different setups to see how this affect the distributions of the fermions in the system.

Finally, in chapter 4, we will use the results of chapter 3 as the new distribution of the quasi-particles in a superconductor, as if it was an open quantum system. Indeed, because of the coupling to the environment, the quasi-particles in the system are no longer in thermal equilibrium and therefore we cannot assume that they are distributed according to the Fermi-Dirac distribution, the standard assumption in the BCS model of superconductivity and the HFB algorithm. By modifying the HFB algorithm implemented in chapter 2 by taking into account the environment and the new distribution of the quasi-particles derived in chapter 3, we will explore how compare the numerical results of chapter 2 with the results of the out of equilibrium system.

Throughout the whole master thesis, we will work in units such that $\hbar = k_B = 1$.

Chapter 1

Many-body quantum theory

Since this thesis will deal with systems consisting of many particles it seems important to remind the reader how quantum mechanics deals with such systems and to introduce the specific tools and concepts needed.

We will start with the first approach for a quantum treatment of many-body systems, that is with a wavefunction in a many body Hilbert space constructed as a product of one particle Hilbert spaces and then make sure this wavefunction is (anti)symmetric depending of the statistic of the particles involved in the system. We will see that this process is quite laborious and not adapted to deal with systems with variable number of particles. A new formalism will thus be introduced, leading to a simpler description allowing for changing the number of particles in the system via *creation* and *annihilation* operators. This chapter is based on the lectures notes of Prof. P. Schlagheck [24] and on the books of C. Cohen-Tannoudji, B. Diu and F. Laloë [25, 26]

1.1 The many-body space

Let us consider a quantum system of N *indistinguishable* particles, meaning particles exhibiting the same properties (same mass, same charge, same spin,...). Indistinguishability implies that in such a system one cannot label the particles, for example in a system of N electrons there is no way to tell which electron is in position r_1, which one is in position r_2 and so on. One can only tell that there is an electron in position r_1, an electron in position r_2 and so on.

The state of the system is characterized at any time by a wavefunction of the form

$$\psi \equiv \psi(\xi_1, ...\xi_N) \equiv \psi(\mathbf{r}_1\sigma_1, ..., \mathbf{r}_N\sigma_N) \tag{1.1}$$

where $\xi_i \equiv (\mathbf{r}_i, \sigma_i)$ is the generalized coordinates for the *ith* particle with r its position and σ its spin.

This wavefunction contains all the information about the system and $|\psi(\xi_1, \ldots, \xi_N)|^2$ represents the probability density to find particle 1 in position $\mathbf{r}_1$ and with spin σ_1, particle 2 in position $\mathbf{r}_2$ and with spin σ_2, etc. To have physical meaning this density should be normalized such that

$$\int d\xi_1 ... \int d\xi_N |\psi(\xi_1, ..., \xi_N)|^2 \equiv \int d^3r_1 \sum_{\sigma_1} ... \int d^3r_N \sum_{\sigma_N} |\psi(\mathbf{r}_1\sigma_1, ..., \mathbf{r}_N\sigma_N)|^2 = 1, \tag{1.2}$$

mathematically translating the fact that the N particles must be found somewhere in space.

We know that the wavefunction of a single-particle system must belong to a Hilbert space $\mathcal{H}_1$ of square integrable functions $L^2(\mathbb{R}^3)$

$$\mathcal{H}_1 = \{\psi : \mathbb{R}^3 \times I \to \mathbb{C}, \xi \equiv (\mathbf{r}, \sigma) \mapsto \psi(\xi) \equiv \psi(\mathbf{r}, \sigma) \text{ with } \int d\xi |\psi(\xi))|^2 < \infty\} \tag{1.3}$$

with I the spin space (e.g. $I = \{-\frac{1}{2}, \frac{1}{2}\}$ for electrons). In this Hilbert space one can construct an orthonormal basis :

$$\mathcal{B}_1 = (|\phi_0\rangle, |\phi_1\rangle, ...) \equiv (|\phi_k\rangle)_{k \in \mathbb{N}_0} \tag{1.4}$$

where the ϕ_k are functions of $\mathcal{H}_1$ such that (orthogonality relation):

$$\langle \phi_k | \phi_{k'} \rangle = \int d\xi \, \langle \phi_k | \xi \rangle \, \langle \xi | \phi_{k'} \rangle = \int d\xi \phi_k^*(\xi) \phi_{k'}(\xi) = \delta_{kk'}. \tag{1.5}$$

Now that we have a basis we can use it to represent operators acting in $\mathcal{H}_1$

$$A = \sum_{k,k'=0}^{\infty} A_{kk'} |\phi_k\rangle \langle \phi_k'| \text{ with } A_{kk'} = \langle \phi_k | A | \phi_{k'} \rangle . \tag{1.6}$$

The Hilbert space describing a N body system is then given by the tensor product of N single-particle Hilbert space $\mathcal{H}_1$

$$\mathcal{H}_N = \underbrace{\mathcal{H}_1 \otimes ... \otimes \mathcal{H}_1}_{\text{N times}} \tag{1.7}$$

and an orthonormal basis $\mathcal{B}_N$ of this space is made of N one-state basis

$$\mathcal{B}_N = (|\phi_{k_1}\rangle, |\phi_{k_2}\rangle, ..., |\phi_{k_N}\rangle)_{k_1,...k_N \in \mathbb{N}_0}. \tag{1.8}$$

We can write the **total operator** $\hat{\mathrm{A}}$[1] in this basis

$$A = \sum_{k_1,...,k_N=0}^{\infty} \sum_{n=1}^{N} \sum_{k_n'=0}^{\infty} A_{k_n k_n'} |\phi_{k_1}, ..., \phi_{k_n}, ..., \phi_{k_N}\rangle \langle \phi_{k_1}, ..., \phi_{k_n}, ..., \phi_{k_N} | . \tag{1.9}$$

1.2   The symmetry postulate

As we said earlier, in quantum mechanics it is postulate that two **identical** particles are **indistinguishable**, this implies that the wavefunction of a system of N identical particles must be **invariant** under transposition of two particles:

$$\Pi_{nn'} \psi(\xi_1, ..., \xi_n, ..., \xi_{n'}, ...\xi_N) = \psi(\xi_1, ..., \xi_{n'}, ..., \xi_n, ...\xi_N) \tag{1.10}$$

where $\Pi_{nn'}$ is the **transposition** operator. Obvious properties of $Pi_{nn'}$ are : $\Pi_{nn'} = \Pi_{n'n} = \Pi_{nn'}^{\dagger}$ and $\Pi_{nn'}^2 = \mathbb{1}$. Meaning that $\Pi_{nn'}$ is a hermitian, unitary operator having eigenvalues ± 1. Therefore its eigenfunctions are either symmetric (for eigenvalue +1) or antisymmetric (for eigenvalue -1) under exchange of coordinates. This invariance imposes that the transposition operators should commute with the Hamiltonian : $[H, \Pi_{nn'}] = 0$. We would be tempted to choose a common basis of all $\Pi_{nn'}$ in which the Hamiltonian is diagonal. However, for $N > 2$ the transposition operators do not commute with each other in general. For them to commute we must impose that ψ is either **entirely symmetric** or **entirely antisymmetric** with respect to exchange of coordinates then defining two orthogonal subspaces $\mathcal{H}_N^{\pm}$ of the Hilbert space, the (anti)symmetric subspace which contain entirely (anti)symmetric wavefunctions:

$$\mathcal{H}_N^{\pm} = \{ \psi \in \mathcal{H}_N : \Pi_{nn'} \psi = \pm \psi \, \forall \, n, n' = 1, ..., N \}. \tag{1.11}$$

The symmetry postulate then state that any physical system of N identical will be represented by either an entirely symmetric or entirely antisymmetric many-body wavefunction and a many-body wavefunction initially in $\mathcal{H}_N^+$ (respectively in $\mathcal{H}_N^-$) will always stay in this subspace. For the symmetric case the particles are called **bosons** while for the antisymmetric case they are called **fermions**. Since we will only deal with fermionic particles we will from now on only consider them in the developments and drop the superscript.

We can now construct the antisymmetric basis $\mathcal{B}_N$ of the antisymmetric subspace. Let us start by the simplest case $N = 2$: the Hilbert space $\mathcal{H}_2$ is spanned by the basis $\mathcal{B}_2 = (|\phi_{k_1}\phi_{k_2}\rangle)_{k_1,k_2 \in \mathbb{N}_0}$. After antisymmetrization we obtain the following basis

$$|\phi_{k_1 k_2}\rangle = \mathcal{A}_{k_1,k_2}(|\phi_{k_1}\phi_{k_2}\rangle - |\phi_{k_2}\phi_{k_1}\rangle) \tag{1.12}$$

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[1]For a system of N **indistinguishable** particles it would not be relevant to use operator acting on a single particle since we cannot tell the particles apart it is thus logical to speak of **total** operator.

with $\mathcal{A}_{k_1,k_2}$ a normalization constant to be determined. We directly see that we cannot have two fermions occupying the same state. Indeed, we have

$$|\phi_{k_1 k_1}\rangle = \mathcal{A}_{k_1,k_1}(|\phi_{k_1}\phi_{k_1}\rangle - |\phi_{k_1}\phi_{k_1}\rangle) = 0, \tag{1.13}$$

which mathematically expresses the **Pauli exclusion principle**. Finally, the normalization condition $\langle\phi_{k_1 k_2}|\phi_{k_1' k_2'}\rangle = \delta_{k_1 k_1'}\delta_{k_2 k_2'}$ lead to $\mathcal{A}_{k_1 k_2} = 1/\sqrt{2}$, for $k_1 > k_2$[2].

When considering $N > 2$ we need to introduce the **permutation** group

$$\Pi_N = \{\pi : \{1,...,N\} \to 1,...,N, n \mapsto \pi(n) : \pi(n) = \pi(n') \Leftrightarrow n = n' \;\forall\; n, n' = 1,...,N\}. \tag{1.14}$$

This group contains N! elements and each one is either **even** or **odd** depending on the number of transposition operators needed to represent it, defining the signature of the permutation $(\pm 1)^\pi$. Our normalized and symmetric basis are then expressed by

$$|\phi_{k_1...k_N}\rangle = \frac{1}{\sqrt{N!}} \sum_{\pi \in \Pi_N} (\pm 1)^\pi |\phi_{k_{\pi(1)}}...\phi_{k_{\pi(N)}}\rangle. \tag{1.15}$$

In conclusion, the procedure to construct the ket representing a system of N identical particles is the following :

- We arbitrary label the particles then we construct the ket $|\psi\rangle$ corresponding to the physical state in consideration and the labeling.

- We symmetrize or antisymmetrize $|\psi\rangle$ depending of the nature of the particles.

- Finally, we normalize the vector.

1.3   Second quantization : Fock space

The framework developed above has three majors problems, firstly the idea of labeling the particles is inconsistent with the indistinguishability of particles, secondly applying the symmetry postulate becomes very thorough task when the number of particles become large and finally it does not allow to work with a variable number of particle. Thus a more useful framework is presented using **creation** and **annihilation** operators acting in the **Fock space**.

Instead of putting the ith particle in the state $|\phi_{k_i}\rangle$ like we did previously we are now going to give the number of particles n_k we have in each state k. To this end we rewrite the basis $\mathcal{B}_N$

$$|\phi_{k_1...k_N}\rangle \equiv |n_0, n_1, n_2, ...\rangle \tag{1.16}$$

and a given $|n_0, n_1, n_2, ...\rangle$ will be called **Fock state**. The space in which live all those state is called the **Fock space**

$$\mathcal{H}^\pm = \bigoplus_{N=0}^\infty \mathcal{H}_N^\pm = \mathcal{H}_0 \oplus \mathcal{H}_1 \oplus \mathcal{H}_2^\pm \oplus \mathcal{H}_3^\pm \oplus ... \tag{1.17}$$

which is the direct sum of all the spaces $\mathcal{H}_N^\pm$. The Fock space basis is then the union of the individual basis $\mathcal{B} = \cup_{N=0}^\infty \mathcal{B}_N$ with $\mathcal{B}_N$ defined in (1.16):

$$\mathcal{B}_N^\pm = \left\{ |n_0, n_1, n_2, ...\rangle : \sum_{k=0}^\infty n_k = N \right\} \tag{1.18}$$

with $n_k \in \{0, 1\}$ for fermions, since we cannot have two fermions in the same state k due to the Pauli exclusion principle.

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[2]we impose $k_1 > k_2$ to avoid double counting of identical states

Now that the Fock space and the Fock states living inside we can define those creation ($c_k^\dagger$) and annihilation (c_k) operators we talked about before by their action on the Fock states

$$c_k^\dagger \left| n_0, n_1, ..., n_k, ... \right\rangle = (-1)^{n_0 + ... + n_{k-1}} (1 - n_k) \left| n_0, n_1, ..., n_k + 1, ... \right\rangle, \tag{1.19}$$

$$c_k \left| n_0, n_1, ..., n_k, ... \right\rangle = (-1)^{n_0 + ... + n_{k-1}} n_k \left| n_0, n_1, ..., n_k - 1, ... \right\rangle. \tag{1.20}$$

We see that the names of these operators is appropriate considering their effect on a Fock state, $c_k^\dagger$ will create a particle in the state $\left| \phi_k \right\rangle$ and c_k will destroy a particle in $\left| \phi_k \right\rangle$. Those operators follows the rules of fermionic algebra

$$\{c_k, c_{k'}^\dagger\} = \delta_{kk'}, \tag{1.21}$$

$$\{c_k, c_{k'}\} = \{c_k^\dagger, c_{k'}^\dagger\} = 0. \tag{1.22}$$

Finally, note that any operator can be written in terms of the creation and annihilation operators the simplest example being the number operator $n_k = c_k^\dagger c_k$ which gives the number of particles occupying the state k.

Chapter 2

BCS theory

The BCS theory is a fundamental theory for standard superconductors. It is thus important the explains the basis of this theory. This theory developed by John Bardeen, Leon N. Cooper, and Robert Schrieffer in 1957 [27, 28] finds the origin of superconductivity in the creation of bound pairs of electrons, known as Cooper pairs, due to an attractive interaction between them.

We will see in this chapter that if we consider an attractive interaction between electrons at $T=0$K in a simplified many electrons system then a bound state between two electrons is energetically favorable compared to free electrons. Then we shall discuss what is the origin of this attraction between the electrons in standard materials. We will then derive mathematically the new state made of these pairs of electrons first at zero then at finite temperature. Finally, we will end this chapter by explaining how to numerically simulate such systems using a self consistent approach and by numerically verifying a few properties of the theory.

A thorough derivation of the BCS theory would require some advanced mathematical tools such as Green's functions and Feynman diagrams[1]. Nevertheless, one can get a good understanding of the phenomenon using more basic tools of quantum mechanics. This is the path we will choose here, with a derivation mainly inspired by the book of M. Tinkham "Introduction to superconductivity" [30].

2.1 Cooper pairs

Before diving in the theory of superconducting material, we should make a brief reminder of the classic theory of metals. In metals, the electrons will fill the levels from the lowest the to the highest energy, respecting the Pauli exclusion principle, up the Fermi energy. All these electrons form what is called the **Fermi sea** and the surface of this sea is the **Fermi level**. Only the electrons at the Fermi level are really relevant for the properties of the material (such as electrical or thermal conductivity, magnetic properties,...) since the other electrons are more deeply "tied" to the material and are screened by each other. Those surface electrons can be considered as free electrons (plane waves), and have thus an energy dispersion given by

$$\epsilon_{\mathbf{k}} = \frac{\mathbf{k}^2}{2m} \tag{2.1}$$

with $\mathbf{k}$ the wave vector and m the (effective) mass of the electron[2]. This energy dispersion is showed in fig 2.1.

It was in 1956 that Cooper proposed that an attraction, not matter how weak, will lead to an instability in the Fermi sea and the pairing of electrons in pairs [31].

To show that the binding happens, let us consider a simple model composed of a Fermi sea at $T=0$ K to which is added two electrons at positions $\mathbf{r_1}$ and $\mathbf{r_2}$ respectively. The electrons are only

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[1]See for example the book by Carsten Timm [29] for such a derivation.

[2]For the sake of simplicity here, we consider an isotropic effective mass, i.e., $m_x = m_y = m_z = m$ where m_α ($\alpha = x, y, z$) are the effectives masses in the α direction.
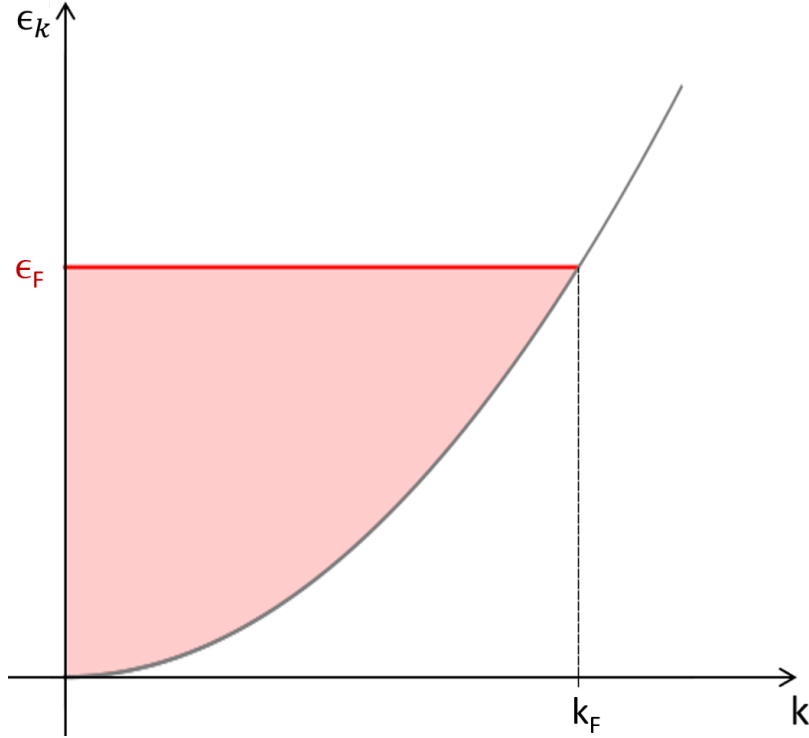
Figure 2.1: Energy dispersion of electrons in metal. The electrons fill all available states up to the Fermi energy (or Fermi level) forming the Fermi sea.

interacting between each other and not with the Fermi sea (except for the Pauli exclusion principle). The simplest wavefunction for these two electrons is a combination of Gaussian wave packets with the two momentum $\mathbf{k}$ being opposite so that the energy is the lowest possible. Such a wavefunction writes like

$$\psi_0(\mathbf{r}_1, \mathbf{r}_2) = \sum_{k > k_F} g_{\mathbf{k}} e^{i\mathbf{k}.\mathbf{r_1}} e^{-i\mathbf{k}.\mathbf{r_2}}. \tag{2.2}$$

Where the $g_{\mathbf{k}}$ are normalization constants. Now, since electrons are fermionic particles, we know that our wavefunction has to be antisymmetric. There is two ways for our wavefunction to be antisymmetric. First possibility is as a product of $\cos \mathbf{k}.(\mathbf{r}_1 - \mathbf{r}_2)$ with the antisymmetric singlet spin state $(\uparrow_1\downarrow_2 - \downarrow_1\uparrow_2)$ where the subscripts tell us to which electron is the spin. Second possibility is as a product of $\sin \mathbf{k}.(\mathbf{r}_1 - \mathbf{r}_2)$ with the symmetric triplet spin state $(\uparrow_1\uparrow_2, \uparrow_1\downarrow_2 + \downarrow_1\uparrow_2, \downarrow_1\downarrow_2)$. Since we expect an attraction between the electrons we choose the first combination because the cosine gives a larger probability for the two electrons to be close to each other. We can then rewrite our wavefunction as

$$\psi_0(\mathbf{r}_1, \mathbf{r}_2) = \left[\sum_{k > k_F} g_{\mathbf{k}} \cos \mathbf{k}.(\mathbf{r}_1 - \mathbf{r}_2)\right] (\uparrow_1\downarrow_2 - \downarrow_1\uparrow_2) \tag{2.3}$$

where the up and down arrows refer to the spin state of the electron. Schrodinger equation gives us [32]

$$(E - 2\epsilon_{\mathbf{k}})g_{\mathbf{k}} = \sum_{k' > k_F} V_{\mathbf{k}\mathbf{k'}} g_{\mathbf{k'}} \tag{2.4}$$

with ϵ_k the energies of the plane-wave and $V_{kk'}$ the matrix element of the interaction potential

$$V_{\mathbf{k}\mathbf{k'}} = \frac{1}{\Omega} \int V(\mathbf{r}) \exp\{i(\mathbf{k'}\text{-}\mathbf{k}).\mathbf{r}\} d\mathbf{r} \tag{2.5}$$

with $\mathbf{r}$ the distance between the two electrons and Ω the normalization volume. The elements $V_{\mathbf{kk'}}$ give the value of the potential for scattering a pair of electrons with initial momenta ($\mathbf{k}$',-$\mathbf{k}$') to a momenta ($\mathbf{k}$,-$\mathbf{k}$). If we can find a set of $g_{\mathbf{k}}$ satisfying (2.4) with $E < 2E_F$ then the bound state is energetically favorable.

In order to simplify the analysis, Cooper introduced an approximation for the potential

$$V_{kk'} = \begin{cases} -V & \text{if } \xi_{\mathbf{k}} \text{ and } \xi_{\mathbf{k'}} < \omega_c \\ 0 & \text{otherwise,} \end{cases} \tag{2.6}$$

with the energy taken relative to the Fermi level, $\xi_{\mathbf{k}} = E_{\mathbf{k}} - E_F$. That is only the electrons with energies up to a cutoff frequency ω_c from the Fermi level will feel a constant interaction of strength V, then (2.4) can be rewritten as

$$g_{\mathbf{k}} = V \frac{\sum_{k'>k_F} g_{k'}}{2\epsilon_{\mathbf{k}} - E}. \tag{2.7}$$

Now we can sum over all $|\mathbf{k}| > k_F$ and simplify the sums on $g_{\mathbf{k}}$ and $g_{\mathbf{k'}}$

$$\frac{1}{V} = \frac{1}{\sum_{k>k_F}(2\epsilon_{\mathbf{k}} - E)}. \tag{2.8}$$

Now let us replace the sum by an integration and introduce $D(F)$, the density of states (DOS) for one spin orientation electrons at the Fermi level

$$\frac{1}{V} = D(F) \int_{E_F}^{E_F+\omega_c} \frac{d\epsilon}{2\epsilon - E} = \frac{1}{2} ln \frac{2E_F - E + 2\omega_c}{2E_F - E}$$

$$\Leftrightarrow e^{\frac{2}{D(F)V}} = \frac{2E_F - E + 2\omega_c}{2E_F - E}$$

$$\Leftrightarrow e^{\frac{2}{D(F)V}} = 1 + \frac{2\omega_c}{2E_F - E}$$

$$\Rightarrow e^{\frac{2}{D(F)V}} = \frac{2\omega_c}{2E_F - E} \quad \text{if} \quad e^{\frac{2}{N(F)V}} \gg 1.$$

In most superconductor we observe that $D(F)V < 0.3$ we can thus make the above **weak coupling approximation**. Finally solving for E we have

$$E = 2E_F - 2\omega_c e^{\frac{-2}{D(F)V}} \tag{2.9}$$

we indeed find an energy smaller than $2E_F$ for an arbitrary small V. Meaning than if we have an attractive potential, no matter its strength, a bound state is favorable in small range of energies above the Fermi level. This bound state of electrons is called **Cooper pairs**.

If we come back to equation (2.7) we see that $g_{\mathbf{k}}$ depends on $\mathbf{k}$ only through $\epsilon_{\mathbf{k}} = k^2/2m$ meaning only on the absolute value of $\mathbf{k}$. That means that the wavefunction of Eq. (2.2) has a spherical symmetry. The Cooper pair wavefunction is a s-wave.

2.2   Origin of the attraction

The BCS theory requires the matrix elements $V_{\mathbf{kk'}} \equiv V(\mathbf{k} - \mathbf{k'}) \equiv V(\mathbf{q})$ which give the strength of the potential for scattering a pair of electrons of momenta $(\mathbf{k'}, -\mathbf{k'})$ to momenta $(\mathbf{k}, -\mathbf{k})$ to be negative. These matrix elements are given by :

$$V_{\mathbf{kk'}} = \Omega^{-1} \int V(\mathbf{r}) e^{i\mathbf{q} \cdot \mathbf{r}} d\mathbf{r} \tag{2.10}$$

with $\mathbf{r}$ the distance between the two electrons and Ω the normalization volume If we consider bare electrons then our potential V($\mathbf{r}$) is the Coulomb potential

$$V(\mathbf{r} - \mathbf{r'}) = \frac{e^2}{4\pi\epsilon_0 |\mathbf{r} - \mathbf{r'}|}, \tag{2.11}$$

its Fourier transform yields

$$V_{\mathbf{q}} = \frac{e^2}{\epsilon_0 q^2} \tag{2.12}$$

which is obviously always positive thus giving a repulsive interaction.

If we consider the electrons in a metal then we need to take into account the medium, i.e. the other conduction electrons and the positive ion cores giving the new matrix elements

$$V_{\mathbf{q}} = \frac{e^2}{\epsilon_r(\mathbf{q},\omega)\epsilon_0 q^2} \tag{2.13}$$

with $\epsilon_r(\mathbf{q},\omega)$ the relative permittivity of the medium For electrons in a metal we know that due to the ion cores and the other electrons we have a screening effect. A simple model for this screening is the Thomas-Fermi screening, which takes the form

$$V(\mathbf{r} - \mathbf{r}') = \frac{e^2}{4\pi\epsilon_0|\mathbf{r} - \mathbf{r}'|}e^{-|\mathbf{r}-\mathbf{r}'|/r_{\mathrm{TF}}} \tag{2.14}$$

and which leads to a reduced interaction (especially, contrary to Coulomb repulsion, the potential vanish for a great enough distance $|\mathbf{r} - \mathbf{r}'| \gg r_{\mathrm{TF}}$, r_{TF} being the Thomas-Fermi screening length). However this is still a repulsive one.

We see that considering only the electrons will not lead to an attraction. The only way to have an attractive potential is to consider the electron-phonon interactions. Fröhlich was among the first to show how to treat such a electron-phonon system [33]. A very simple way of modelling the electron-phonon system is the "jellium model" in which a solid is approximated by a fluid of electrons and point ions in place of nuclei. This is this model that was applied in the context of superconductivity by Pines to show how an attraction can occur between two electrons [34]. The jellium model gives a potential in the form [35]

$$V(\mathbf{q},\omega) = \frac{4\pi e^2}{q^2 + k_s^2} + \frac{4\pi e^2}{q^2 + k_s^2}\frac{\omega_{\mathbf{q}}^2}{\omega^2 - \omega_{\mathbf{q}}^2} \tag{2.15}$$

we see that for $\omega < \omega_{\mathbf{q}}$ we have $V < 0$ thanks to the second term coming from the phonon mediated interaction while the first one is the classic screened coulomb repulsion. Even if this model is very simple it shows that an attraction of the same order of the repulsion can happen if we take into account the presence of the phonons.

Finally, note that the BCS theory requires an attractive potential for the formation of Cooper pairs but that an attraction could have other origins than electron-phonon interactions and that is a possible explanation for non classical superconductivity.

2.3 The BCS ground state: variational method

Since we showed that the Fermi sea is unstable for the scattering of electrons in state $|\mathbf{k},\uparrow\rangle$ and $|-\mathbf{k},\downarrow\rangle$ we need to define a new ground state considering it. The new ground state was proposed as an ansatz by Bardeen, Cooper and Schrieffer and they considered that it is a superposition of cooper pairs states

$$|\psi_{\mathrm{BCS}}\rangle = \prod_{\mathbf{k}}\left(u_{\mathbf{k}} + v_{\mathbf{k}}c_{\mathbf{k}\uparrow}^{\dagger}c_{-\mathbf{k}\downarrow}^{\dagger}\right)|0\rangle \tag{2.16}$$

where the product of creation operators $c_{\mathbf{k}\uparrow}^{\dagger}c_{-\mathbf{k}\downarrow}^{\dagger}$ creates the Cooper pair of electrons with opposite momentum and spin on the vacuum state $|0\rangle$ and $u_{\mathbf{k}}, v_{\mathbf{k}}$ are complex coefficients to be determined.

This grounds state should be normalized leading to

$$
\begin{aligned}
1 &= \langle \psi_{\mathrm{BCS}} | \psi_{\mathrm{BCS}} \rangle \\
&= \langle 0 | \prod_{\mathbf{k}} \left(u_{\mathbf{k}}^* + v_{\mathbf{k}}^* c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} \right) \prod_{\mathbf{k}'} \left(u_{\mathbf{k}'} + v_{\mathbf{k}'} c_{\mathbf{k}'\uparrow}^\dagger c_{-\mathbf{k}'\downarrow}^\dagger \right) |0\rangle \\
&= \langle 0 | \prod_{\mathbf{k}} \left(|u_{\mathbf{k}}|^2 + u_{\mathbf{k}}^* v_{\mathbf{k}} c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger + u_{\mathbf{k}} v_{\mathbf{k}}^* c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} + |v_{\mathbf{k}}|^2 \right) |0\rangle \\
&= \prod_{\mathbf{k}} \left(|u_{\mathbf{k}}|^2 + |v_{\mathbf{k}}|^2 \right).
\end{aligned}
\tag{2.17}
$$

Which is satisfied if we impose $|u_{\mathbf{k}}|^2 + |v_{\mathbf{k}}|^2 = 1$ for all $\mathbf{k}$. That lead to the interpretation that $|v_{\mathbf{k}}|^2$ is the probability of the pair being occupied and $|u_{\mathbf{k}}|^2$ is the probability of the pair being unoccupied.

We now have to determine the value of the coefficients $u_{\mathbf{k}}, v_{\mathbf{k}}$. We first rely on a variational method by minimizing the expectation value of the energy $\langle \psi_{\mathrm{BCS}} | H | \psi_{\mathrm{BCS}} \rangle$. The Hamiltonian is given by[3]

$$
H = \sum_{\mathbf{k}\sigma} \xi_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} + \frac{1}{N} \sum_{\mathbf{k}\mathbf{k}'} V_{kk'} c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger c_{-\mathbf{k}'\downarrow} c_{\mathbf{k}'\uparrow}.
\tag{2.18}
$$

We will consider the same approximation for $V_{\mathbf{k}\mathbf{k}'}$ as in (2.6),

$$
V_{kk'} = \begin{cases} -V & \text{if } \xi_{\mathbf{k}} \text{ and } \xi_{\mathbf{k}'} < \omega_c \\ 0 & \text{otherwise.} \end{cases}
\tag{2.19}
$$

The energy of the BCS ground state is defined as the expectation value of the Hamiltonian in that state:

$$
\begin{aligned}
\langle H \rangle_{\psi_{BCS}} &= \langle \psi_{\mathrm{BCS}} | H | \psi_{\mathrm{BCS}} \rangle \\
&= \sum_{\mathbf{k}\sigma} \xi_{\mathbf{k}} \langle 0 | \prod_{\mathbf{q}} \left(u_{\mathbf{q}}^* + v_{\mathbf{q}}^* c_{-\mathbf{q}\downarrow} c_{\mathbf{q}\uparrow} \right) c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} \prod_{\mathbf{q}'} \left(u_{\mathbf{q}'} + v_{\mathbf{q}'} c_{\mathbf{q}'\uparrow}^\dagger c_{-\mathbf{q}'\downarrow}^\dagger \right) |0\rangle \\
&\quad + \frac{1}{N} \sum_{\mathbf{k}\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} \langle 0 | \prod_{\mathbf{q}} \left(u_{\mathbf{q}}^* + v_q^* c_{-\mathbf{q}\downarrow} c_{\mathbf{q}\uparrow} \right) c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger c_{-\mathbf{k}'\downarrow} c_{\mathbf{k}'\uparrow} \prod_{\mathbf{q}'} \left(u_{\mathbf{q}'} + v_{\mathbf{q}'} c_{\mathbf{q}'\uparrow}^\dagger c_{-\mathbf{q}'\downarrow}^\dagger \right) |0\rangle \\
&= \sum_{\mathbf{k}} \xi_{\mathbf{k}} \langle 0 | |v_{\mathbf{k}}|^2 c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} c_{\mathbf{k}\uparrow}^\dagger c_{\mathbf{k}\uparrow} c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger |0\rangle \\
&\quad + \sum_{\mathbf{k}} \xi_{\mathbf{k}} \langle 0 | |v_{-\mathbf{k}}|^2 c_{\mathbf{k}\downarrow} c_{-\mathbf{k}\uparrow} c_{\mathbf{k}\downarrow}^\dagger c_{\mathbf{k}\downarrow} c_{-\mathbf{k}\uparrow}^\dagger c_{\mathbf{k}\downarrow}^\dagger |0\rangle \\
&\quad + \frac{1}{N} \sum_{\mathbf{k}\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} \langle 0 | u_{\mathbf{k}}^* u_{\mathbf{k}'}^* u_{\mathbf{k}} u_{\mathbf{k}'} c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger c_{-\mathbf{k}'\downarrow} c_{\mathbf{k}'\uparrow} c_{\mathbf{k}'\uparrow}^\dagger c_{-\mathbf{k}'\downarrow}^\dagger |0\rangle \\
&= \sum_{\mathbf{k}} 2\xi_{\mathbf{k}} |v_{\mathbf{k}}|^2 + \frac{1}{N} \sum_{\mathbf{k}\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} v_{\mathbf{k}}^* u_{\mathbf{k}} u_{\mathbf{k}'}^* v_{\mathbf{k}'} := E_{\mathrm{BCS}}.
\end{aligned}
\tag{2.20}
$$

We can choose $u_{\mathbf{k}}, v_{\mathbf{k}}$ to be real thus the normalization constraint simplifies as $u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2 = 1$ which can be easily satisfied by

$$
\begin{aligned}
u_{\mathbf{k}} &= \cos \theta_{\mathbf{k}}, \\
v_{\mathbf{k}} &= \sin \theta_{\mathbf{k}}.
\end{aligned}
\tag{2.21}
$$

This leads to

$$
E_{\mathrm{BCS}} = \sum_{\mathbf{k}} \xi_{\mathbf{k}} (1 - \cos 2\theta_{\mathbf{k}}) + \frac{1}{N} \sum_{\mathbf{k}\mathbf{k}'} \frac{V_{\mathbf{k}\mathbf{k}'}}{4} \sin 2\theta_{\mathbf{k}} \sin \theta_{\mathbf{k}'}.
\tag{2.22}
$$

We can now minimize the energy with respect to any $\theta_{\mathbf{q}}$ by setting

$$
\frac{\partial E_{BCS}}{\partial \theta_{\mathbf{q}}} = 2\epsilon_{\mathbf{q}} \sin 2\theta_{\mathbf{q}} + \frac{1}{N} \sum_{\mathbf{k}'} V_{\mathbf{q}\mathbf{k}'} \cos 2\theta_{\mathbf{q}} \sin 2\theta_{\mathbf{k}'} \overset{!}{=} 0.
\tag{2.23}
$$

---

[3]Note the order of the operators in the second term !

For convenience we replace $\mathbf{q}$ by $\mathbf{k}$ and define the gap $\Delta_{\mathbf{k}}$ through

$$\sin 2\theta_{\mathbf{k}} := \frac{\Delta_{\mathbf{k}}}{\sqrt{\xi_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2}}. \tag{2.24}$$

We can finally rewrite (2.23) as

$$\Delta_{\mathbf{k}} = -\frac{1}{N}\sum_{\mathbf{k'}} V_{\mathbf{kk'}}\frac{\Delta_{\mathbf{k'}}}{2\sqrt{\xi_{\mathbf{k'}}^2 \Delta_{\mathbf{k'}}^2}}. \tag{2.25}$$

This is called the **BCS gap equation**. Let us consider our simplified interaction and introduce a similar one for $\Delta_{\mathbf{k}}$, i.e.:

$$\Delta_{\mathbf{k}} = \begin{cases} \Delta > 0 & \text{for } |\xi_{\mathbf{k}}| < \omega_c \\ 0 & \text{otherwise.} \end{cases} \tag{2.26}$$

By taking into account both simplifications in (2.25), switching to the limit and using the argument of weak coupling we already used in section 2.1 we finally find

$$\Delta = 2\omega_c e^{-1/D(F)V} \tag{2.27}$$

with $D(F)$ the density of state at the Fermi level. We see that, except for the coefficient in the exponential, the simple model with just two electrons added to the Fermi sea predicted the value of the gap in (2.9). Using (2.24) we can rewrite our coefficients $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ in terms of Δ

$$u_{\mathbf{k}}^2 = \frac{1}{2}\left(1 + \frac{\xi_{\mathbf{k}}}{\sqrt{\xi_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2}}\right) \tag{2.28}$$

$$v_{\mathbf{k}}^2 = \frac{1}{2}\left(1 - \frac{\xi_{\mathbf{k}}}{\sqrt{\xi_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2}}\right). \tag{2.29}$$

We see that if $V \to 0$ then $\Delta_{\mathbf{k}} \to 0$ and we have $u_{\mathbf{k}}^2 \to 1$ and $v_{\mathbf{k}}^2 \to 0$ which is consistent with the interpretation we made previously stating that $u_{\mathbf{k}}^2$ is the probability of the pair being unoccupied and $v_{\mathbf{k}}^2$ is the probability of the pair being occupied. Indeed, if there is no interaction then there is no formation of pairs.

2.4   Bogoliubov-Valatin transformation

The variational approach presented in the previous section and that was used in the original BCS paper [28] has allowed us to determine the ground state of a superconductor but it is not adapted to model superconducting excited states. To treat those we will rely on two more modern methods. Let us start with the same Hamiltonian as in previous section

$$H = \sum_{\mathbf{k}\sigma} \xi_{\mathbf{k}} c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma} + \frac{1}{N}\sum_{\mathbf{kk'}} V_{kk'} c_{\mathbf{k}\uparrow}^{\dagger} c_{-\mathbf{k}\downarrow}^{\dagger} c_{-\mathbf{k'}\downarrow} c_{\mathbf{k'}\uparrow}. \tag{2.30}$$

Now the first new method we will use is a **mean field approximation** which consists of replacing an operator O as $O = \langle O \rangle + \delta O$ with $|\delta O| \ll \langle O \rangle$ where $\langle O \rangle$ is the expectation value of O and δO quantum fluctuation around the expectation value. With that replacement we can rewrite the product of two operators AB as

$$\begin{aligned} \delta A \delta B &= \left(A - \langle A \rangle\right)\left(B - \langle B \rangle\right) \\ \Leftrightarrow \quad 0 &\approx AB - \langle A \rangle B - \langle B \rangle A + \langle A \rangle \langle B \rangle \\ \Leftrightarrow \quad AB &\approx \langle A \rangle B + A \langle B \rangle - \langle A \rangle \langle B \rangle, \end{aligned} \tag{2.31}$$

where we neglect the product of δA and δB. The last term is just a number leading to a shift of energy that we will neglect from now on. For the treatment of BCS theory it is adequate to choose

$A = c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow}$ and $B = c_{-\mathbf{k'}\downarrow} c_{\mathbf{k'}\uparrow}$, i.e. A creates a cooper pair and B destroys one. With that choice for A and B our Hamiltonian now reads

$$H_{\mathrm{BCS}} = \sum_{\mathbf{k}\sigma} \xi_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \frac{1}{N} \sum_{\mathbf{kk'}} V_{kk'} \left(\langle c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow} \rangle c_{-\mathbf{k'}\downarrow} c_{\mathbf{k'}\uparrow} + c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow} \langle c_{-\mathbf{k'}\downarrow} c_{\mathbf{k'}\uparrow} \rangle \right). \tag{2.32}$$

Now we define

$$\Delta_{\mathbf{k}} := -\frac{1}{N} \sum_{\mathbf{k'}} V_{\mathbf{kk'}} \langle c_{-\mathbf{k'}\downarrow} c_{\mathbf{k'}\uparrow} \rangle \tag{2.33}$$

and therefore have

$$\Delta^*_{\mathbf{k}} = -\frac{1}{N} \sum_{\mathbf{k'}} V_{\mathbf{kk'}} \langle c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow} \rangle. \tag{2.34}$$

The choice of the name $\Delta_{\mathbf{k}}$ is naturally not random as we will later see that this is the same quantity as the one introduced in the previous section in 2.25. We can write the Hamiltonian in term of $\Delta_{\mathbf{k}}$ as

$$H_{\mathrm{BCS}} = \sum_{\mathbf{k}\sigma} \xi_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} - \sum_{\mathbf{k}} \Delta^*_{\mathbf{k}} c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} - \sum_{\mathbf{k}} \Delta_{\mathbf{k}} c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow}. \tag{2.35}$$

The Hamiltonian contains terms in cc and $c^\dagger c^\dagger$ hence in the basis $\{c_{\mathbf{k}\uparrow}, c^\dagger_{-\mathbf{k}\uparrow}, c_{\mathbf{k}\downarrow}, c^\dagger_{-\mathbf{k}\downarrow}\}$ it is non diagonal. The goal is to find a new basis in which it has a diagonal form. To do so we will perform a transformation on the creation and annihilation operators $c^\dagger$ and c called **Bogoliubov-Valatin transformation** [36, 37]. This transformation consists in defining a new set of creation-annihilation operators as[4]

$$\begin{aligned} \gamma_{\mathbf{k}\uparrow} &= u^*_{\mathbf{k}} c_{\mathbf{k}\uparrow} - v_{\mathbf{k}} c^\dagger_{-\mathbf{k}\downarrow}, \\ \gamma^\dagger_{-\mathbf{k}\downarrow} &= v^*_{\mathbf{k}} c_{\mathbf{k}\uparrow} + u_{\mathbf{k}} c^\dagger_{-\mathbf{k}\downarrow}. \end{aligned} \tag{2.36}$$

Those new operators should satisfy anticommutation relations

$$\{\gamma_{\mathbf{k}\uparrow}, \gamma^\dagger_{\mathbf{k}\uparrow}\} \overset{!}{=} 1 \tag{2.37}$$

leading to

$$|u_{\mathbf{k}}|^2 + |v_{\mathbf{k}}|^2 = 1. \tag{2.38}$$

The inverse relation of (2.36) is

$$\begin{aligned} c_{\mathbf{k}\uparrow} &= u_{\mathbf{k}} \gamma_{\mathbf{k}\uparrow} + v_{\mathbf{k}} \gamma^\dagger_{-\mathbf{k}\downarrow}, \\ c^\dagger_{-\mathbf{k}\downarrow} &= -v^*_{\mathbf{k}} \gamma_{\mathbf{k}\uparrow} + u^*_{\mathbf{k}} \gamma^\dagger_{-\mathbf{k}\downarrow}, \end{aligned} \tag{2.39}$$

that we can insert in the BCS Hamiltonian leading to

$$\begin{aligned} H_{\mathrm{BCS}} = \sum_{\mathbf{k}} \Big[&\left(\xi_{\mathbf{k}} |u_{\mathbf{k}}|^2 - \xi_{\mathbf{k}} |v_{\mathbf{k}}|^2 + \Delta^*_{\mathbf{k}} v_{\mathbf{k}} u_{\mathbf{k}} + \Delta_{\mathbf{k}} u^*_{\mathbf{k}} v^*_{\mathbf{k}} \right) \gamma^\dagger_{\mathbf{k}\uparrow} \gamma_{\mathbf{k}\uparrow} \\ &+ \left(\xi_{\mathbf{k}} |u_{\mathbf{k}}|^2 - \xi_{\mathbf{k}} |v_{\mathbf{k}}|^2 + \Delta^*_{\mathbf{k}} u_{\mathbf{k}} v_{\mathbf{k}} + \Delta_{\mathbf{k}} u^*_{\mathbf{k}} v^*_{\mathbf{k}} \right) \gamma^\dagger_{-\mathbf{k}\downarrow} \gamma_{-\mathbf{k}\downarrow} \\ &+ \left(\xi_{\mathbf{k}} u^*_{\mathbf{k}} v_{\mathbf{k}} + \xi_{\mathbf{k}} u^*_{\mathbf{k}} v_{\mathbf{k}} + \Delta^*_{\mathbf{k}} v^2_{\mathbf{k}} - \Delta_{\mathbf{k}} (u^*_{\mathbf{k}})^2 \right) \gamma^\dagger_{\mathbf{k}\uparrow} \gamma^\dagger_{-\mathbf{k}\downarrow} \\ &+ \left(\xi_{\mathbf{k}} v^*_{\mathbf{k}} u_{\mathbf{k}} + \xi_{\mathbf{k}} v^*_{\mathbf{k}} u_{\mathbf{k}} - \Delta^*_{\mathbf{k}} u^2_{\mathbf{k}} + \Delta_{\mathbf{k}} (v^*_{\mathbf{k}})^2 \right) \gamma_{-\mathbf{k}\downarrow} \gamma_{\mathbf{k}\uparrow} \Big]. \end{aligned} \tag{2.40}$$

The Hamiltonian will be diagonal if we choose the $u_{\mathbf{k}}, v_{\mathbf{k}}$ such that the terms in $\gamma\gamma$ and $\gamma^\dagger\gamma^\dagger$ vanish. This happens if

$$2\xi_{\mathbf{k}} u^*_{\mathbf{k}} v_{\mathbf{k}} + \Delta^*_{\mathbf{k}} v^2_{\mathbf{k}} - \Delta_{\mathbf{k}} (u^*_{\mathbf{k}})^2 = 0. \tag{2.41}$$

Multiplying by $\Delta^*_{\mathbf{k}}/(u^*_{\mathbf{k}})^2$ leads to a quadratic equation whose solution is

$$\frac{\Delta^*_{\mathbf{k}} v_{\mathbf{k}}}{u^*_{\mathbf{k}}} = \sqrt{\xi^2_{\mathbf{k}} + |\Delta_{\mathbf{k}}|^2} - \xi_{\mathbf{k}} \tag{2.42}$$

---

[4]Once again, the choice of u and v is not arbitrary since it will turn out they are the same coefficients as in section 2.3

that we can solve along with (2.38) finding

$$|u_{\mathbf{k}}|^2 = 1 - |v_{\mathbf{k}}|^2 = \frac{1}{2}\left(1 + \frac{\xi_{\mathbf{k}}}{\sqrt{\xi_{\mathbf{k}}^2 + |\Delta_{\mathbf{k}}^2|^2}}\right) \tag{2.43}$$

in perfect agreement with (2.28) in the previous section. The Hamiltonian finally simply reads

$$H_{BCS} = \sum_{\mathbf{k}\sigma} \sqrt{\xi_{\mathbf{k}}^2 + |\Delta_{\mathbf{k}}|^2}\gamma_{\mathbf{k}\sigma}^{\dagger}\gamma_{\mathbf{k}\sigma} \tag{2.44}$$

we see that even when $\xi_{\mathbf{k}} = 0$ (i.e. at the Fermi surface) an energy $|\Delta_{\mathbf{k}}|$ is required to create an excitation, $\Delta_{\mathbf{k}}$ play the role of an **energy gap**. The Hamiltonian (2.44) gives us the energy dispersion

$$E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + |\Delta_{\mathbf{k}}|^2}. \tag{2.45}$$

If we take the special case $\Delta_{\mathbf{k}} = 0$ then we have $E_{\mathbf{k}} = |\xi_{\mathbf{k}}|$ and

$$u_{\mathbf{k}}^2 = \frac{1}{2}\left(1 + \frac{\xi_{\mathbf{k}}}{|\xi_{\mathbf{k}}|}\right), \tag{2.46}$$

$$v_{\mathbf{k}}^2 = \frac{1}{2}\left(1 - \frac{\xi_{\mathbf{k}}}{|\xi_{\mathbf{k}}|}\right), \tag{2.47}$$

meaning that below the Fermi surface (i.e., for $\xi_{\mathbf{k}} < 0$ the quasiparticles are holes ($v_{\mathbf{k}}^2 = 1$ and $u_{\mathbf{k}}^2 = 0$) while above Fermi surface they are electrons, as shown in figure 2.2. For the general case
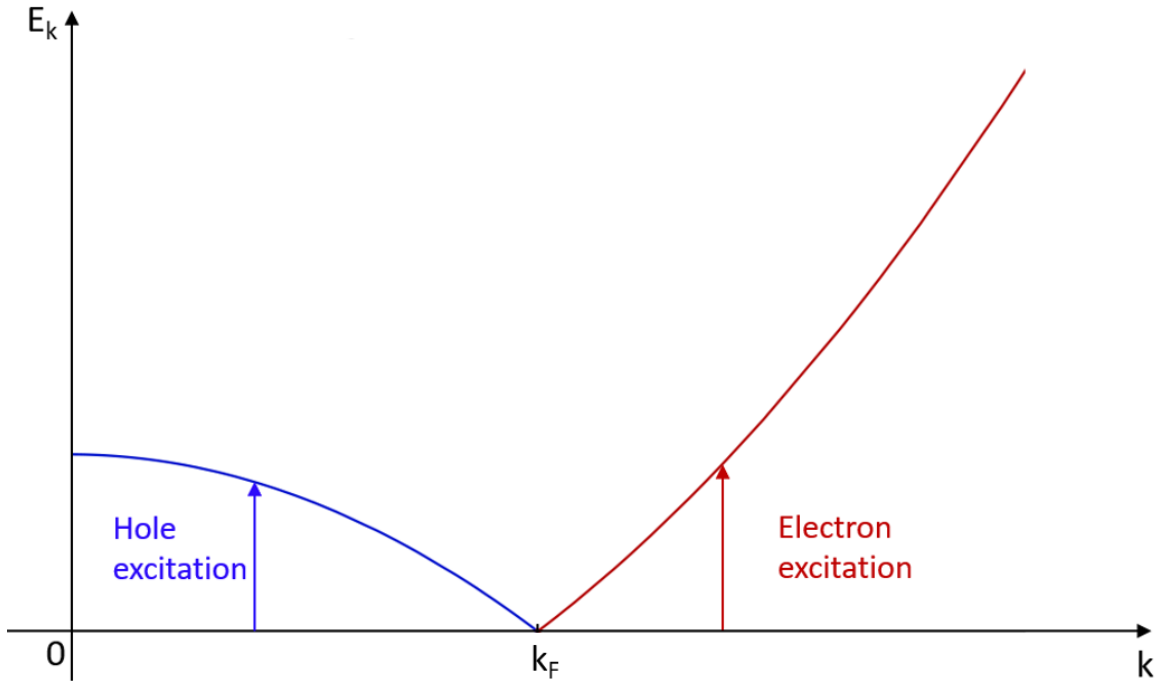

Figure 2.2: Energy dispersion of the Bogoliubov quasi-particles when $\Delta = 0$. In that case those quasiparticles are holes below the Fermi level k_F and electrons above. Note that the hole dispersion relation is the opposite of the electron one (i.e., an inverted parabola), as a hole corresponds to the absence of an electron.

when Δ_{k_F} is non zero the electron pairing opens an energy gap of dimension Δ_{k_F} as shown in 2.3
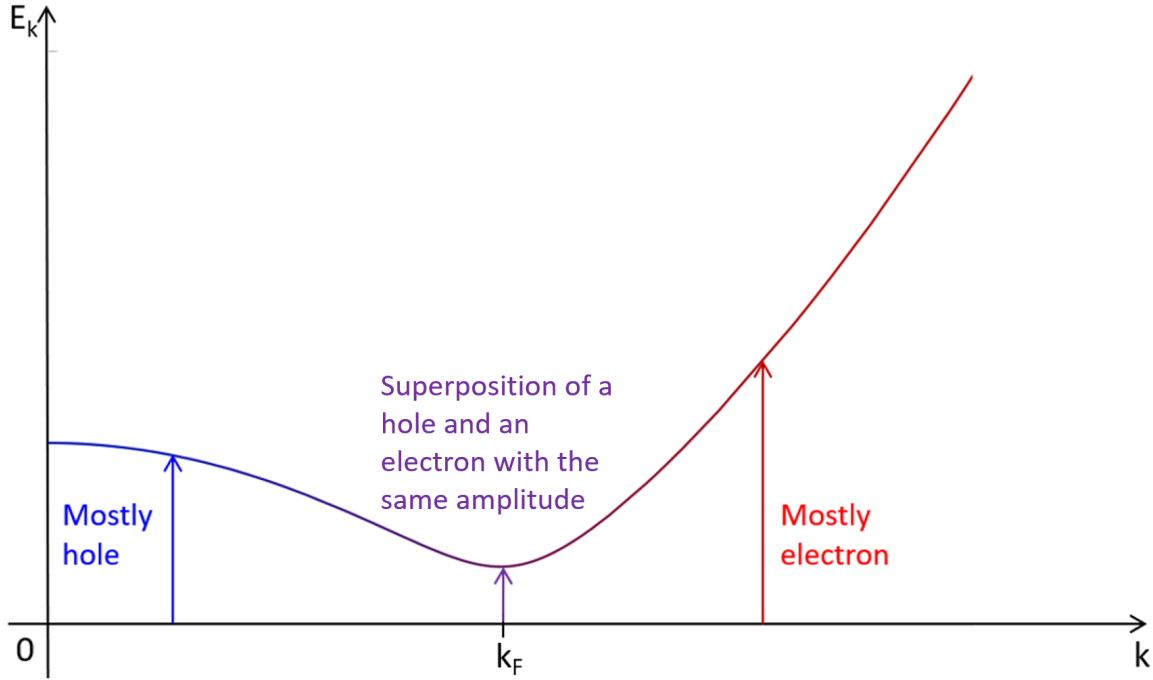
Figure 2.3: Energy dispersion of the Bogoliubov quasiparticles when pairing of electrons occurs, opening a gap in the energy spectrum at the Fermi level k_F. In this case, the quasiparticles are superposition of holes and electrons. Far above the Fermi level they mostly are electrons, far below mostly holes and at Fermi level the amplitudes of the superposition are equal.

Now we can apply the Bogoliubov transformation to the definition of $\Delta_{\mathbf{k}}$ (2.33) yielding

$$\Delta_{\mathbf{k}} = -\frac{1}{N} \sum_{\mathbf{k'}} V_{\mathbf{kk'}} \left(-v_{\mathbf{k'}} u_{\mathbf{k'}} \langle \gamma^{\dagger}_{\mathbf{k'}\uparrow} \gamma_{\mathbf{k'}\uparrow} \rangle - v^2_{\mathbf{k'}} \langle \gamma^{\dagger}_{\mathbf{k'}\uparrow} \gamma^{\dagger}_{-\mathbf{k'}\downarrow} \rangle + u^2_{\mathbf{k'}} \langle \gamma_{-\mathbf{k'}\downarrow} \gamma_{\mathbf{k'}\uparrow} \rangle + u_{\mathbf{k'}} v_{\mathbf{k'}} \langle \gamma_{-\mathbf{k'}\downarrow} \gamma^{\dagger}_{-\mathbf{k'}\downarrow} \rangle \right) .$$
(2.48)

The averages are evaluated using H_{BCS} and we consider the quasiparticles to be at thermal equilibrium meaning they are distributed according to the Fermi-Dirac distribution

$$n_f(E_{\mathbf{k}}) = \frac{1}{e^{E_{\mathbf{k}}/T} + 1}$$
(2.49)

leading to

$$\langle \gamma^{\dagger}_{\mathbf{k}\uparrow} \gamma_{\mathbf{k}\uparrow} \rangle = n_f(E_{\mathbf{k}}) \tag{2.50}$$

$$\langle \gamma^{\dagger}_{\mathbf{k}\uparrow} \gamma^{\dagger}_{-\mathbf{k}\downarrow} \rangle = 0 \tag{2.51}$$

$$\langle \gamma_{-\mathbf{k}\downarrow} \gamma_{\mathbf{k}\uparrow} \rangle = 0 \tag{2.52}$$

$$\langle \gamma_{-\mathbf{k}\downarrow} \gamma^{\dagger}_{-\mathbf{k}\downarrow} \rangle = 1 - n_f(E_{\mathbf{k}}). \tag{2.53}$$

This is an element important of standard BCS theory which is at the heart of this master thesis. Indeed, in the next chapters, we will investigate how to go beyond this assumption by coupling the system to external reservoirs to transform these quasi-particles distributions into out-of-equilibrium ones and explore in this way how to realise dissipative engineering of the gap.

We now have the **BCS gap equation** at arbitrary temperature

$$\Delta_{\mathbf{k}} = -\frac{1}{N} \sum_{\mathbf{k'}} V_{\mathbf{kk'}} \frac{\Delta_{\mathbf{k'}}}{2\sqrt{\xi^2_{\mathbf{k'}} + \Delta^2_{\mathbf{k'}}}} \left[1 - 2n_f(E_{\mathbf{k'}}) \right]$$
(2.54)

as in section 2.3 we can make simplifications on the interaction and the gap given by (2.19) and (2.26) respectively which simplify the equation

$$1 = -\frac{V_0}{N} \sum_{\mathbf{k'}} \frac{1 - 2n_f(E_{\mathbf{k'}})}{2\sqrt{\xi_{\mathbf{k'}}^2 + \Delta^2}}. \tag{2.55}$$

We can then take the limit to integral assuming the density of states to be roughly constant around the Fermi level

$$1 \approx V_0 D(E_F) \int_{-\omega_D}^{\omega_D} d\xi \frac{\tanh \frac{\beta}{2}\sqrt{\xi^2 + \Delta^2}}{2\sqrt{\xi^2 + \Delta^2}}. \tag{2.56}$$

By solving numerically the integral in the weak-coupling limit we get the temperature dependence of Δ which is a universal curve that can be seen in Fig. 2.4 and that holds (or at least is a good approximation) for most conventional superconductors.
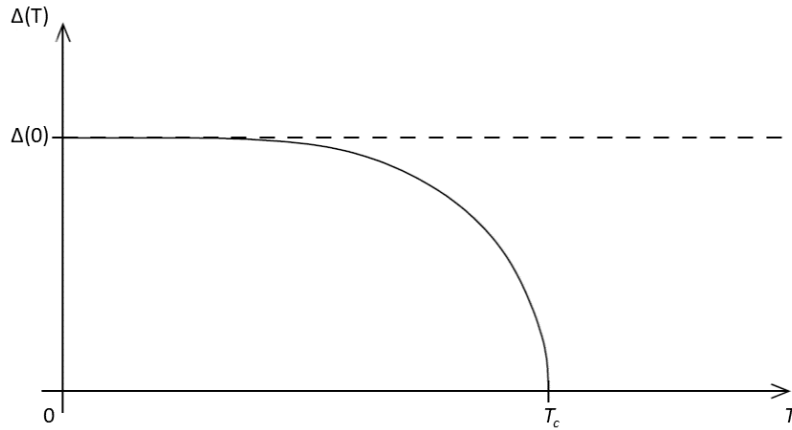

Figure 2.4: Gap versus temperature in the weak-coupling approximation.

This gives us interesting information about the thermodynamic of the superconducting transition. Indeed, the curve shape is typical of the order parameter of a second order phase transition thus the superconducting transition is a second order one whose order parameter is the gap.

2.5   A comment on dimension

Multiple times in this chapter we have been using the density of states (DOS) of free electrons to replace sums by integrals. But as we know the density of states depends on the dimension of the system, 1D DOS goes as $E^{-1/2}$, 2D DOS is constant and 3D DOS goes as $E^{1/2}$.

For our numerical study we will expose afterwards, we chose to work in 1D in order to simplify and quicken the algorithm but it would be obviously possible to extend the algorithm to treat systems in 2 or 3D. This choice to work in 1D has another implication, The Mermin–Wagner theorem [38] forbids phase transitions in 1D and 2D. More precisely, it forbids the establishment of long-range order due to the importance of phase fluctuations in 1D, which hampers the emergence of real superconductivity [39]. Strictly speaking, our model for the interactions should thus be interpreted as a model to describe pairing of fermions without superconductivity, as has been observed in some materials [40, 41]. Nonetheless, a recent approach of phase transitions, the Berezinskii–Kosterlitz–Thouless (BKT) transition, shows the appearance of a quasi ordered phase for sufficiently low temperature in two dimensional system [42]. In addition, out of equilibrium, the Mermin-Wagner theorem can be violated, as described in [43] for a 2D system, which also motivates the study of the impact of out-of-equilibrium quasi-particles distributions performed in the next chapters.

Hence, the question of the emergence of real phase transitions in low dimensions, while interesting, is not the direct scope of this thesis. We will still be misusing the word while talking about superconductivity later in the text.

2.6   Self-consistent Hartree-Fock-Bogoliubov algorithm

The value of the gap Δ could be numerically determined using the BCS gap equation (2.54) but this method presents two downsides. First, the gap equation is only valid when the single-particle energy is spin-independent. Thus, if we want to model a system which contains a magnetic field we cannot use that equation. For the second downside we need to come back to the mean field approximation we made in the beginning of section 2.4, a complete treatment of the problem is done by using Wick's theorem [44]

$$
\begin{aligned}
c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow} c_{-\mathbf{k'}\downarrow} c_{\mathbf{k'}\uparrow} \approx {} & \left\langle c^\dagger_{\mathbf{k}\uparrow} c_{\mathbf{k'}\uparrow} \right\rangle c^\dagger_{-\mathbf{k}\downarrow} c_{-\mathbf{k'}\downarrow} + \left\langle c^\dagger_{-\mathbf{k}\downarrow} c_{-\mathbf{k'}\downarrow} \right\rangle c^\dagger_{\mathbf{k}\uparrow} c_{\mathbf{k'}\uparrow} \\
& - \left\langle c^\dagger_{\mathbf{k}\uparrow} c_{-\mathbf{k'}\downarrow} \right\rangle c^\dagger_{-\mathbf{k}\downarrow} c_{\mathbf{k'}\uparrow} - \left\langle c^\dagger_{-\mathbf{k}\downarrow} c_{\mathbf{k'}\uparrow} \right\rangle c^\dagger_{-\mathbf{k}\downarrow} c_{\mathbf{k'}\uparrow} \\
& + \left\langle c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow} \right\rangle c_{-\mathbf{k'}\downarrow} c_{\mathbf{k'}\uparrow} + \langle c_{-\mathbf{k'}\downarrow} c_{\mathbf{k'}\uparrow} \rangle c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow}.
\end{aligned}
\tag{2.57}
$$

We see that it gives rise to three types of terms:

1. Terms in $\langle c^\dagger_\uparrow c_\uparrow \rangle$ or $\langle c^\dagger_\downarrow c_\downarrow \rangle$ are the **Hartree** terms describing the electrostatic potential felt by the k'-th electron due to the $N-1$ other electrons. They give rise to the Hartree mean-field through the definition

$$
\Sigma_s = \frac{U}{2\pi} \int_{-\infty}^{\infty} \langle c^\dagger_{sk} c_{sk} \rangle dk
\tag{2.58}
$$

   where U is the interaction strength (with dimensions of energy x length) and $s = \{\uparrow, \downarrow\}$ denotes the spin.

2. Terms in $\langle c^\dagger_\uparrow c_\downarrow \rangle$ or $\langle c^\dagger_\downarrow c_\uparrow \rangle$ are the **Fock** terms describing spin flips. Note that these terms give 0 if there is no interaction to mediate spin-spin interaction. They give rise to the Fock mean-field through the definition

$$
\chi = \frac{U}{2\pi} \int_{-\infty}^{\infty} \langle c^\dagger_{\uparrow k} c_{\downarrow k} \rangle dk
\tag{2.59}
$$

3. Terms in $\langle c^\dagger_\uparrow c^\dagger_\downarrow \rangle$ or $\langle c_\downarrow c_\uparrow \rangle$ are the **Bogoliubov** terms describing electron pairing. They give rise to the Bogoliubov mean-field through the definition

$$
\Delta = \frac{U}{2\pi} \int_{-\infty}^{\infty} \langle c_{\uparrow k} c_{\downarrow -k} \rangle dk
\tag{2.60}
$$

The definition of those three fields is valid only in one dimension as can be guessed by the simple integral. To work in 3 dimension would require to integrate over k_x, k_y and k_z.

To implement a more complete and physically realistic numerical method we will rather use the self consistent Hartree-Fock-Bogoliubov method. For this method we start from the BCS Hamiltonian (2.35) which, as this formulation suggest, can be written as a matrix in the basis $\mathbf{b_k} = \{c_{\mathbf{k}\uparrow}, c^\dagger_{-\mathbf{k}\uparrow}, c_{\mathbf{k}\downarrow}, c^\dagger_{-\mathbf{k}\downarrow}\}$. This matrix form of the Hamiltonian is

$$H_{\text{BCS}} =$$

$$
\sum_{\mathbf{k}} \mathbf{b_k}
\begin{pmatrix}
E_{k\uparrow} - E_F + \Sigma_\uparrow & 0 & 0 & \Delta \\
0 & -(E_{k\uparrow} - E_F + \Sigma_\uparrow) & -\Delta & 0 \\
0 & -\Delta & E_{-k\downarrow} - E_F + \Sigma_\downarrow & 0 \\
\Delta & 0 & 0 & -(E_{-k\downarrow} - E_F + \Sigma_\downarrow)
\end{pmatrix}
\mathbf{b_k}^T.
\tag{2.61}
$$

Where $\mathbf{b_k}^T$ is the transpose of $\mathbf{b_k}$, $E_{k\sigma}(\sigma =\uparrow,\downarrow)$ is the non interacting energy, Σ is the Hartree mean field and Δ is the Bogoliubov mean field [5]. To determine those mean fields we need to perform the Bogoliubov transformation (i.e. diagonalize the Hamiltonian). The self-consistent HFB algorithm can be summarized as follows:

Step 1: Choose an initial trial value for Δ and both Σ called Δ_0 and Σ_0[6].

Step 2: Diagonalize the matrix appearing in the Hamiltonian given by (2.61).

Step 3: Determine the new value of Δ called Δ_1 using Eq. (2.48) and Eqs (2.50) to (2.53) (similarly, you can find the new value of Σ, called Σ_1).

Step 4: Evaluate the difference $|\Delta_1 - \Delta_0|, |\Sigma_1 - \Sigma_0|$. If it is smaller than the desired precision ϵ then the simulation has converged and the mean fields are $\Delta = \Delta_1, \Sigma = \Sigma_1$.

Step 5: If $|\Delta_1 - \Delta_0| > \epsilon$ or $|\Sigma_1 - \Sigma_0| > \epsilon$ then we start back to step 1 with Δ_1 as the new Δ_0 and Σ_1 as the new Σ_0 until we get convergence for both field.

The self consistent HFB has been implemented on Mathematica and was used to verify the theoretical properties derived earlier.

2.6.1   Energy dispersion

We first computed the energy dispersion of the quasiparticles when the interaction between electrons is zero. In that case there can be no pairing and the energy dispersion is the classical energy of an electron given by $k^2/(2m) - \mu$ above the Fermi level k_F and the energy of a hole (that is the opposite of the energy of the electron) below the Fermi level. For our computation we used $\mu = -2.5$meV. The numerical plot of the energy dispersion is shown in fig 2.5
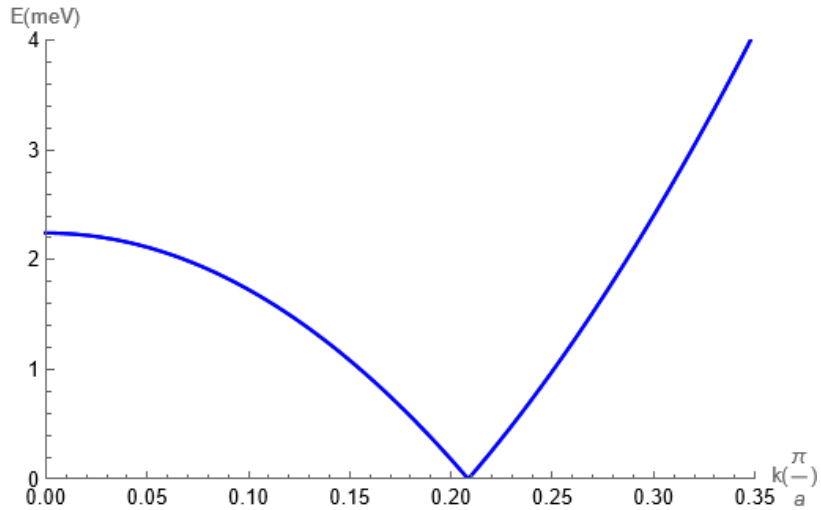

Figure 2.5: Numerical energy dispersion of a superconductor without pairing ($\Delta = 0$) and with a chemical potential of $\mu = 2.5$meV. The numerical results give a dispersion relation consistent with the theoretical curve in fig 2.2. Parameters for the simulation are: the effective mass $m = 2m_e = 2 \times 9.109 \times 10^{-31}$ kg, the interaction strength $U = 0$ meVnm, the precision $\epsilon = 10^{-30}$ meV and the parameter $a = 2 \times 10^{-9}$ nm which serves as a cutoff for the integration over k in Eqs. (2.59)-(2.60). Indeed numerically we cannot integrate from $-\infty$ to ∞.

---

[5]In this thesis we have not considered any process to mediate spin flip there will therefore not be any Fock mean field.

[6]If a Fock mean field is considered we should obviously also assume an initial value for it.

Now let us turn on electron interactions by setting $U = 0.1$meV in the algorithm leading to the emergence of Hartree and Bogoliubov fields. The energy dispersion plot is shown in fig 2.6 where we can see the gap opening.
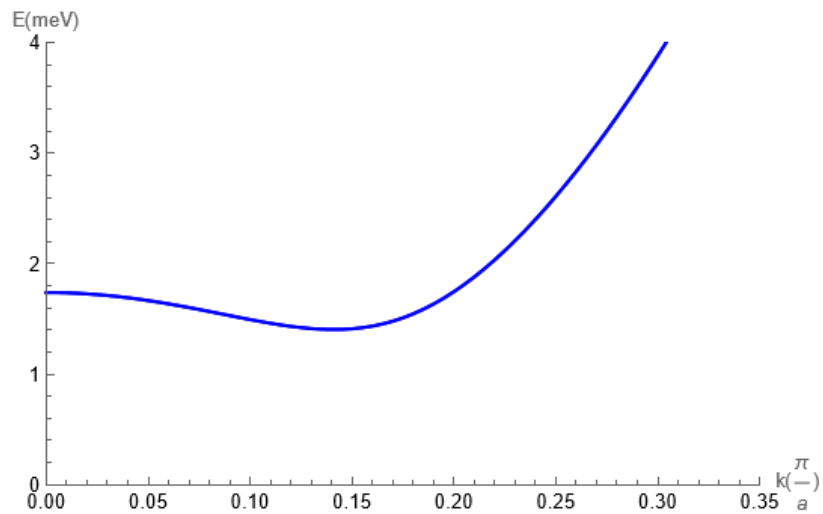

Figure 2.6: Energy dispersion of the Bogoliubov quasiparticles when pairing interaction is turned on. We still have a chemical potential of $\mu = 2.5$meV but we also set a potential for the Bogoliubov and Hartree fields of $U = 0.1$ meVnm so that we can use the algorithm presented before. Once again the numerical results are consistent with the theoretical curve of Fig 2.3. Parameters for the simulation are: the effective mass $m = 2m_e = 2 \times 9.109 \times 10^{-31}$ kg, the precision $\epsilon = 10^{-30}$ meV and the parameter $a = 2 \times 10^{-9}$ nm.

In both cases we see the numerical results are in accordance with the theory showed in figures 2.2 and 2.3.

2.6.2   Temperature dependence of the gap

Now let us see the plot of our gap versus the temperature which will give us the critical temperature. The parameters are the same as before ($\mu = -2.5$meV, $U = 0.1$ meV) and at $T = 0K$ the Fermi-Dirac distribution (2.49) is replaced by the Heaviside function $\Theta(-E_{\mathbf{k}})$. The plot is shown below in fig 2.7.
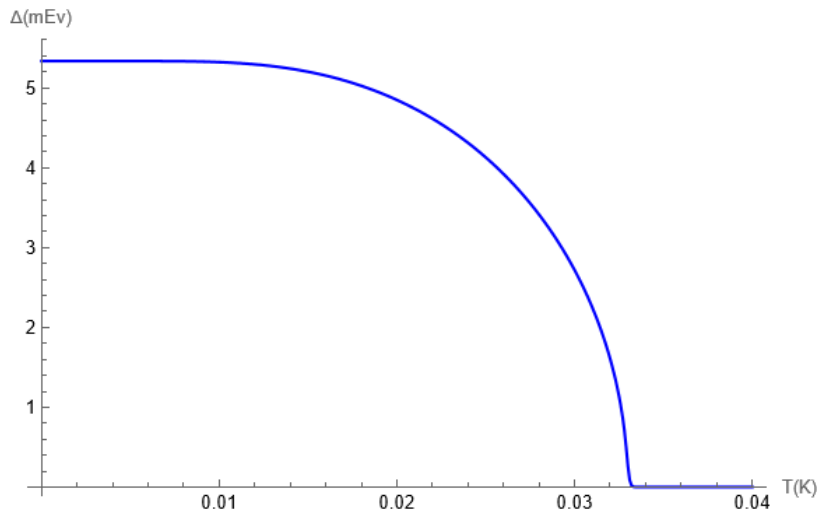
Figure 2.7: Temperature dependence of the pairing gap of a classical superconductor in thermal equilibrium and with a chemical potential $\mu = -1\text{meV}$. In this case we have a critical temperature T_c of around 33mK. Parameters for the simulation are: the effective mass $m = 2m_e = 2 \times 9.109 \times 10^{-31}$ kg, the precision $\epsilon = 10^{-30}$ meV, the strength of interaction between electrons $U = 0.1$ meVnm and the parameter $a = 2 \times 10^{-9}$ nm.

Once again the numerical analysis reproduces the theory and we see the characteristic curve of a second order phase transition.

This ends up this chapter dedicated to the development of the BCS theory of superconductivity and to a benchmark of a HFB algorithm on some of its properties. As mentioned earlier, the standard BCS theory assumes that the quasiparticles are at thermal equilibrium (see Eqs. (2.50) to (2.53)). What happens if they are not ? The remainder of this master thesis is dedicated to that question. First, in the next chapter, we will see how the coupling of a system to external reservoirs make it possible to reach out-of-equilibrium states. Then, in the last chapter, we will modify the BCS theory to account for quasiparticle distributions pushed out of equilibrium in this way and investigate their impact on the gap.

Chapter 3

Theory of open quantum systems

This chapter will be dedicated to explain how open systems are treated in the context of quantum mechanics. Indeed, just like in classical mechanics, there is no quantum system (except for the whole universe) that is really isolated which underlines the importance of developing a theory to model those. Open quantum systems have a lot of applications in physics, e.g. in quantum optics [45], quantum control [46], quantum computation [47] and even in other field like quantum biology [48]. Once considered as undesirable, especially in the trending field of quantum computing, because of the associated decoherence [49, 50, 51] interaction with the environment can now be exploited as an advantage. Indeed, improvements in experimental tools in the fields of quantum optics and solid-states has allowed the emergence of what is commonly called **dissipation engineering**. This emerging field has already proved itself very useful for applications such as state preparation [52, 53], quantum transport [54] or quantum technologies [55, 56]. Dissipation engineering enables to reach far from equilibrium states that otherwise would be hardly or not reachable at all making it a tool worth developing.

In section 3.1 will start by presenting an essential tool for describing quantum states. In section 3.2, we will derive the most common equation describing the evolution of an open quantum system as can be obtained using some approximations. Such an equation is called a **master equation** for the reduced density operator of the system. Finally, we will apply what we did previously to a simple system which will be implemented numerically.

3.1 Density operator

In a first course of quantum mechanics we learn that a quantum system is described by a wavefunction, also called ket vector, $|\psi(t)\rangle$ that provides all the information about the state of the system and whose time evolution is governed by the Schrodinger equation

$$i\frac{d}{dt}|\psi(t)\rangle = H|\psi(t)\rangle. \tag{3.1}$$

But a ket vector is not the most general way to describe a quantum system. Indeed it only describe a **pure state**[57], that is a system for which we know exactly its state. Unfortunately, it often happens that we do not know exactly in what state our system is, especially when working with open quantum system. If we start with a system in a pure state $|\psi(t=0)\rangle$ it will evolve due to the environment in a way we will not be able to tell its exact state at a later time t. Even if we cannot tell the exact state of our system we can say that it has a probability p_i to be in the state $|\psi_i\rangle$ (we obviously need $\sum_i p_i = 1$). This is what we call a **mixed state**, that is a probabilistic mixture of multiple pure states[1], as elaborated on in more detail below.

---

[1]One should not confuse a mixed state and a quantum superposition ! A quantum superposition is a **pure** state $|\psi\rangle = c_1|\psi_1\rangle + c_2|\psi_2\rangle$ with $c_1, c_2 \in \mathbb{C}, |c_1|^2 + |c_2|^2 = 1$ while for a mixed state the probability p_i are real numbers such that $\sum p_i = 1$

3.1.1   Definition and properties

We define the ***density operator***[58] ρ as

$$\rho = \sum_j p_j \, |\psi_j\rangle \, \langle\psi_j| \,, \quad \text{with} \quad 0 \le p_j \le 1 \quad \text{and} \quad \sum p_j = 1 \tag{3.2}$$

we then say that the system is in the (mixed) state ρ. Note that a pure state is just the special case of mixed state $\rho = |\psi\rangle \, \langle\psi|$.

To better understand the concept of density operator let us suppose a simple two dimensional system. Then the system can be either in the state $|1\rangle$ or in the state $|2\rangle$. If the system is prepared in the equal probability mixture we have

$$\rho = \frac{1}{2} \, |1\rangle \, \langle 1| + \frac{1}{2} \, |2\rangle \, \langle 2|$$

which gives in matrix form

$$\rho = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

We thus see that the diagonal elements give the probability the find the system in each state. For this reason they are called the ***populations***. Now if the system in prepared in the pure superposed state (again with equal probability) we have

$$\rho \equiv |\psi\rangle \, \langle\psi| = \left(\frac{1}{\sqrt{2}} (|1\rangle + |2\rangle) \right) \left(\frac{1}{\sqrt{2}} (\langle 1| + \langle 2|) \right)$$

$$\Leftrightarrow \rho = \frac{1}{2} (|1\rangle \, \langle 1| + |2\rangle \, \langle 2| + |1\rangle \, \langle 2| + |2\rangle \, \langle 1|).$$

Where the two first terms are the diagonal elements and the two last the off-diagonal elements giving

$$\rho = \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}.$$

We now have off-diagonal elements called the ***coherences***. These coherences indicate that the state of the system is necessarily a mixture of pure states that are superposition of the basis states.

Let us give a few important properties of the density operator[59]:

1. ρ is positive-definite, i.e. ρ is hermitian and $\langle\phi| \, \rho \, |\phi\rangle \ge 0 \quad \forall |\phi\rangle$. Indeed, ρ is a projection operator and all projection operator are hermitian and we have

$$\langle\phi| \, \rho \, |\phi\rangle = \sum_j p_j \, \langle\phi|\psi_j\rangle \, \langle\psi_j|\phi\rangle = \sum_j p_j |\langle\phi|\psi_j\rangle|^2 \ge 0. \tag{3.3}$$

2. $\text{Tr}(\rho) = 1$. Indeed if $|i\rangle$ is a basis of the system

$$\text{Tr}(\rho) = \sum_i |i\rangle \, \rho \, \langle i| = \sum_{i,j} |\langle i|\psi_j\rangle|^2 = \sum_j p_j = 1. \tag{3.4}$$

   This is a direct consequence of the fact that the diagonal elements are the probability to find the system in each possible basis state.

3. $\text{Tr}(\rho^2) \le 1$, the equality happens only if ρ describe a pure state. indeed, let $|i\rangle$ be a basis then

$$\text{Tr}(\rho^2) = \sum_i \langle i| \, \rho^2 \, |i\rangle = \sum_{i,j,k} p_j p_k \, \langle i|\psi_j\rangle \, \langle\psi_j|\psi_k\rangle \, \langle\psi_k|i\rangle = \sum_{j,k} p_j p_k |\langle\psi_j|\psi_k\rangle|^2 \le \sum_{j,k} p_j p_k = 1.$$
$$\tag{3.5}$$

   Equality can only occurs if there is only one element $|\psi\rangle$ that is if we have a pure state.

4. If the $|\psi_i\rangle$ evolve according to the Schrodinger equation then the density operator evolve according to the equation

$$i\frac{d}{dt}\rho = [H, \rho] \tag{3.6}$$

called the **Liouville–von Neumann equation.** Indeed,

$$
\begin{aligned}
i\frac{d}{dt}\rho &= i\frac{d}{dt}\sum_j p_j \left|\psi_j\right\rangle\left\langle\psi_j\right| \\
&= i\sum_j \left[\left|\frac{d}{dt}\psi_j\right\rangle\left\langle\psi_j\right| + i\left|\psi_j\right\rangle\left\langle\frac{d}{dt}\psi_j\right|\right] \\
&= \sum_j \left[\left|i\frac{d}{dt}\psi_j\right\rangle\left\langle\psi_j\right| - \left|\psi_j\right\rangle\left\langle i\frac{d}{d}\psi_j\right|\right] \\
&= \sum_j \left[\left|H\psi_j\right\rangle\left\langle\psi_j\right| - \left|\psi_j\right\rangle\left\langle H\psi_j\right|\right] \\
&= \sum_j \left[H\left|\psi_j\right\rangle\left\langle\psi_j\right| - \left|\psi_j\right\rangle\left\langle\psi_j\right|H^\dagger\right] \\
&= H\rho - \rho H = [H, \rho].
\end{aligned}
\tag{3.7}
$$

5. The expectation value of an observable described by an hermitian operator O is

$$\langle O \rangle = \mathrm{Tr}(O\rho). \tag{3.8}$$

Indeed, let once again $|i\rangle$ designate a basis of the system then

$$
\langle\psi|O|\psi\rangle = \sum_{i,j} \langle\psi|i\rangle\langle i|O|j\rangle\langle j|\psi\rangle = \sum_{i,j} \langle i|O|j\rangle\langle j|\psi\rangle\langle\psi|i\rangle
$$
$$
= \sum_{i,j} \langle i|O|j\rangle\langle j|\rho|i\rangle = \sum_i \langle i|O\rho|i\rangle = \mathrm{Tr}(O\rho).
$$

3.1.2   Reduced density operator

Suppose a system S composed of two subsystems, $S = A + B$. We know that the Hilbert space $\mathcal{H}_S$ of the system is given by the tensor product of the two Hilbert subspaces

$$\mathcal{H}_S = \mathcal{H}_A \otimes \mathcal{H}_B \tag{3.9}$$

and that a basis of S is the tensor product of the two basis of A and B

$$\left|\phi_i^S\right\rangle = \left|\phi_i^A\right\rangle \otimes \left|\phi_i^B\right\rangle \tag{3.10}$$

As we said just before, the state of the system is described by the density operator ρ. The **reduced density matrix** ρ_A is defined as

$$\rho_A = \mathrm{Tr}_B(\rho) = \sum_i \left(I_A \otimes \left\langle\phi_i^B\right|\right) \rho \left(I_A \otimes \left|\phi_i^B\right\rangle\right) \tag{3.11}$$

with I_A is the identity matrix on the Hilbert space $\mathcal{H}_A$. The operation Tr_B is called the **partial trace** over B and is just a trace as usually defined but only on the subspace B. Contrary to the classical trace, the partial trace does not return a number but returns an operator which is the density operator describing the subsystem A. We obviously get the reduced density operator ρ_B by tracing ρ over A.

Let O_A be an operator acting exclusively on the subspace $\mathcal{H}_A$. It can be extended to the whole system

$$O = O_A \otimes I_B. \tag{3.12}$$

Also, we have, by using (3.8)

$$
\begin{aligned}
\langle O \rangle &= \mathrm{Tr}(O\rho) \\
&= \sum_{ij} \langle \phi_i^A \otimes \phi_j^B | \, O\rho \, | \phi_i^A \otimes \phi_j^B \rangle \\
&= \sum_{iji'j'} \langle \phi_i^A \otimes \phi_j^B | \, O \, | \phi_{i'}^A \otimes \phi_{j'}^B \rangle \langle \phi_{i'}^A \otimes \phi_{j'}^B | \, \rho \, | \phi_i^A \otimes \phi_j^B \rangle \\
&= \sum_{ii'} \langle \phi_i^A | \, O_A \, | \phi_{i'}^A \rangle \langle \phi_{i'}^A | \, \rho_A \, | \phi_i^A \rangle \\
&= \mathrm{Tr}_A(O_A \rho_A).
\end{aligned}
\tag{3.13}
$$

This result means that for an operator only acting on $\mathcal{H}_A$ you can evaluate its expectation value without knowing the state of the other subsystem ρ_B. This is an extremely important result in the context of open quantum systems since, in general, the environment has a very large (if not infinite) Hilbert space so that it would not be possible in general to work with its density operator. But since we are only interested in describing the system we do require to describe the complex environment.

3.2 Markovian master equation derivation

We consider a system S in interaction with an environment B that together form a larger, isolated system. Then, considering the previous section the system is described by a density operator ρ_S that acts on $\mathcal{H}_S$, the environment by a density operator ρ_B that acts on $\mathcal{H}_B$ and the composite system by a density operator ρ that acts on $\mathcal{H}_A \otimes \mathcal{H}_B$. At any time the composite system can be written as

$$
\rho(t) = \rho_S(t) \otimes \rho_B(t) + \rho_{corr}(t),
\tag{3.14}
$$

where $\rho_{corr}(t)$ is the part of the density operator that cannot be put into a separable form $\cdot \otimes \cdot$.

Since the composite system is isolated its density operator evolves according to the Liouville–Von Neumann equation

$$
i\frac{d}{dt}\rho(t) = [H, \rho(t)]
\tag{3.15}
$$

H being the Hamiltonian of the composite system

$$
H = H_S \otimes I_B + I_S \otimes H_B + H_{int}
\tag{3.16}
$$

with H_S, H_B and H_{int} the Hamiltonians of the open system, the environment and of the interaction between both respectively. But, in general, we are only interested in the evolution of the subsystem S which we can get by taking the partial trace of (3.15)

$$
\frac{d}{dt}\rho_S(t) = -i\,\mathrm{Tr}_B([H, \rho(t)]).
\tag{3.17}
$$

We still have to get rid of the density operator of the composite system in the commutator to obtain a closed evolution equation for $\rho_S(t)$ that is what we will be doing in the following. We will derive the master equation by making approximations invoking physical arguments but it should be noted that it has been demonstrated [60] that a master equation is valid only if it can be written in the standard form

$$
\frac{d\rho_S(t)}{dt} = -i\left[H_S + H_{LS}, \rho_S(t)\right] + \sum_{i,j=1}^{d_S^2} a_{ij}\left(F_i \rho_S(t) F_j^\dagger - \frac{1}{2}\left\{ F_j^\dagger F_i, \rho_S(t) \right\} \right).
\tag{3.18}
$$

The first term of the equation describes the unitary evolution of the system. H_{LS} is called the **Lamb-Shift** Hamiltonian which cause a modification of the energy levels of H_S due to the coupling with the environment. The second term describes the irreversible, non-unitary, evolution and is often
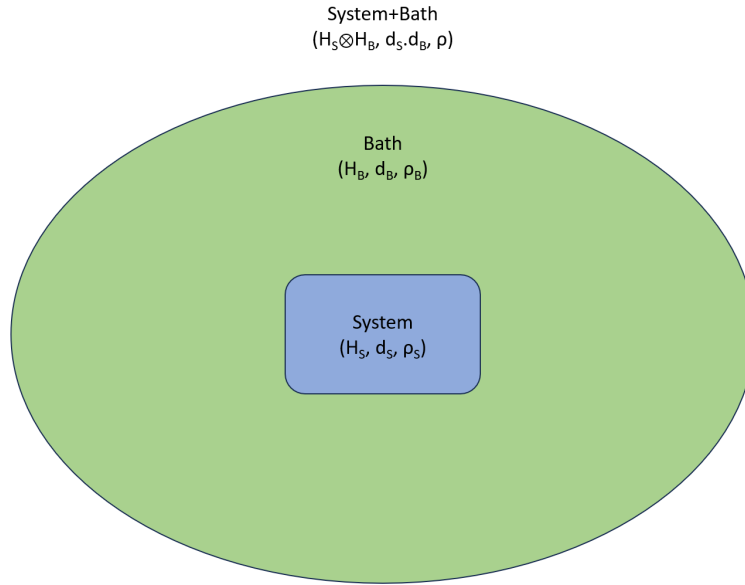
Figure 3.1: Schematic representation of an open quantum system. The system of interest has the dimension d_S and is describe by the density matrix ρ_S whose time evolution is generated by the Hamiltonian H_S. This system is in interaction with a Bath (or environment) of dimension d_B (usually very large if not infinite), describe by the density operator ρ_B which evolves due to the Hamiltonian H_B. The combination System+bath forms a **_closed_** system.

called **_dissipator_**. The operators F_i involved in this dissipator form with the identity operator a complete basis of the Liouville space, the operation $\{.,.\}$ is the anti-commutator and the a_{ij} define a positive matrix.

For the derivation it is convenient to work in the interaction picture. In this picture the density operator becomes

$$\rho_I(t) = e^{iH_0 t} \rho(t) e^{-iH_0 t} \tag{3.19}$$

with $H_0 = H_S \otimes I_B + I_S \otimes H_B$. The interaction Hamiltonian transforms in the same way

$$H_{int,I}(t) = e^{iH_0 t} H_{int} e^{-iH_0 t}. \tag{3.20}$$

Then the Liouville-Von Neumann equation in interaction picture is

$$i\frac{d\rho_I(t)}{dt} = [H_{int,I}(t), \rho_I(t)]. \tag{3.21}$$

In this picture, we see that the evolution of the density operator over time depends only on the interaction Hamiltonian. By integrating the equation we have

$$\rho_I(t) = \rho_I(0) - i \int_0^t [H_{int,I}(t'), \rho_I(t')] \, dt'. \tag{3.22}$$

Now, we insert this result back in (3.21) and we trace the equation over the environment which yields

$$\frac{d\rho_{S,I}(t)}{dt} = -i \operatorname{Tr}_B \left([H_{int,I}(t), \rho_I(0)] \right) - \int_0^t \operatorname{Tr}_B \left([H_{int,I}(t), [H_{int,I}(t'), \rho_I(t')]] \right) dt'. \tag{3.23}$$

It is now time to introduce three approximations in order to simplify this equation.

3.2.1   Born approximation

This approximation considers that

- The system S has a very small interaction with the environment B.

- The environment is stationary, $\rho_B(t) = \rho_B$.

That means that the state of the composite system is, at any time, a product state

$$\rho(t) = \rho_S(t) \otimes \rho_B \tag{3.24}$$

meaning we consider $\rho_{corr} = 0$. We also consider

$$\text{Tr}_B\left([H_{int}(t), \rho_S(0) \otimes \rho_B]\right) = 0 \tag{3.25}$$

this is not really an approximation as we can always absorb terms in the system Hamiltonian H_S in order to cancel this term [61]. Equation (3.23) becomes

$$\frac{d\rho_S(t)}{dt} = -\int_0^t \text{Tr}_B\left([H_{int}(t), [H_{int}(t'), \rho_S(t') \otimes \rho_B]]\right) dt'. \tag{3.26}$$

3.2.2   Markov approximation

Let us do the substitution $t' \to t - t'$ yielding to

$$\frac{d\rho_S(t)}{dt} = -\int_0^t \text{Tr}_B\left([H_{int}(t), [H_{int}(t - t'), \rho_S(t - t') \otimes \rho_B]]\right) dt'. \tag{3.27}$$

We now rewrite the interaction Hamiltonian as

$$H_{int}(t) = \alpha V(t), \tag{3.28}$$

where α represents the strength of the coupling so that in this form it will allow us to consider a weak coupling. Our evolution equation then reads

$$\frac{d\rho_S(t)}{dt} = -\alpha^2 \int_0^t \text{Tr}_B\left([V(t), [V(t - t'), \rho_S(t - t') \otimes \rho_B]]\right) dt'. \tag{3.29}$$

But in that case when $\alpha \to 0$ the variations of the density operator also go to zero so we cannot observe the dynamic of the system. To work around this problem we do the substitution $t'' = \alpha^2 t'$

$$\frac{d\rho_S(t)}{dt} = -\int_0^{\alpha^2 t} \text{Tr}_B\left([V(t), [V(t - t''/\alpha^2), \rho_S(t - t''/\alpha^2) \otimes \rho_B]]\right) dt''. \tag{3.30}$$

So that if we want the derivative to be different than zero we need to extend the integration to the infinity. By doing so the variations of the state of the system at a time t does not depend anymore of the states at previous times, physically this means that with this approximation we neglect the memory of the system. Let us also note that if $\alpha \to 0$ then $\rho_S(t)$ evolves slowly and we can assume it to be constant. So now we have the Born-Markov equation

$$\frac{d\rho_S(t)}{dt} = -\int_0^\infty \text{Tr}_B\left([H_{int}(t), [H_{int}(t - t'), \rho_S(t) \otimes \rho_B]]\right) dt'. \tag{3.31}$$

There still is a problem remaining, the Born-Markov equation does not, in general, guarantee a positive-definite ρ_S. We will then make a last approximation, the secular approximation also called rotating wave approximation (RWA).

3.2.3   Secular approximation

The most general form for the interaction Hamiltonian in Schrodinger picture is

$$H_{int,S} = \sum_{\alpha} A_{\alpha} \otimes B_{\alpha} \tag{3.32}$$

With A_{α} and B_{α} hermitian operators that act on the system and on the environment respectively. Now we will decompose $H_{int,S}$ into eigenoperators[2] of the system Hamiltonian. If we suppose for simplicity that the spectrum of H_S is discrete, we denote its eigenvalues by ϵ and the projectors onto the eigenspace related to the eigenvalue ϵ by $\mathcal{P}(\epsilon)$. We can now define

$$A_{\alpha}(\omega) \equiv \sum_{\omega = \epsilon' - \epsilon} \mathcal{P}(\epsilon) A_{\alpha} \mathcal{P}(\epsilon'). \tag{3.33}$$

Then we have

$$[H_S, A_{\alpha}(\omega)] = -\omega A_{\alpha}(\omega) \tag{3.34}$$

$$[H_S, A_{\alpha}^{\dagger}(\omega)] = +\omega A_{\alpha}^{\dagger}(\omega), \tag{3.35}$$

the operators $A_{\alpha}(\omega)$ and $A_{\alpha}^{\dagger}(\omega)$ are eigenoperators of H_S of eigenvalue $-\omega$ and $+\omega$. By summing over all energies and because the eigenspace on which we project A_{α} is complete we have

$$\sum_{\omega} A_{\alpha}(\omega) = A_{\alpha} \tag{3.36}$$

The interaction Hamiltonian now has the form

$$H_{int,S} = \sum_{\alpha\omega} A_{\alpha}(\omega) \otimes B_{\alpha} \tag{3.37}$$

We now need to write the interaction Hamiltonian in the interaction picture in order to cast it in the Born-Markov equation (3.31). Considering the commutation relations, the eigenoperators read in interaction picture

$$e^{iH_S t} A_{\alpha}(\omega) e^{-iH_S t} = e^{-i\omega t} A_{\alpha}(\omega) \tag{3.38}$$

$$e^{iH_S t} A_{\alpha}^{\dagger}(\omega) e^{-iH_S t} = e^{i\omega t} A_{\alpha}^{\dagger}(\omega). \tag{3.39}$$

By also taking B_{α} in the interaction picture $(B_{\alpha}(t) = e^{iH_B t} B_{\alpha} e^{-iH_B t})$, the interaction Hamiltonian in the interaction picture now has the particular form

$$H_{int,I}(t) = \sum_{\alpha\omega} e^{-i\omega t} A_{\alpha}(\omega) \otimes B_{\alpha}(t). \tag{3.40}$$

Inserting this Hamiltonian in the Born-Markov equation (3.31) we get after simplifications

$$\frac{d\rho_S(t)}{dt} = \sum_{\omega,\omega'} \sum_{\alpha,\beta} e^{i(\omega'-\omega)t} \Gamma_{\alpha\beta}(\omega) \left(A_{\beta}(\omega)\rho_S(t)A_{\alpha}^{\dagger}(\omega') - A_{\alpha}^{\dagger}(\omega')A_{\beta}(\omega)\rho_S(t) \right) + h.c. \tag{3.41}$$

Where h.c. is the hermitian conjugate and we introduced the environment correlation functions $\Gamma_{\alpha\beta}(\omega)$ defined as

$$\Gamma_{\alpha\beta}(\omega) \equiv \int_0^{\infty} dt' e^{i\omega t'} \operatorname{Tr}_B(B_{\alpha}^{\dagger}(t)B_{\beta}(t-t')\rho_B) \equiv \int_0^{\infty} dt' e^{i\omega t'} \left\langle B_{\alpha}^{\dagger}(t)B_{\beta}(t-t') \right\rangle. \tag{3.42}$$

The secular approximation consists in neglecting the terms in $\omega' \neq \omega$ so that we have

$$\frac{d\rho_S(t)}{dt} = \sum_{\omega} \sum_{\alpha\beta} e^{i(\omega'-\omega)t} \Gamma_{\alpha\beta}(\omega) \left(A_{\beta}(\omega)\rho_S(t)A_{\alpha}^{\dagger}(\omega) - A_{\alpha}^{\dagger}(\omega)A_{\beta}(\omega)\rho_S(t) \right) + h.c. \tag{3.43}$$

---

[2] An eigenoperator O of eigenvalue λ of a matrix M is a linear operator such that $[M,O] = \lambda M$

3.2.4   Standard form

Finally the secular Born-Markov equation (3.43) can be expressed in the standard form (3.18) if we decompose the environment correlation functions (3.42) as

$$\Gamma_{\alpha\beta}(\omega) = \frac{1}{2}\gamma_{\alpha\beta}(\omega) + iS_{\alpha\beta}(\omega) \tag{3.44}$$

with

$$\gamma_{\alpha\beta}(\omega) = \Gamma_{\alpha\beta}(\omega) + \Gamma_{\beta\alpha}^*(\omega) = \int_{-\infty}^{\infty} dt'e^{i\omega t'}\left\langle B_\alpha^\dagger(t')B_\beta(0)\right\rangle \tag{3.45}$$

$$S_{\alpha\beta}(\omega) = \frac{1}{2i}\left(\Gamma_{\alpha\beta}(\omega) - \Gamma_{\beta\alpha}^*(\omega)\right). \tag{3.46}$$

Using these we finally obtain our master equation in the interaction picture

$$\frac{d\rho_S(t)}{dt} = -i\left[H_{LS}, \rho_S(t)\right] + \mathcal{D}(\rho_S(t)). \tag{3.47}$$

Where the hermitian operator H_{LS} is called the Lamb shift Hamiltonian

$$H_{LS} = \sum_\omega \sum_{\alpha\beta} S_{\alpha\beta}(\omega)A_\alpha^\dagger(\omega)A_\beta(\omega) \tag{3.48}$$

and the dissipator $\mathcal{D}(\rho_S(t))$ is a shortened form of

$$\mathcal{D}(\rho_S(t)) = \sum_\omega \sum_{\alpha\beta} \gamma_{\alpha\beta}(\omega)\left(A_\beta(\omega)\rho_S(t)A_\alpha^\dagger(\omega) - \frac{1}{2}\left\{A_\alpha^\dagger(\omega)A_\beta(\omega), \rho_S(t)\right\}\right). \tag{3.49}$$

3.3   4-level open system

In this section we will apply the master equation derivation from the previous section to a specific open system. The chosen system is the simplest system we can imagine for spin one half fermions, that is a 4-level system $\{|0\rangle, |\downarrow\rangle, |\uparrow\rangle, |\downarrow\uparrow\rangle\}$ where $|0\rangle$ is the non-occupied state, $|\uparrow\rangle$ and $|\downarrow\rangle$ are the single occupied states and $|\downarrow\uparrow\rangle$ is the double occupied state. Here, to make the connection with a BCS superconductor, we can interpret the fermions of this 4-level system as Bogoliubov quasiparticles and the fact that we have only one level for each spin as if we were focusing on a specific energy $E_{\mathbf{k_0}} \equiv \omega_S$ (i.e., a specific value of $\mathbf{k}_0$) among the full quasi-particle spectrum $E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + \Delta^2}$ (i.e., among all $\mathbf{k}$). We consider that this system is coupled to two (non superconducting) reservoirs that are considered to be at thermal equilibrium and that their energy can be controlled by adding a chemical potential μ as described below in figure 3.2.

Our open system is then described by different Hamiltonians:

- The 4-level system Hamiltonian H_S

$$H_S = \omega_S\left(\sum_{s=\downarrow,\uparrow}\gamma_s^\dagger\gamma_s\right) \tag{3.50}$$

  which is an Hamiltonian of the form of (2.44) for only one value of $\mathbf{k}$. Here the γ operators are creation/annihilation operators for Bogoliubov quasiparticles. Note that this Hamiltonian is usually used to model quantum dots [62, 63].

- The Hamiltonians of the two reservoirs

$$H_{reservoirs} = \sum_k \sum_{s=\downarrow,\uparrow} \sum_{l=L,R} (\omega_k + \mu_l)b_{ksl}^\dagger b_{ksl} \tag{3.51}$$

  are standard Hamiltonians with b being creation/annihilation operators for normal particles.
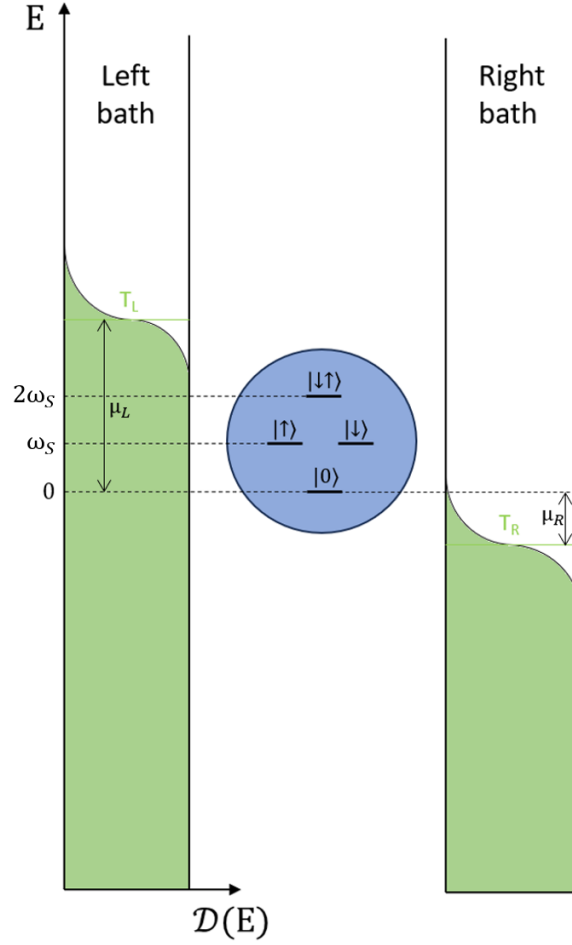
Figure 3.2: Schematic description of our four level system. The four states are the vacuum state $|0\rangle$ of energy zero, the degenerate single spin-states $|\uparrow\rangle$ and $|\downarrow\rangle$ of energy ω_s and the double-spin state of energy $2\omega_s$. This system is connected to two fermionic baths at different temperature T_L and T_R and chemical potentials (i.e., Fermi energies) μ_L and μ_R. The density of states $\mathcal{D}(E)$ are assumed to be constant over the range of the relevant transitions energies of the system.

- The interaction Hamiltonian

$$H_{int} = \sum_k \sum_{s=\downarrow,\uparrow} \sum_{l=L,R} \left(t_{ksl} b_{ksl}^\dagger c_s + t_{ksl}^* c_s^\dagger b_{ksl} \right). \tag{3.52}$$

  Where the t_{ksl} are tunneling amplitudes. This Hamiltonian describes exchange of particles with the reservoirs.

In order to derive the master equation for our specific system we need to write our interaction Hamiltonian in the interaction picture. But before, since we have a superconducting system we should apply the Bogoliubov transformation to the c_s operators so that H_{int} becomes

$$H_{int} = \sum_{k,l} \Big[t_{kl} \left(b_{kl\downarrow}^\dagger (-v\gamma_\uparrow^\dagger + u\gamma_\downarrow) + b_{kl\uparrow}^\dagger (u\gamma_\uparrow + v\gamma_\downarrow^\dagger) \right)$$

$$+ t_{kl}^* \left((-v^*\gamma_\uparrow + u^*\gamma_\downarrow^\dagger) b_{kl\downarrow} + (u^*\gamma_\uparrow^\dagger + v^*\gamma_\downarrow) b_{kl\uparrow} \right) \Big]. \tag{3.53}$$

Now we write it in the interaction picture

$$H_{int}^I = \sum_{k,l} \left[t_{kl} \left(b_{kl\downarrow}^{\dagger,I}(t)(-v\gamma_\uparrow^{\dagger,I}(t) + u\gamma_\downarrow^I)(t) + b_{kl\uparrow}^{\dagger,I}(t)(u\gamma_\uparrow^I(t) + v\gamma_\downarrow^{\dagger,I}(t)) \right) \right.$$
$$\left. + t_{kl}^* \left((-v^*\gamma_\uparrow^I(t) + u^*\gamma_\downarrow^{\dagger,I}(t))b_{kl\downarrow}(t) + (u^*\gamma_\uparrow^{\dagger,I}(t) + v^*\gamma_\downarrow^I(t))b_{kl\uparrow}^I(t) \right) \right]. \quad (3.54)$$

where

$$b_{kls}^I(t) = e^{iH_B t} b_{kls} e^{-iH_B t} = e^{-i(\omega_k + \mu_l)t} b_{kls} \quad (3.55)$$
$$\gamma_s^I(t) = e^{iH_S t} \gamma_s e^{-iH_S t} = e^{-i\omega_S t} \gamma_s. \quad (3.56)$$

We define

$$B_{ls}^I(t) = \sum_k t_{kl}^* b_{kls}^I(t). \quad (3.57)$$

The following derivation we be done entirely in the interaction picture but we will omit the superscript I to simplify the notation.

We start with

$$\frac{d\rho_S(t)}{dt} = -\int_0^t \text{Tr}_B \left([H_{int}(t), [H_{int}(t'), \rho(t')]] \right) dt' \quad (3.58)$$

developing the double commutator gives

$$\frac{d\rho_S(t)}{dt} = -\int_0^t \text{Tr}_B \left(H_{int}(t)H_{int}(t')\rho(t') - H_{int}(t')\rho(t')H_{int}(t) - H_{int}(t)\rho(t')H_{int}(t') \right.$$
$$\left. + \rho(t')H_{int}(t')H_{int}(t) \right) \quad (3.59)$$

Now we have to replace H_{int} by its definition. The complete derivation is quite long but mainly repetitive so we will only develop the first term here.

$$-\int_0^t \text{Tr}_B \left[\left(B_\downarrow^\dagger(t)(-v\gamma_\uparrow^\dagger(t) + u\gamma_\downarrow(t)) + B_\uparrow^\dagger(t)(u\gamma_\uparrow(t) + v\gamma_\downarrow^\dagger(t)) + B\downarrow(t)(-v^*\gamma_\uparrow(t) + u^*\gamma_\downarrow^\dagger(t)) \right. \right.$$
$$\left. + B_\uparrow(t)(u^*\gamma_\uparrow^\dagger(t) + v^*\gamma_\downarrow(t)) \right)$$
$$\left(B_\downarrow^\dagger(t')(-v\gamma_\uparrow^\dagger(t') + u\gamma_\downarrow(t')) + B_\uparrow^\dagger(t')(u\gamma_\uparrow(t') + v\gamma_\downarrow^\dagger(t')) + B\downarrow(t')(-v^*\gamma_\uparrow(t') + u^*\gamma_\downarrow^\dagger(t')) \right.$$
$$\left. + B_\uparrow(t')(u^*\gamma_\uparrow^\dagger(t') + v^*\gamma_\downarrow(t')) \right)$$
$$\rho(t') \Big] dt'. \quad (3.60)$$

Since the baths are in normal state this yields that only the terms in $B_s^\dagger B_s$ and $B_s B_s^\dagger$ will be non zero. Spin flips for the quasiparticles are also not considered so that only the products involving gamma operators for the same spin will survive.

$$-\int_0^t \text{Tr}_B \left[B_\downarrow^\dagger(t)B_\downarrow(t') \left(|v|^2 \gamma_\uparrow^\dagger(t)\gamma_\uparrow(t') + |u|^2 \gamma_\downarrow(t)\gamma_\downarrow^\dagger(t') \right) \rho(t') \right.$$
$$+ B_\uparrow^\dagger(t)B_\uparrow(t') \left(|u|^2 \gamma_\uparrow(t)\gamma_\uparrow^\dagger(t') + |v|^2 \gamma_\downarrow^\dagger(t)\gamma_\downarrow(t') \right) \rho(t')$$
$$+ B_\downarrow(t)B_\downarrow^\dagger(t') \left(|v|^2 \gamma_\uparrow(t)\gamma_\uparrow^\dagger(t') + |u|^2 \gamma_\downarrow^\dagger(t)\gamma_\downarrow(t') \right) \rho(t')$$
$$\left. + B_\uparrow(t)B_\uparrow^\dagger(t') \left(|u|^2 \gamma_\uparrow^\dagger(t)\gamma_\uparrow(t') + |v|^2 \gamma_\downarrow(t)\gamma_\downarrow^\dagger(t') \right) \rho(t') \right] dt'. \quad (3.61)$$

Once again, the development for each term is always the same we will thus only keep the first term. We will now introduce the Born approximation $\rho(t') = \rho_S(t') \otimes \rho_B$.

$$-\int_0^t \text{Tr}_B \left(B_\downarrow^\dagger(t)B_\downarrow(t')\rho_B \right) |v|^2 \gamma_\uparrow^\dagger(t)\gamma_\uparrow(t')\rho_S(t') dt'. \quad (3.62)$$

By definition $\text{Tr}_B \left(B_\downarrow^\dagger(t) B_\downarrow(t') \rho_B \right) = \left\langle B_\downarrow^\dagger(t) B_\downarrow(t') \right\rangle$ which gives using (3.57) and writing explicitly the time dependence

$$\left\langle B_\downarrow^\dagger(t) B_\downarrow(t') \right\rangle = \sum_{kk'} t_k^* t_{k'}^* e^{i\omega_k t} e^{-i\omega_k t'} \left\langle b_{k\downarrow}^\dagger b_{k'\downarrow} \right\rangle. \tag{3.63}$$

The particles of the bath are at thermal equilibrium so we have $\left\langle b_{k\downarrow}^\dagger b_{k'\downarrow} \right\rangle = n(\omega_k)\delta_{kk'}$. We can go from the sum over k to an integral over ω_k by introducing the density of states $\mathcal{D}(\omega_k)$

$$\int_\infty^\infty d\omega_k |t_k|^2 \mathcal{D}(\omega_k) e^{i\omega_k(t-t')} n(\omega_k). \tag{3.64}$$

The product $|t_k|^2 \mathcal{D}(\omega_k)$ is just the tunneling rate Γ divided by π. Equation (3.62) now reads

$$-\frac{\Gamma}{\pi} \int_0^t dt' \int_\infty^\infty d\omega_k e^{i\omega_k(t-t')} n(\omega_k) |v|^2 \gamma_\uparrow^\dagger(t) \gamma_\uparrow(t') \rho_S(t') dt'. \tag{3.65}$$

We will perform the time integral first but before we apply the Markov approximation by extending the integration domain to ∞ and by considering $\rho_S(t') \approx \rho_S(t)$. By also writing explicitly the time dependence of the gamma operators we have

$$-\frac{\Gamma}{\pi} \int_\infty^\infty d\omega_k n(\omega_k) |v|^2 e^{i(\omega_k + \omega_S)t} \left(\int_0^\infty dt' e^{-i(\omega_k + \omega_S)t'} \right) \gamma_\uparrow^\dagger \gamma_\uparrow \rho_S(t). \tag{3.66}$$

The time integral yields $\pi\delta(\omega + \omega_S)$ if we neglect the principal value, the delta in omega simplify greatly the remaining integral so that we finally have one of the term of our master equation

$$\frac{d\rho_S(t)}{dt} = -\Gamma n(-\omega_S) |v|^2 \gamma_\uparrow^\dagger \gamma_\uparrow \rho_S(t) + ... \tag{3.67}$$

After repeating what we did for all terms and after simplification by exploiting the facts that $n(-\omega_S) = 1 - n(\omega_S)$ and $|v|^2 + |u|^2 = 1$ we obtain the master equation

$$\frac{d\rho_S(t)}{dt} = \sum_{i=1}^4 \sum_{l=L,R} \eta_{i,l} \left(L_i \rho_S(t) L_i^\dagger - \frac{1}{2} \left\{ L_i^\dagger L_i, \rho_S(t) \right\} \right). \tag{3.68}$$

Where the L_i and η_i are elements of the vectors

$$\mathbf{L} = (L_1, L_2, L_3, L_4) = (\gamma_\downarrow, \gamma_\uparrow, \gamma_\downarrow^\dagger, \gamma_\uparrow^\dagger) \tag{3.69}$$

$$\boldsymbol{\eta}_l = \Gamma_l(\eta_{1l}, \eta_{2l}, \eta_{3l}, \eta_{4l}) = \Gamma_l \left(1 - n(\omega_S - \mu_l), 1 - n(\omega_S - \mu_l), n(\omega_S - \mu_l), n(\omega_S - \mu_l)\right) \tag{3.70}$$

We can now solve our master equation (3.68) numerically to see how the system evolve depending on the characteristics of the two reservoirs. To do so, we just need to project the master equation onto the basis $\{|0\rangle, |\downarrow\rangle, |\uparrow\rangle, |\downarrow\uparrow\rangle\}$, which yields a linear system of differential equations for the density matrix elements. Let us see how the populations in the system evolve depending on the chemical potentials of the two reservoirs. In the following, we study two configurations, first the case where both baths have a positive chemical potential and second the case where one bath has a positive chemical potential and the other one a negative chemical potential. Both cases were numerically implemented and the results are shown below in figures 3.3 and 3.4.
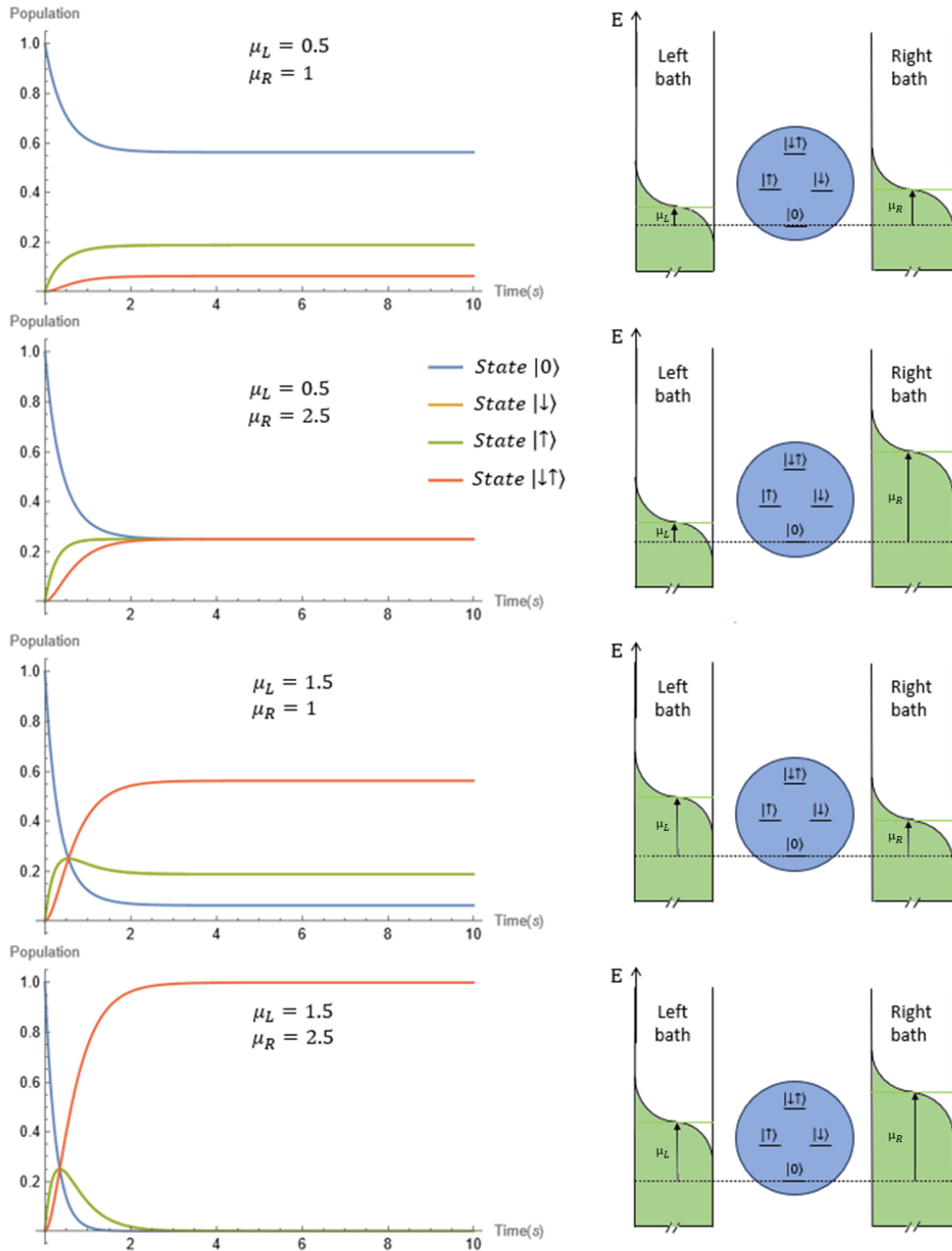
Figure 3.3: Left: evolution of the populations of the system when both chemical potentials are positive for different values of chemical potentials. Right: schematic description of the configuration of the system corresponding to the left plot. In the four cases we start in the state $|0\rangle$. We observe than the more we increase both chemical potentials the more we populate the double spin state. Finally, here the chemical potentials are expressed in unit of ω_S.
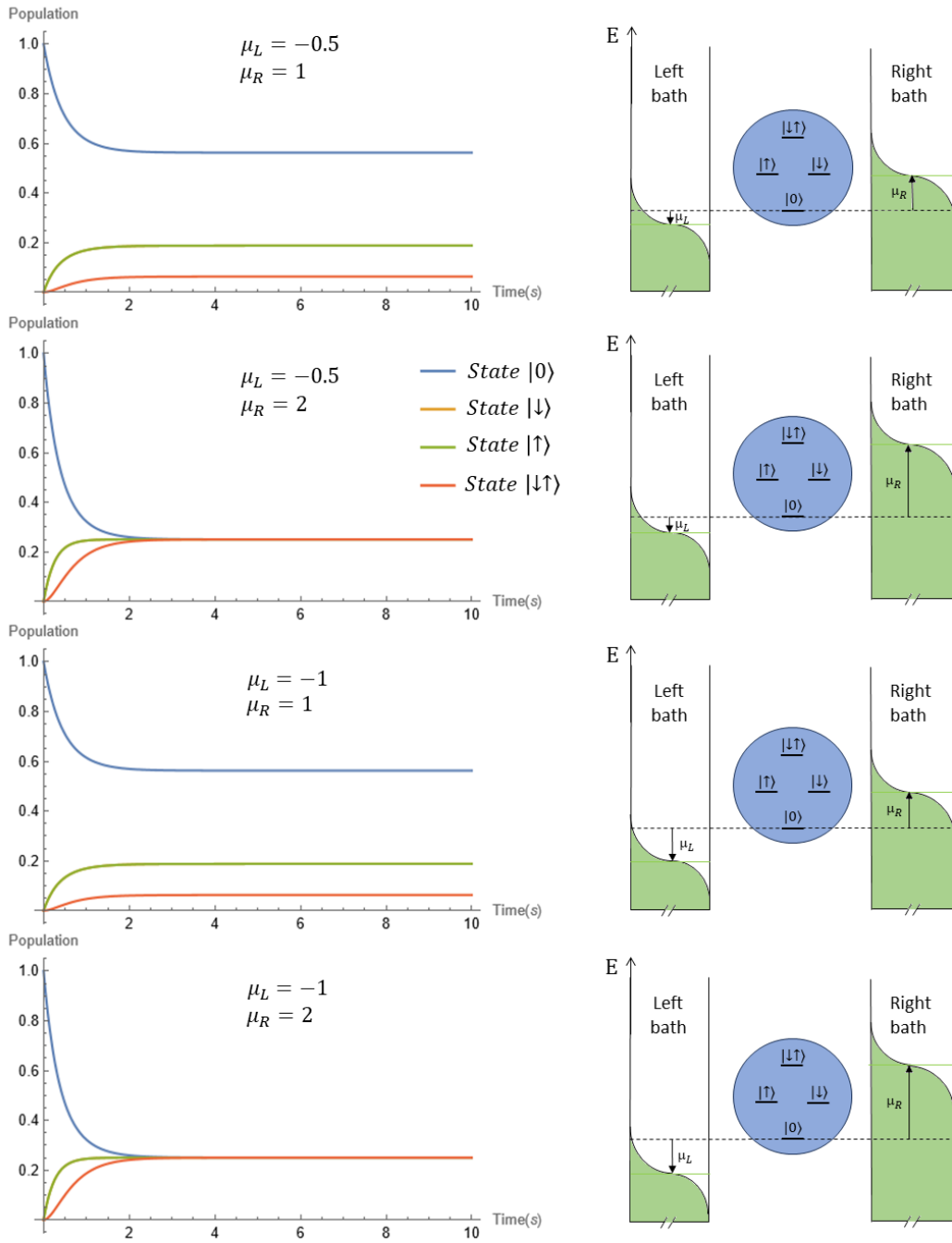
Figure 3.4: Left: evolution of the populations of the system when one chemical potential is positive and the othe negative for different values of chemical potentials. Right: schematic description of the configuration of the system corresponding to the left plot. In the four cases we start in the state $|0\rangle$. In this configuration increasing (in absolute value) the chemical potentials only lead to an even population of the four states. Finally, here the chemical potentials are expressed in unit of ω_S.

Finally, to introduce what we will be doing in the next chapter and what is the main interest of this thesis, we can determine the expectation values $\langle \gamma^\dagger \gamma \rangle, \langle \gamma \gamma^\dagger \rangle$ needed to compute the gap Δ. Indeed, because our system is out of equilibrium the quasiparticles are no longer distributed according the Fermi-Dirac distribution. The fact that the system is no more at equilibrium can be understood as follows: each bath tends to push the system at thermal equilibrium at their own temperature by filling the system with quasi-particles up to their chemical potential according to their Fermi-Dirac distributions. But since the system is coupled to two baths at different temperature and chemical potentials, this creates a kind of frustration yielding an out-of-equilibrium steady state.

To compute these expectation values we first evaluate the density operator in the steady state ρ_{SS} by setting the left member of the master equation (3.68) to zero and by imposing the condition that the sum of the diagonal elements of the density operator must be one. We then just need to solve the system of equations

$$
\begin{cases}
0 = \displaystyle\sum_{i=1}^{4} \sum_{l=L,R} \eta_{i,l} \left(L_i \rho_{SS} L_i^\dagger - \frac{1}{2} \left\{ L_i^\dagger L_i, \rho_{SS} \right\} \right). \\
\displaystyle\sum_{j=1}^{4} \langle j | \rho_{SS} | j \rangle = 1
\end{cases}
\tag{3.71}
$$

to get the density operator in the steady state. We then just need to apply the definition of the expectation value

$$
\langle \gamma_s^\dagger \gamma_s \rangle = \mathrm{Tr}\big(\gamma_s^\dagger \gamma_s \rho_{SS}\big) \equiv n(\omega_S),
\tag{3.72}
$$

$$
\langle \gamma_s \gamma_s^\dagger \rangle = \mathrm{Tr}\big(\gamma_s \gamma_s^\dagger \rho_{SS}\big) \equiv 1 - n(\omega_S).
\tag{3.73}
$$

By computing the traces we get the following distribution for the quasiparticles as a function of the energy ω_S in our system

$$
n(\omega_S) = \frac{\Gamma_L}{\Gamma_L + \Gamma_R} n(\omega_S - \mu_L) + \frac{\Gamma_R}{\Gamma_L + \Gamma_R} n(\omega_S - \mu_R)
\tag{3.74}
$$

Where the subscript L and R refer to the left and right bath respectively, the $\Gamma_{L,R}$ are the tunneling rates describing how probable are the tunneling of particles between the system and the two baths and the $n_{L,R}$ are the Fermi-Dirac distributions of the baths. Hence, we see that the new distribution of the quasi-particles is a weighted sum of the thermal distributions of the two baths.

Chapter 4

Out of equilibrium HFB

In this last chapter we will go back to our self-consistent HFB algorithm and replace the Fermi-Dirac distribution by the distribution (3.74) we found at the end of the last chapter. By doing so we will be able to compute the gap of our 4-level system depending on the characteristics of the two reservoirs and compare the results with the ones we had in the classic case. In the previous chapter we considered our system to be in the single mode $\mathbf{k}_0$ as expressed by Eq. (3.50). But all the development made for that single mode can be extended to any mode $\mathbf{k}$, as we can assume the quasi-particles behave independently. We will do so in this chapter and consider a continuum of mode $\mathbf{k}$ and thus retrieve a one dimensional configuration to apply our HFB algorithm.

The quasiparticles now satisfy

$$\langle \gamma_{\mathbf{k}\uparrow}^{\dagger} \gamma_{\mathbf{k}\uparrow} \rangle = \frac{\Gamma_L}{\Gamma_L + \Gamma_R} n(E_{\mathbf{k}} - \mu_L) + \frac{\Gamma_R}{\Gamma_L + \Gamma_R} n(E_{\mathbf{k}} - \mu_R) \tag{4.1}$$

$$\langle \gamma_{\mathbf{k}\uparrow}^{\dagger} \gamma_{-\mathbf{k}\downarrow}^{\dagger} \rangle = 0 \tag{4.2}$$

$$\langle \gamma_{-\mathbf{k}\downarrow} \gamma_{\mathbf{k}\uparrow} \rangle = 0 \tag{4.3}$$

$$\langle \gamma_{-\mathbf{k}\downarrow} \gamma_{-\mathbf{k}\downarrow}^{\dagger} \rangle = 1 - \frac{\Gamma_L}{\Gamma_L + \Gamma_R} n(E_{\mathbf{k}} - \mu_L) - \frac{\Gamma_R}{\Gamma_L + \Gamma_R} n(E_{\mathbf{k}} - \mu_R). \tag{4.4}$$

that is a weighted sum of the distributions of the reservoirs, where the energy $E_{\mathbf{k}}$ is given by

$$E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + |\Delta_{\mathbf{k}}|^2}. \tag{4.5}$$

Here, we set the chemical potential of the system (its Fermi level) to zero, so that $\xi_{\mathbf{k}} = \epsilon_{\mathbf{k}} = \mathbf{k}^2/(2m)$. Hence, the distributions of the quasi-particles of the system are no more control directly by its chemical potential, but by the chemical potentials and temperatures of the left and right reservoirs.

4.1 Gap versus temperature

To start we will see how the pairing gap evolves with the temperature in three different configurations of the reservoirs: when they both have a positive chemical potential, when one has a positive chemical potential while the other is kept at zero chemical potential and lastly when one bath has a positive and the other a negative chemical potential. We see that when both baths have a positive chemical potential (Fig 4.1) the gap holds under an higher temperature ($T_c \approx 10\text{K}$) as we have an augmentation of the critical temperature of two orders of magnitude compared to the case investigated in Fig. 2.7, where $T_c = 0.033\text{K}$ was found. That improvement is substantial and we will give a possible explication of why it happens later. It should be noted that the end part of the numerical data (Blue curve) shows oscillations that are due to the precision of the algorithm and does not have any physical meaning. In order to this problem a quartic fit has been made on the end of the numerical data the give an intuition of what physically happens. Now when one bath
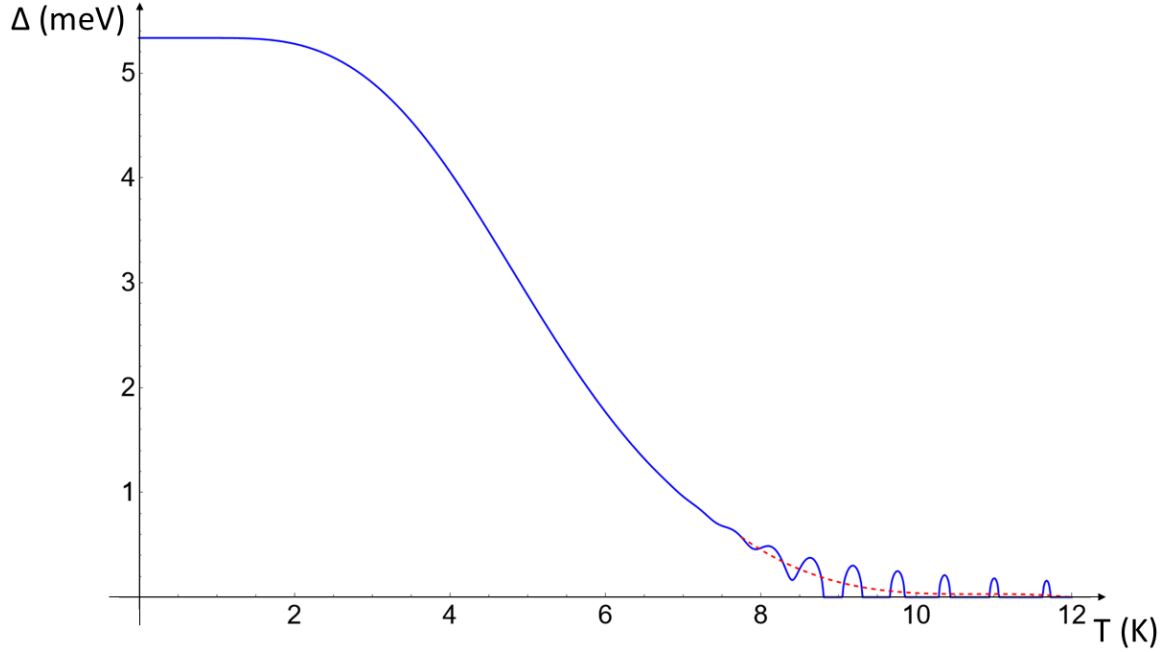
Figure 4.1: Evolution of the pairing gap with the temperature of the reservoirs when both baths have a chemical potential of $\mu_L = \mu_R = 1$ meV. We observe that the gap keeps its maximal value when the temperature is below 3K before it starts decreasing. Note that the gap does not vanish suddenly at a critical temperature like we saw at the end of section 2.4 but instead decreases exponentially. Finally, we see that the simulation failed to converge properly in the last part leading to oscillations in the blue curve. To compensate, we did a quartic on this last part displayed in dashed red. Other parameters used for the simulations are the tunneling rates $\Gamma_L = \Gamma_R$, the effective mass $m = 2m_e = 2 \times 9.109 \times 10^{-31}$ kg, the strength of the electrons interaction $U = 1$ meVnm and a precision $\epsilon = 10^{-14}$ meV and the cutoff length $a = 2 \times 10^{-9}$ nm.

has a positive chemical potential when is other is kept a zero (Fig 4.2) we still have an improvement of the critical temperature and on how gap is holding with temperature but not as good as in the previous configuration as we do not have the large plateau of constant Δ at the beginning anymore. Finally, when we have one positive and one negative chemical potential (Fig 4.3) we have the same dependence as in the classical BCS theory with a closed system but with a smaller critical temperature. From the three configurations this is the only one that does not lead to an enhancement of the pairing gap.

We should underline the fact that in Figs 4.1 and 4.2 the dependence of the gap on the temperature does no longer reflect a second order phase transition. Even if we did say we had improvement of the critical temperature we cannot really talk about a critical temperature anymore since the gap no longer goes abruptly to zero at a specific temperature but rather goes to zero asymptotically.

4.2 Delta versus chemical potentials

Since we saw in the previous section that the configuration with two positive chemical potentials lead to the best enhancement of our superconducting system we shall investigate it deeper. In this section, we will see how the gap evolves as a function of the chemical potentials of the baths for fixed temperatures.

We see in Fig 4.4 that for a given temperature a sufficiently large chemical potential is required to reach the maximum gap possible. Furthermore, the higher the temperature the larger the chemical potential to reach the maximum gap.
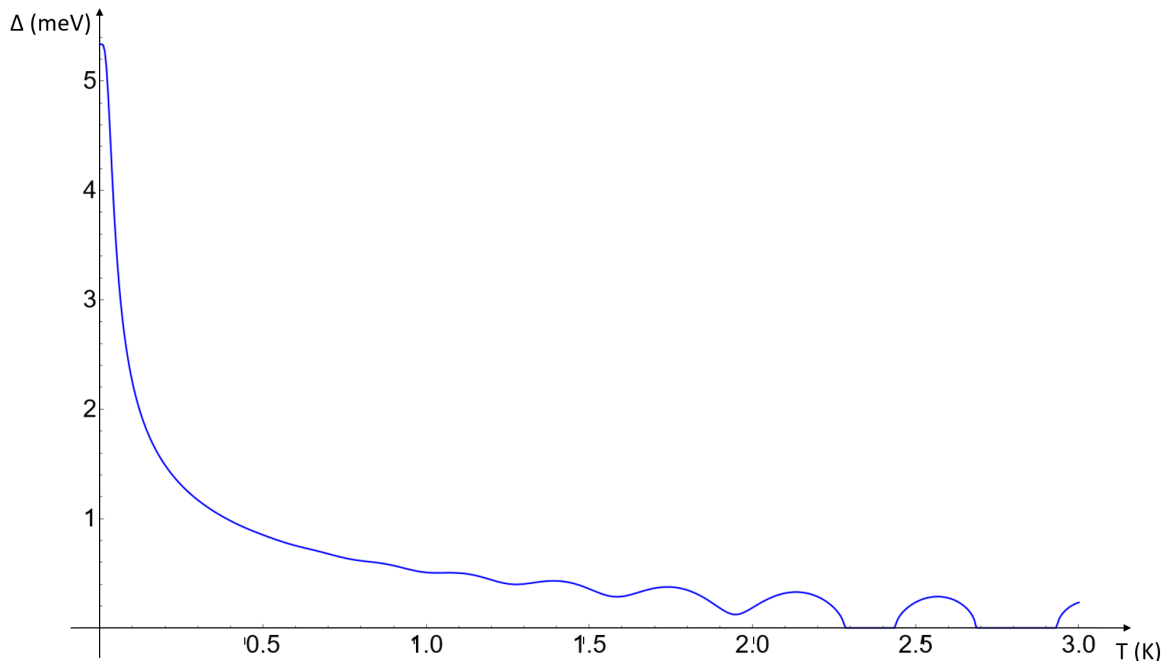
Figure 4.2: Evolution of the pairing gap with the temperature when one bath has a chemical potential of $\mu_L = 1$ meV and the other $\mu_R = 0$ meV. Contrary to the previous case here the gap decreases as soon as the temperature is increased. Like previously, the gap decreases exponentially instead of vanishing at a given temperature like in the equilibrium BCS theory. Other parameters used for the simulations are the tunneling rates $\Gamma_L = \Gamma_R$, the effective mass $m = 2m_e = 2 \times 9.109 \times 10^{-31}$ kg, the strength of the electrons interaction $U = 1$ meVnm and a precision $\epsilon = 10^{-14}$ meV and the cutoff length $a = 2 \times 10^{-9}$ nm.

We see for example that if we want the gap to remain at $T = 6$K (meaning having a dependence like in Fig. 4.1 but where the gap stays constant until 6K) we need to increase the chemical potentials to $\mu \approx +4$meV.

4.3   Explanation for the gap improvement

It is now time to give a possible explanation for why the gap is conserved at way higher temperature once the two reservoirs are set at positive chemical potential. The explanation is the following, both baths are filled with electrons and specially with electrons of momentum $+k$ and spin up and with electrons of momentum $-k$ and spin down. In that configuration the system can absorb electrons from both bath and in particular the system can absorb one of each electron we previously mentioned and once in the superconducting system those electrons will form a cooper pair an thus we will observe a pairing gap. A schematic description is shown below in Fig 4.5. While the temperature is kept low enough this mechanism will compensate for the loss of cooper pairs due to thermal excitation into Bogoliubov quasiparticles. When the temperature increases two mechanisms will lead to the destruction of the cooper pairs and therefore of the gap. First, as we already said when the temperature is not zero there is thermal excitation of the cooper pairs that lead to their destruction. Second, with greater temperature we know that the Fermi-Dirac distribution of the two reservoirs will have a more gradual transition which will allow the system to emit electrons to the empty states of the reservoirs which will also contribute to destroying Cooper pairs. That reasoning also explain why the two others configurations we tried were not as efficient as the one with two positive baths. When we have a positive chemical potential bath and one kept at zero chemical potential then the system will absorb electrons from the first bath but will be able to absorb from
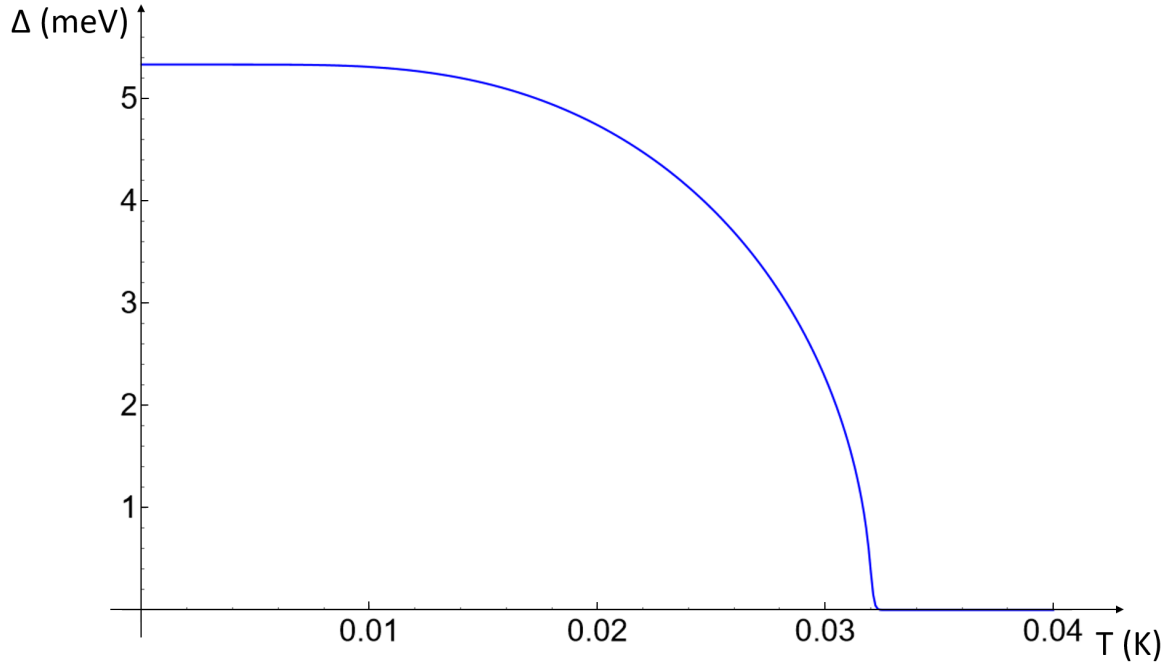
Figure 4.3: Evolution of the pairing gap with the temperature when one bath has a chemical potential of $\mu_L = 1$ µeV and the other $\mu_R = -1$ µeV. In this configuration we find the same dependence as the equilibrium case, with a characteristic shape of a second order phase transition. We have a non negligible critical temperature only for very small values of the chemical potentials, if we increase them then the gap only exists at $T = 0$ K. Other parameters used for the simulations are the tunneling rates $\Gamma_L = \Gamma_R$, the effective mass $m = 2m_e = 2 \times 9.109 \times 10^{-31}$ kg, the strength of the electrons interaction $U = 1$ meVnm and a precision $\epsilon = 10^{-14}$ meV and the cutoff length $a = 2 \times 10^{-9}$ nm.

as much as emit to the second bath leading to the splitting of the Cooper pairs and the decreasing of the gap as soon as the temperature is non zero as we saw in Fig 4.2. And when one bath has a positive chemical potential and the other a negative one then the system will absorb electrons from a bath as much as it emits to the other bath and therefore we have no improvement of the gap dependence in temperature as shown in Fig 4.3.
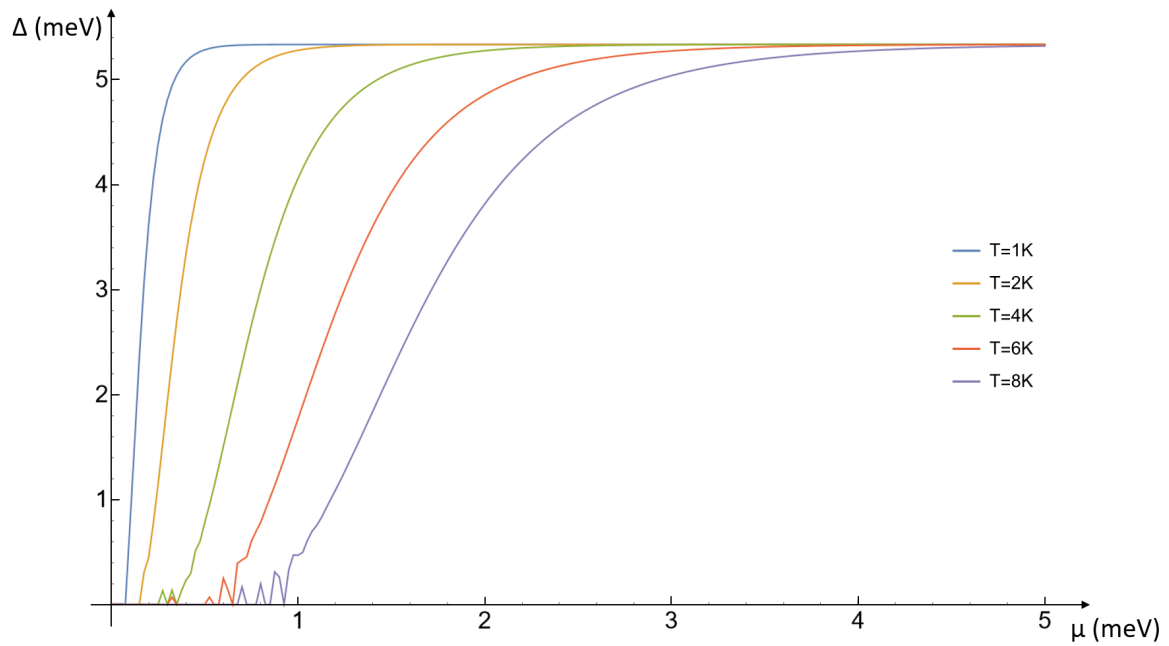
Figure 4.4: Evolution of the gap with the chemical potential μ when $\mu_L = \mu_R = +\mu$ for different temperatures. We see that the complete gap is reach when μ is sufficiently high and that this required μ is higher when the temperature is higher. Once again, we observe non physical oscillations for small values of Δ. Other parameters used for the simulations are the tunneling rates $\Gamma_L = \Gamma_R = 1$, the effective mass $m = 2m_e = 2 \times 9.109 \times 10^{-31}$ kg, the strength of the electrons interaction $U = 1$ meVnm and a precision $\epsilon = 10^{-14}$ meV and the cutoff length $a = 2 \times 10^{-9}$ nm.
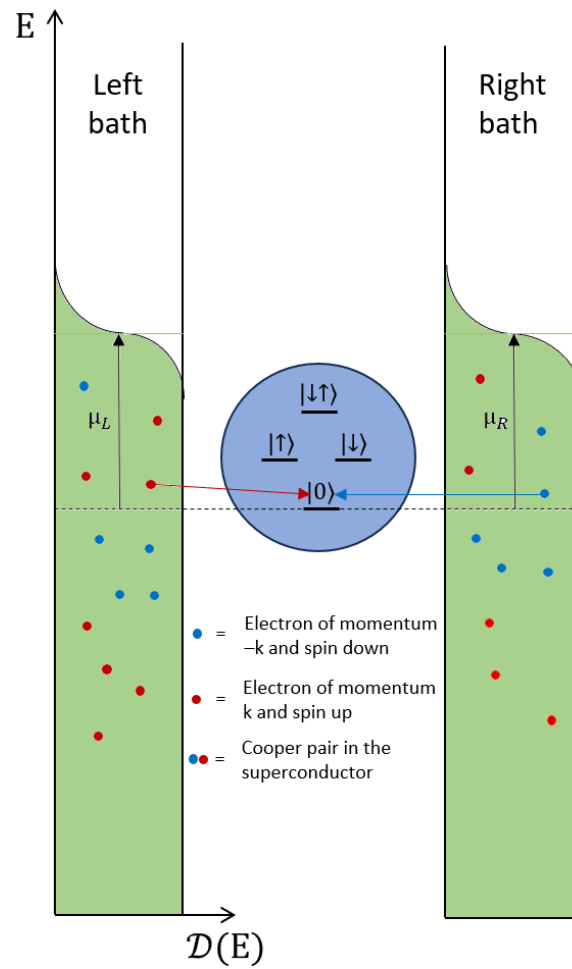
Figure 4.5: Schematic depiction of the mechanism improving the gap dependence on temperature when the two reservoirs are at positive chemical potential. Both reservoirs are filled with electrons in states $|\mathbf{k}, \uparrow\rangle$ and $|-\mathbf{k}, \downarrow\rangle$ that the system can absorb due to the positive chemical potential. Since the system is superconducting one electron in each state can combine in a Cooper pair leading to the apparition of a gap. This electron absorption can counterbalance the Cooper pair destruction due to thermal excitation if the temperature is not to high . Therefore the gap remains at higher temperatures compared to the case of a non-interacting superconductor.

Conclusion

4.4 General summary

In this master thesis, we applied the tools of open quantum systems to study theoretically the control of superconductivity via dissipation engineering. Indeed, as we said in the introduction of the thesis, we have good reasons to think that a well designed environment could be a source of enhancement of the superconductivity of the system. Because the second quantization formalism is used throughout all the thesis it was necessary to dedicate the first chapter to give a basic understanding of that formalism and of the creation and annihilation operators.

In the second chapter we developed the BCS theory which is the theory explaining all standard superconductors at a microscopic level. This theory explain superconductivity by the pairing of opposite spin and momentum electrons which, in the case of classical superconducting materials, happens due to phonon-electrons interaction. We considered the new BCS ground state as a superposition of Cooper pairs with a standard Hamiltonian that is a sum of a kinetic part and of a potential part, the latter being the interactive potential between the electrons. This Hamiltonian allowed us to compute the energy of the BCS ground state in order to apply a variational method, that is stating we are in a minimal energy state. We then were able to define the gap which is the minimal energy required to break a Cooper pair. This approach while giving interesting information does not allow to treat thermal excitation of the cooper pairs. To resolve his problem we used a more modern approach, the Bogoliubov-Valatin transformation. This method consists of defining new creation and annihilation operators for Bogoliubov quasiparticles, which are superposition of hole and electron and are the excited states of Cooper pair. The gap could then be defined through the average number of quasiparticles which, because we considered the quasiparticles to be in thermal equilibrium, is given by the Fermi-Dirac distribution. We can then now find the gap for any temperature. Finally, we explained and implemented the self-consistent Hartree-Fock-Bogoliubov (HFB) algorithm, the most common way to numerically solve BCS superconductor, and used it to verify some properties previously given.

In the third chapter the theory of open quantum system was presented. It was necessary to define the density operator, an extension of the notion of ket vector essential when working with open quantum systems. Afterwards we showed how to derive a Markovian master equation, the equation governing the evolution of a quantum system when it is weakly coupled to an environment. We then applied that formalism to derive in full details an original master equation for a 4-level fermionic system, the fermion being a Bogoliubov quasiparticle, coupled to two fermionic reservoirs at thermal equilibrium that can interact between each others with electron tunneling. We then solved the master equation of this system for different configuration of the reservoirs to see how the population of the system evolve depending on the configuration. Lastly, we also computed the new distribution for the quasiparticle that is no longer in thermal equilibrium.

Finally, in the last chapter we came back to our HFB algorithm but we modified the Fermi-Dirac distribution of the quasiparticles to be the new distribution found at then end of chapter 3. We were therefore able to compute the gap for our out-of-equilibrium system in different configurations of the reservoirs and compare it with the equilibrium case of chapter 2. When the two reservoirs have a positive chemical potential we observe very satisfying results. Indeed, in that case the gap hold under temperature of the order of the Kelvin, a substantial improvement compared to the critical temperature of a few milli Kelvin obtained in chapter 2. Interestingly, this new configuration

yields actually an equilibrium distribution for the quasi-particles, as the two reservoirs are at the same temperature and chemical potential. We finally proposed an explanation for that considerable improvement, we supposed that the reservoirs act as source of electrons for the system to absorb and form Cooper pairs thus counterbalancing the loss of Cooper pairs by thermal excitations.

4.5   Outlook

There are many ways to develop the work of this thesis and the improvements can be done on all three parts that make our system.

4.5.1   Improve the system

The first improvement we could make on the system would be working in two or three dimensions, the latter would allow for phase transition and "true" superconductivity. Another modification would be to model the superconductivity of our system with other theories than BCS. A first modification in describing the superconductor would be to assume the spin-triplet state for the Cooper pair wavefunction. Indeed, even if we chose the spin-singlet at the beginning of chapter 2 because most of the standard superconductors exhibit a spin-singlet Cooper pair, spin-triplet superconductors do exist [64]. One suggested explanation for exotic superconductivity is a d-wave [65] or p-wave [66] pairing instead of the classic s-wave we considered in this thesis. Such pairings imply that the gap has a more complex definition and is no longer isotropic. This already gives a few ways to complexify the modelling of our superconductor.

4.5.2   Improve the environment

Applying electromagnetic fields to the system could have multiple impacts. It would differentiate the up and down spins as they would no longer be treated as equivalent. Moreover it could enable spin-orbit coupling (thus giving rise to Fock field) which can enhance electron pairing [67] and as we said in the introduction electromagnetic fields have already been used to enhance superconductivity [22, 23]. We could also assume baths that are themselves superconducting which would result in richer exchange with the system (exchange of electrons, of pairs, of quasiparticles).

4.5.3   Improve the system-environment coupling

Instead of considering weak coupling between the system and the environment, we could also assume a strong coupling and consider non-Markovian regime. Also, in this master thesis, we considered only the case where we first solve the master equation for the quasi-particles to find the steady states *before* solving the self-consistent Hamiltonian problem. An alternative (but much involved) approach would be to solve a self-consistent Liouvillian problem. That is, it would correspond to find the steady state of the master equation self-consistently to calculate the new correlations functions.

4.5.4   Experimental considerations

In this master thesis, we focused on looking at theoretical protocols to explore possibilities of enhancing the gap. In the future, it would be interesting to look at how our models could be implemented in real experimental setups, in condensed matter systems with superconductors and normal leads as reservoirs (NSN junctions), but also in other systems like in cold atoms with e.g. ^{6}Li fermionic atoms as the relevant fermions [68]. Indeed, the rapid development of this platform makes it possible to study more and more quantum transport problems. It also allows for the exploration of new ways of controlling transport properties in different regimes, such as via reservoir engineering, which inspired in part this work of this master thesis.

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