UNIVERSIDADE FEDERAL DE PERNAMBUCO
DEPARTAMENTO DE FÍSICA – CCEN
PROGRAMA DE PÓS-GRADUAÇÃO EM FÍSICA

RODRIGO HENRIQUE DE BRAGANÇA

THEORY OF SUPERCONDUCTIVITY:

PHENOMENOLOGY, MEAN FIELD AND FLUCTUATIONS

Recife
2019

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Dissertação apresentada ao Programa de Pós-Graduação em Física da Universidade Federal de Pernambuco, como requisito parcial para a obtenção do título de Mestre em Física.

Área de Concentração: Física da Matéria Condensada e de Materiais

Orientador: Prof. Arkady Shanenko

Recife
2019

Catalogação na fonte
Bibliotecária Arabelly Ascoli CRB4-2068

B813t Bragança, Rodrigo Henrique de
Theory of superconductivity: phenomenology, mean field and fluctuations / Rodrigo Henrique de Bragança. – 2019.
105 f.: il. fig.

Orientador: Arkady Shanenko
Dissertação (Mestrado) – Universidade Federal de Pernambuco. CCEN. Física. Recife, 2019.
Inclui referências.

1. Física da matéria condensada e de materiais. 2. Equações GL. 3. Teoria BCS. 4. FFLO. I. Shanenko, Arkady (orientador). II. Título.

530.41 CDD (22. ed.) UFPE-CCEN 2020-53

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Aprovada em: 09/08/2019.

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This work is dedicated to my mom, my first teacher.

ACKNOWLEDGMENTS

I would like to acknowledge the help of the people who made this thesis as the culmination of 2 years of work possible. First, I would like to thank my mother, Sulamita, for teaching me how to read and to write but most of all for all her dedication to teach me how to be a decent human being.

I would also like to thank my scientific adviser Arkady Shanenko for helping me to learn so much about physics and mathematics, for telling me so many good stories about Russia and about the life of scientists and for believing in me as a physicist.

I also thank my colleagues for helping me with my calculations.

I appreciate help of Mihail Croitoru both with his lectures and outside his lectures.

Finally, I thank for the financial support the CNPq and the Department of Physics of the Federal University of Pernambuco.

ABSTRACT

More than one century has passed since Heike Kamerlingh Onnes discovered the phenomena of superconductivity but this field is still full of potential. This work will consider how we can understand the phenomena of superconductivity using quantum mechanics and how we can go beyond the standard superconducting model developed in the middle of the 20th century. We will start our consideration by discussing the basic experimental facts of a superconductor and the work of the London brothers that explains the Meissner effect by using the two-fluid theory where some of the electrons would condense into a super-fluid. The physical explanation of how this happens done by Leon Cooper who explained that at sufficiently low temperatures electrons can form stable pairs and condensate as bosons is discussed. This, though, is not enough to explain the phenomena of superconductivity. The first attempt at an explanation was the phenomenological theory by Ginzburg and Landau(GL) which we derive by considering the necessity of an order-parameter, a quantity which is small near the critical temperature, allowing us to write the free-energy as a expansion on this small parameter. By using the variational principle we are able get the two GL equations. However, there is still the need for a theory based on microscopic arguments. We will calculate the BCS Hamiltonian which lies at the heart of the theory developed by Bardeen, Cooper and Schrieffer by using mean-field theory and quasiparticles. This theory explains the behavior of a clean s-wave superconductor and naturally arrive at the conclusion that the spectrum of the excitation of the quasiparticles has a gap. To complete our analysis of basic theory we will discuss how we can link GL theory with BCS theory by the Green function formalism first develop by Gor'kov. We are going to clearly see that the GL equations which were obtained by phenomenological arguments can be derived from microscopic arguments. Following this discussion the application of this formalism is done by considering a system with just spin-magnetic interaction and a system with more than one electronic band, broadening therefore the scope of the BCS theory. For this two situations, the values for the critical temperature will change from the mean-field result. And, as a last topic we will tackle fluctuations. The mean-field theory is an approximation and has its limits of application. Going beyond we can use the fluctuation theory. How this theory is obtained and the so-called "Fluctuation driven shift of the critical temperature" are presented at the end of this dissertation.

Keywords: GL equations. BCS theory. FFLO. Multi-band. Fluctuations.

RESUMO

Mais de um século se passou desde que Heike Karmerlingh Onnes descobriu o fenômeno da supercondutividade, mas essa área ainda contém muito potencial. Essa tese considerará como podemos entender o fenômeno da supercondutividade e como podemos ir além dos modelos de supercondutores padrões que foram desenvolvidos durante o meio do século XX. Nós começamos nossa consideração por discutir os fatos experimentais básicos e o trabalho dos irmãos Fritz e Heinz London que explica o efeito Meissner usando a teoria de dois-fluidos onde alguns elétrons são condensados em um super fluido. A explicação física de como isso pode acontecer, dada por Leon Cooper ao demonstrar que em temperaturas suficientemente baixas elétrons podem formar pares estáveis e criar um condensado como se fossem bósons, é discutida. Isto, no entanto, não foi suficiente para explicar todos os efeitos da supercondutividade. A primeira tentativa de explicar ela foi a teoria fenomenológica de Ginzburg e Landau (GL) a qual nós derivamos por introduzir o conceito de um parâmetro de ordem,uma quantidade que é nula acima da temperatura crítica e não nula abaixo mas é pequeno perto da temperatura crítica. Isso nos permite expandir a energia livre em potências do parâmetro de ordem e então usar o princípio variacional chegando assim nas duas equações GL. No entanto, ainda havia necessidade de uma teoria baseada em argumentos microscópicos. A teoria Bardeen-Cooper-Schrieffer (BCS) resolveu essa necessidade. Nós derivamos a Hamiltoniana de BCS usando "Mean-Field Theory" e "quasiparticles". Essa teoria explica o comportamento de um supercondutor limpo e s-wave chegando naturalmente na conclusão de que o espectro energético possue um "gap". Para completar a nossa análise da teoria basica nós investigamos como a teoria GL está conectada com a teoria BCS usando o formalismo das funções de Green desenvolvido por Gor'kov. Nós veremos claramente que as equações GL que foram obtidas por meio de argumentos fenomenológicos podem ser derivadas pelo formalismo microscópico. Em seguida a aplicação desse formalismo é feito por considerar sistemas com apenas interação "spin-magnetic" e um sistemas com mais de uma banda eletrônica, ampliando assim o escopo inicial da teoria BCS. Para esses dois casos a temperatura crítica afasta-se do resultado convencional obtido com a teoria de "Mean-Field". O último tópico desse trabalho trata de flutuações térmicas. A teoria de campo médio é uma aproximação e possue um limite para sua aplicação. Indo além nós podemos usar a teoria de flutuações térmicas. Como essa teoria é derivada e o chamado "Fluctuation driven shift of the critical temperature" são discutidos no final dessa dissertação.

Palavras-Chave: Equações GL.Teoria BCS. FFLO. Multi bandas. Flutuações.

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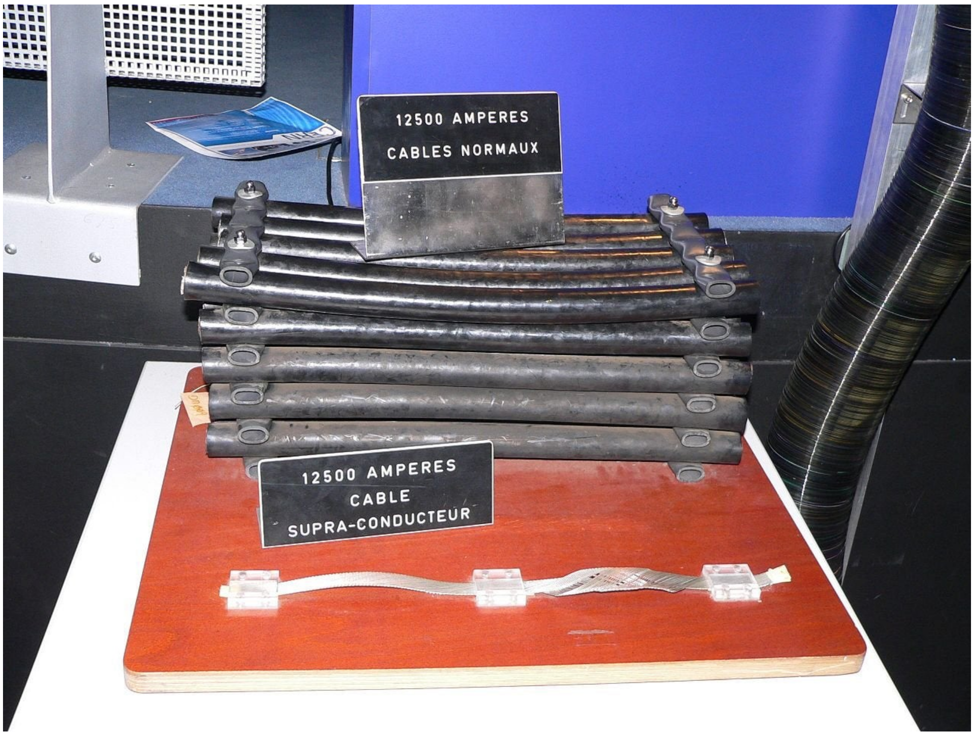
CONTENTS

1 GENERAL INTRODUCTION

An old English adage goes: “A picture is worth a thousand words”. And that proves to be true when someone is introducing the concept of superconductivity. Here I could talk a lot about the technical benefits of the deeper understanding the world around us but I will simply show you the following picture:



Both of these objects are electric cables used at CERN. Both of them conduct a current of 12,500 A. The massive cable at the back was used at the Large Electron Positron Collider and the one in the front is used at the Large Hadron Collider. So, the question is, how can both of them conduct an electric current of 12,500 A? The answer lies in the phenomenon of superconductivity which is going to be discussed in this thesis.

In **Chapter 2** we will discuss how the first steps were taken in understanding the behavior of superconducting materials. We will learn what is the Meissner effect and how Heinz and Fritz London explained it by the idea of electrons forming a superfluid quantum condensate.

Next, **Chapter 3** will consider the phenomenological and microscopical theories of superconductivity and how they are linked to the formalism of Green Functions. We will see examples that will indicate their validity by showing that they give results backed by experimental data.

Chapter 4 will expand the range of application of the theory of superconductivity by considering a system in the paramagnetic limit when the external magnetic field only acts on spins of electrons, leading to electron paring with nonzero momenta. Then we will consider how to deal with a system with two carrier bands and will see that despite having two contributing bands, the GL formalism for this system is single-component but with coefficients given by averages over these available bands.

Finally, in the last chapter **Chapter 5**, we will consider thermal fluctuations. We will see why BCS theory is not always enough to describe superconductors, we will see how the fluctuations shift the critical temperature from its mean field value and what is the Ginzburg number and why it is important in this formalism.

2 INTRODUCTION TO SUPERCONDUCTIVITY

2.1 A little bit of history

In the beginning of the 20th century many investigations were focused on the nature of matter near absolute zero. However, a serious obstacle was achievement of temperatures near 0K. In 1908 Dutch physicist Heike Kamerlingh Onnes, by using new techniques, was able to liquefy helium that can be in such a state below 4 K. This achievement had opened the doors for experiments at very low temperatures. And 3 years later, Onnes found something very exciting when studying the electrical properties of low-temperature metals. The point is that 20 years before this finding, German scientist Georg Simon Ohm had demonstrated that metals have an intrinsic resistance to the flow of electrons because the latter collide with material atoms. This is what we know as electrical resistance. Onnes expected that when the temperature decreases, the averaged kinetic energy of electrons decreases as well so that the interaction between them plays the major role. From the point of view of the classical statistical mechanics, cold particles should produce a lattice (for electrons it is known as the Wigner crystal) and, thus, it is rather hard to arrange a steady current in this case, i.e., the resistance should increase up to infinity. Surprisingly, after cooling mercury down to around 4K and measuring its electrical resistivity, Onnes have found that the resistivity dropped abruptly to zero and the electrons move without losses of energy [1]. Onnes expected a kind of superinsulator but discovered the first superconductor.

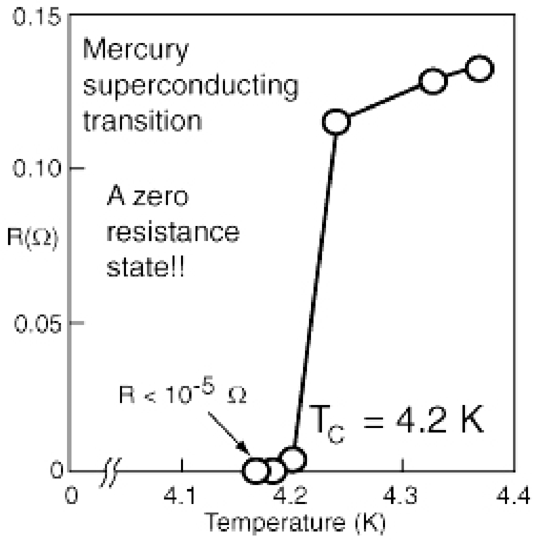


Figure 1: Sharp drop in electrical resistance $R(\Omega)$ bellow critical temperature $T_c = 4.2K$ for mercury

2.2 Basic experimental facts

Although the infinite conductivity is the most obvious characteristic, the true nature of the superconducting state appears more clearly in its magnetic response.

- MEISSNER EFFECT: This next step in the related research has been made by German physicists Walther Meissner and Robert Ochsenfeld [2]. They observed that a superconductor can expel a magnetic field from its core. Their work has demonstrated that the superconducting state has another important property in addition to the zero resistance: it can be perfectly diamagnetic. The perfect diamagnetism means that when the system in question is placed in an external magnetic field, it produces a field in the opposite direction so that in its interior $\mathbf{B} = 0$.

- CRITICAL FIELD: The interplay between the superconducting state and magnetic field is not reduced to the Meissner effect. An increase in the magnitude of the external magnetic field kills superconductivity, similarly to an increase in the temperature. For a given temperature the highest external magnetic field at which the material remains in the superconducting state, is usually called "critical field".

  For type I superconductors this is the thermodynamic critical field denoted as $H_c(T)$. For type II superconductors the transformation under an external field is more complicated, involving the lower critical $H_{c1}(T)$ and upper critical $H_{c2}(T)$ fields. For $H_{c1}(T) < H < H_{c2}(T)$ the mixed (Shubnikov) state appears where the diamagnetic currents are accompanied by paramagnetic ones. The normal state is realized above $H_{c2}(T)$.

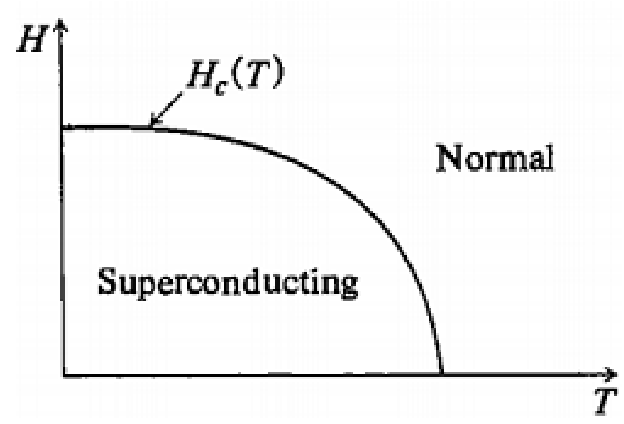


Figure 2: Phase diagram of $H(T)$ for type I superconductors, showing the superconducting region and normal region

- HEAT CAPACITY: Superconductors are also identified by their distinctive thermal properties. In the normal state the heat capacity (or specific heat) C_n is linear in the limit $T \to 0$. However, when the system undergoes the superconducting transition, a sharp peak in the heat capacity appears at the critical temperature T_c[3]. In the superconducting state the heat capacity decays exponentially when the temperature goes to zero.

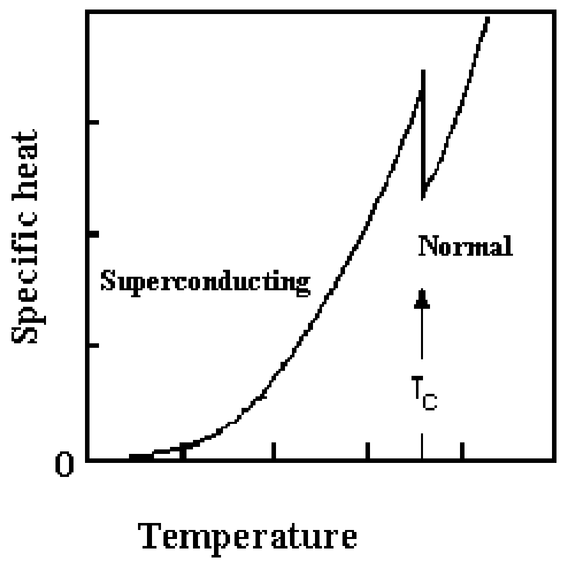


Figure 3: Sketch of the heat capacity (specific heat) temperature dependence in a superconductor

Up to the discovery of the perfect diamagnetism of superconductors there were no successful theory of superconductivity. In 1935 the first successive move was done by the brothers Fritz and Heinz London. They developed the London equations [4] describing the perfect diamagnetism of the Meissner state and postulated that the electrodynamics of superconductors is described by a *massive vector field*.

At the same time Fritz London proposed the derivation of the London equations on the basis of the idea about the macroscopic condensation of electrons in the same single-particle quantum state. The clear link between the *quantum condensate* and massive vector fields, known as the Higgs mechanism today, was first established by Fritz London. However, the remaining problem was that electrons are fermions and a macroscopic occupation of the same quantum state is not possible for fermions by virtue of the Pauli exclusion principle.

The mystery related to the condensation of superfluid electrons was solved in a while by American physicist Leon Cooper who showed that at sufficiently low temperatures, fermions can form stable pairs. The condensation of these pairs, which are in fact composite bosons, produces a superfluid that was anticipated by Fritz London.

2.3 London equations

In 1935 Fritz and Heinz London developed a theory explaining the Meissner effect. To go in more details about the London equations, let us consider a *superelectron* (an electron contributing to a superfluid flow) moving inside a material within the framework of the well-known Drude model. The latter assumes that the motion of an electron is affected by the resistive force $-\frac{\mathbf{v}}{\tau}$, with τ the conductivity-related relaxation time. In this case Newton's second law reads

$$m^* \frac{\partial \mathbf{v}}{\partial t} = e^* \mathbf{E} - \frac{\mathbf{v}}{\tau}, \tag{2.1}$$

where e^* and m^* are the superelectron charge and mass and $\mathbf{E}$ is the electric field. Following the arguments by brothers London, we take the limit $\tau \to \infty$, which means that the electron in question moves without any resistance. Then, for such a superfluid electron we get

$$m^* \frac{\partial \mathbf{v}}{\partial t} = e^* \mathbf{E}. \tag{2.2}$$

The supercurrent density $\mathbf{j}_s$ is given by $\mathbf{j}_s = n_s e^* \mathbf{v}$, where n_s is the density of electrons that conduct electricity without resistance. Therefore the drift velocity of superfluid electrons is $\mathbf{v} = \frac{1}{n_s e^*} \mathbf{j}_s$. Differentiating this expression with respect to the time, we get $\frac{\partial \mathbf{v}}{\partial t} = \frac{1}{n_s e^*} \frac{\partial \mathbf{j}_s}{\partial t}$. Then equation (2.2) yields

$$\frac{\partial \mathbf{j}_s}{\partial t} = \frac{n_s e^{*2}}{m^*} \mathbf{E}, \tag{2.3}$$

which is *the first London equation* connecting the electric field with the supercurrent density. Now, let us take the curl of the both sides of equation (2.3) and express $\nabla \times \mathbf{E}$ in terms of the magnetic field $\mathbf{B}$ from the Maxwell equation $\nabla \times \mathbf{E} = -\frac{1}{c}\frac{\partial \mathbf{B}}{\partial t}$. Then, we arrive at

$$\frac{\partial}{\partial t}\left(\nabla \times \mathbf{j}_s + \frac{n_s e^{*2}}{m^* c}\mathbf{B}\right) = 0. \tag{2.4}$$

One sees that the expression in the parentheses is constant in time. The London brothers argued that it should be zero (a nonzero expression leads to a nonphysical solution) and obtained

$$\nabla \times \mathbf{j}_s = -\frac{n_s e^{*2}}{m^* c}\mathbf{B}, \tag{2.5}$$

which is *the second London equation.* The latter can be rearranged by using Ampere's law $\nabla \times \mathbf{B} = \frac{4\pi}{c}\mathbf{j}_s$ and the homogeneous Maxwell equation $\nabla \cdot \mathbf{B} = 0$ as

$$\nabla^2 \mathbf{B} - \frac{4\pi n_s e^{*2}}{m^* c^2}\mathbf{B} = 0. \tag{2.6}$$

To demonstrate the importance of the London equations, we consider a semi-infinite superconductor ($z > 0$) in an applied field $\mathbf{H} = H\mathbf{e_x}$ parallel to the surface. The magnetic field $\mathbf{B}$ should be equal to $\mathbf{H}$ at the boundary $z = 0$. The corresponding physical solution of equation (2.6) is given by

$$B(z) = He^{-z/\lambda}, \tag{2.7}$$

with *the London penetration depth*

$$\lambda = \sqrt{\frac{m^* c^2}{4\pi n_s e^{*2}}} \tag{2.8}$$

that controls the exponential decay of $B(z)$ inside the superconductor. We note that n_s is not position dependent. but temperature dependent, as it is assumed within the London regime. One sees that the London equations explains the Meissner effect.

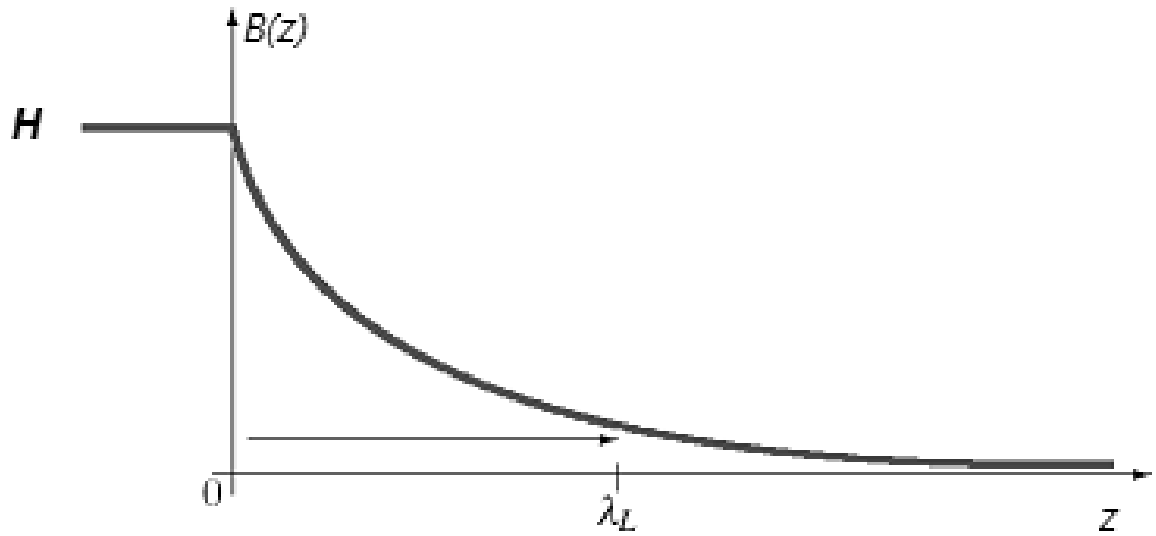


Figure 4: Magnetic-field decay inside the superconducting medium.

The initial arguments by the London brothers in favor of the London equations are heavily based on the assumption that the expression in the parentheses in equation (2.4) is equal to zero. As this assumption assumes additional and extensive calculations[4], not shown in textbooks, it is deductive to give another way to derive (2.6). It is similar to the well-known two-fluid model of liquid helium by Gorter and Casimir. Suppose that a part of electrons in the system move without losses while another part comprises normal electrons. The free energy of the system is given by

$$F = F_N + F_{kin} + F_{mag}, \tag{2.9}$$

where F_N is the free energy of normal electrons, F_{kin} is the contribution of superfluid electrons, and F_{mag} is the energy of the magnetic field. For F_{mag} we have

$$F_{\text{mag}} = \int \frac{\mathbf{B}^2}{8\pi} d\mathbf{r}. \tag{2.10}$$

The kinetic energy of superfluid electrons moving with the velocity $\mathbf{v}(\mathbf{r})$ is of the form

$$F_{\text{kin}} = \int \frac{m^* \mathbf{v}^2}{2} n_s d\mathbf{r}. \tag{2.11}$$

We express F_{kin} in terms of the supercurrent $\mathbf{j}_s$ and, then, use Ampère's equation for the magnetic field. This makes it possible to get the free energy only in terms of integrals of the magnetic field, i.e.,

$$F = F_N + \frac{1}{8\pi} \int \left[\mathbf{B}^2 + \frac{m^* c^2}{4\pi n_s e^{*2}} \left(\boldsymbol{\nabla} \times \mathbf{B} \right)^2 \right] d\mathbf{r}. \tag{2.12}$$

Now we minimize the free energy with respect to the magnetic field. The energy of normal electrons doesn't depend on this field and, hence, we get

$$\delta F = \frac{1}{4\pi} \int \Big[\mathbf{B} \cdot \delta \mathbf{B} + \frac{m^* c^2}{4\pi n_s e^{*2}} \big(\boldsymbol{\nabla} \times \mathbf{B} \big) \cdot \big(\boldsymbol{\nabla} \times \delta \mathbf{B} \big) \Big] d\mathbf{r}. \tag{2.13}$$

We integrate by parts the second term and use the divergence theorem, producing a vanishing surface integral. As a result, we obtain

$$\delta F = \frac{1}{4\pi} \int \Big(\mathbf{B} + \frac{m^* c^2}{4\pi n_s e^{*2}} \boldsymbol{\nabla} \times \boldsymbol{\nabla} \times \mathbf{B} \Big) \cdot \delta \mathbf{B}. \tag{2.14}$$

Now we set $\delta F = 0$ and get exactly (2.6), when keeping in mind the homogeneous Maxwell equation $\boldsymbol{\nabla} \cdot \mathbf{B} = 0$. The London theory provides a clear link between the superfluid electrons moving without losses and the Meissner effect.

We are now in the position to address the critical point about superfluid electrons. Superfluids are made of bosons that form a Bose-Einstein condensate. However, electrons are fermions and obey the Fermi-Dirac statistics that prevents them from the condensation in the same single-particle state. Does it mean that superfluid electrons cannot move with the same superfluid velocity? The answer is “no" and important details are discussed in the next section.

2.4 Cooper pairs

In 1956 Leon Cooper [5] proposed how electrons can form a superfluid: the electron-phonon interaction is responsible for the formation of Cooper pairs that are *composite bosons*. It is well-known that bare electrons repel each other. However, they can attract each other via ions of the crystalline structure inside a metal. A temporary build of positive charge made of displaced ions is created by a moving electron. This charge attracts another electron, providing a weak attraction between electrons in the system. The displacement of ions in the crystalline structure of a metal is characterized by the *phonon field* so that phonons are mediators of the attraction between electrons and the phono-electron interaction is responsible for the formation of Cooper pairs.

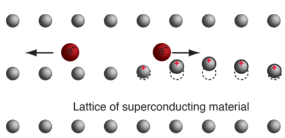


Figure 5: Sketch of the ion displacement in a metal.

However, the competition with the direct Coulomb repulsion makes the effective attraction between electrons rather weak. At the same time, it is well-known from the quantum mechanics that the bound state in three dimensions is not possible when the particle attraction is rather weak. Thus, the question arises: How can a weak electron-phonon interaction produce Cooper pairs? The point is that the fundamental ingredient, which should be mentioned together with the electron-phonon attraction, is the presence of the *Fermi sea*, i.e., the collection of almost fully occupied single-particle states below the Fermi level. This tends to prevent the decay of a bound Cooper pair in two separated (free) electrons because such electrons should have energies larger than the Fermi energy. This favors the Cooper-pair formation even for a rather weak attraction between electrons, as was first mentioned by Leon Cooper.

To find whether or not a weak attraction can produce, in three dimensions, an in-medium bound state called the Cooper pair, let us consider a gas of electrons in a cubic box with the volume L^3, assuming the periodic boundary conditions and zero temperature. The Cooper-pair wave function of two electrons with the spatial coordinates $\mathbf{r}_i$ and spin projections σ_i for $i = 1, 2$ is separable into a product

$$\Psi(\mathbf{r}_1, \sigma_1; \mathbf{r}_2, \sigma_2) = \varphi(\mathbf{R}) g(\mathbf{r}) \chi(\sigma_1, \sigma_2), \tag{2.15}$$

where $\mathbf{R} = \frac{\mathbf{r}_1 + \mathbf{r}_2}{2}$ is the center-of-mass radius vector and $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$ is the relative coordinate vector. The spin part is antisymmetric $\chi(\sigma_1, \sigma_2) = -\chi(\sigma_2, \sigma_1)$ due to the singlet pairing. Then, $g(\mathbf{r}) = g(-\mathbf{r})$, as the Cooper-pair wave function is antisymmetric with respect to the permutation of electrons. For the s-wave case (typical of the Bardeen-Cooper-Schrieffer superconductors) one obtains $g(\mathbf{r}) = g(r)$, with $r = |\mathbf{r}|$. As the medium is homogeneous, the center-of-mass momentum is conserved and we have

$$\varphi(\mathbf{R}) = \frac{1}{L^{3/2}} e^{i\mathbf{QR}}. \tag{2.16}$$

When the in-medium pairs form the quantum condensate, they have the same center-of-mass momentum $\mathbf{Q} = 0$. In the presence of a supercurrent, $\mathbf{Q}$ is nonzero.

Now we have everything at our disposal to investigate the Schrödinger equation for the internal motion of electrons in a Cooper pair. At zero temperature electrons occupy low-energy levels up to the Fermi energy E_F. As the single-particle states are plane waves, we find that the states with $k < k_F = \sqrt{\frac{2mE_F}{\hbar^2}}$ (m is the effective electron mass) are occupied while the states with $k > k_F$ remain free. In this picture we ignore the interaction of electrons producing the Fermi sea below k_F but we do take into account the attraction of two electrons forming a Cooper pair via an attractive potential $V(\mathbf{r})$. Then, we have

$$g(\mathbf{r}) = \sum_{|\mathbf{k}| > k_F} g_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}}, \tag{2.17}$$

where $g_{\mathbf{k}}$ is proportional to the probability amplitude of finding an electron above the Fermi sea (the states with $|\mathbf{k}| < k_F$ are excluded because they are occupied by the Fermi sea). The Schrödinger equation for $g_{\mathbf{k}}$ reads

$$\frac{\hbar^2 k^2}{2m} g_{\mathbf{k}} + \sum_{|\mathbf{k}|>k_F} V_{\mathbf{k},\mathbf{k}'} g_{\mathbf{k}'} = (E + 2E_F) g_{\mathbf{k}}, \tag{2.18}$$

where E is the eigenvalue measured from $2E_F$ and $V_{\mathbf{k},\mathbf{k}'} = \frac{1}{L^3} \int V(\mathbf{r}) e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}} d\mathbf{r}$. Following Cooper's suggestion and to simplify our analysis, we adopt the pseudopotential given by

$$V_{\mathbf{k},\mathbf{k}'} = -\frac{V}{L^3}. \tag{2.19}$$

Then, the Schrödinger equation (2.18) is reduced for $k > k_F$ to

$$g_{\mathbf{k}} = -\frac{V}{L^3} \frac{1}{\left(-\dfrac{\hbar^2 k^2}{m} + E + 2E_F\right)} \sum_{|\mathbf{k}'|>k_F} g_{\mathbf{k}'} \tag{2.20}$$

while for $k < k_F$ we have $g_{\mathbf{k}} = 0$. Making a summation with respect to $\mathbf{k}$, one arrives at

$$\sum_{|\mathbf{k}|>k_F} g_{\mathbf{k}} = -\frac{V}{L^3} \sum_{|\mathbf{k}|>k_F} \frac{1}{\left(-\dfrac{\hbar^2 k^2}{m} + E + 2E_F\right)} \sum_{|\mathbf{k}'|>k_F} g_{\mathbf{k}'}, \tag{2.21}$$

which eventually gives the equation for the eigenvalue E as

$$1 = -\frac{V}{L^3} \sum_{|\mathbf{k}|>k_F} \frac{1}{\left(-\dfrac{\hbar^2 k^2}{m} + E + 2E_F\right)}. \tag{2.22}$$

The sum in the eigenvalue equation suffers of the ultraviolet divergence that is not fundamental but appears due to the use of the pseudopotential. The standard regularization procedure, dating back to Cooper, invokes a cut-off that removes all states with the single-particle energies higher than $E_F + \hbar\omega_D$, with ω_D the cut-off frequency (the Debye frequency for the Bardeen-Cooper-Schrieffer pairing scenario). Now, replacing the discrete sum by an integral and changing variables so that to integrate with respect to $\xi = \frac{\hbar^2 k^2}{2m} - E_F$, we get

$$1 = -V \int_0^{\hbar\omega_D} \frac{N(\xi)}{E - 2\xi} d\xi, \tag{2.23}$$

with $N(\xi)$ the density of states (DOS). As $N(\xi)$ is a sufficiently slow varying function of ξ, we can rewrite the equation (2.23) as

$$1 = VN(0) \int_0^{\hbar\omega_D} \frac{1}{2\xi - E} d\xi = \frac{1}{2} VN(0) \ln\left(\frac{E - 2\hbar\omega_D}{E}\right), \tag{2.24}$$

with $N(0) = \frac{mk_F}{2\pi^2\hbar^2}$ the DOS at the Fermi energy. Keeping in mind that for the weak-coupling regime (it is of interest here) $\frac{\hbar\omega_D}{E} \gg 1$, we find the solution of equation (2.23) as

$$E = -2\hbar w_D e^{-2/N(0)V}. \tag{2.25}$$

As $E < 0$, any pair of free electrons above the Fermi sea is less favorable than a Cooper pair. This is called the *Cooper instability*, i.e., the system of free electrons is not stable with respect to the formation of Cooper pairs. It is important to stress that the result holds even in the limit $V \to 0$. The fact that we did not take into account the interaction of free electrons forming the Fermi sea is not of importance here. It can be taken into account within the mean-field approximation which produces a trivial shift of the Fermi level. For $E < 0$, we have a bound state. This bound state suggests a gap in the energy spectrum, which is consistent with the exponentially falling heat capacity bellow the critical temperature. As we will see in the next chapter, this gap can be calculated precisely by the BCS theory. And as a last property the bound state is obtain regardless of how small V is unlike other systems where there are a minimum value for the attraction.

3 THEORIES OF SUPERCONDUCTIVITY

Normally, to calculate thermodynamic properties like the free energy, entropy or specific heat in an interacting system, it is necessary to perform a long and numerically intensive calculations. However, Lev Landau has realized that near the phase transition one can construct an approximation for the free energy without calculating the microscopic states, just being based on general phenomenological rules. He introduced the concept of the *order parameter*, a quantity that is zero above the phase transition temperature (in the disordered phase) and non-zero below it (in the ordered phase). This idea is the cornerstone the phenomenological Ginzburg-Landau theory.

3.1 Phenomenological theory

3.1.1 Order parameter and free energy functional

Based on the theory of phase transitions developed by Landau, suppose that there is an order parameter ψ which obeys the following property

$$\begin{cases} \psi = 0, & \text{if} \quad T > T_c \\ \psi \neq 0, & \text{if} \quad T < T_c. \end{cases} \tag{3.1}$$

Near T_c, we assume that the order parameter is small (vanishing at T_c) and, therefore, the microscopic free-energy density $f_{s,0}$ of the superconducting state in zero field can be expanded as follows:

$$f_{s,0} = f_{N,0} + a|\psi|^2 + \frac{b}{2}|\psi|^4 + \ldots, \tag{3.2}$$

where $f_{N,0}$ is the free-energy density of the normal state of the system at zero magnetic field, a and b are phenomenological (real) parameters. Following Ginzburg and Landau, we assume b independent of temperature and $a = \alpha(T - T_c)$ and $\alpha > 0$. In the absence of magnetic fields the order parameter is spatially uniform, so Ginzburg and Landau added a term proportional to $|\boldsymbol{\nabla}\psi|^2$ in order to suppress spatial variations. In analogy with the Schroedinger equation, in the absence of magnetic fields this term reads: $\frac{\hbar^2}{2m^*}|-i\boldsymbol{\nabla}\psi|^2$, where m^* is the effective mass of relevant particles (superelectrons which in our modern understanding two bound electrons in a Cooper pair) that contribute to the super-conducting current. When magnetic fields are present then one needs to use the gauge-invariant gradient: $-\frac{\hbar^2}{2m^*}\left(\boldsymbol{\nabla} - \frac{ie^*}{\hbar c}\mathbf{A}(\mathbf{r})\right)^2$ and add the field energy: $\frac{B^2}{8\pi}$. Here $\mathbf{B}$ is the magnetic field and e^* is the charge of superelectrons carrying the supercurrent. In this way the total free energy density of a superconductor in a magnetic field becomes

$$f_s = f_{N,0} + a|\psi|^2 + \frac{1}{2}b|\psi|^4 + \frac{\hbar^2}{2m^*}\left|\left(\boldsymbol{\nabla} - \frac{ie^*}{\hbar c}\mathbf{A}\right)\psi\right|^2 + \frac{\mathbf{B}^2}{8\pi}. \tag{3.3}$$

We need just to integrate over the system volume V, which is localized and correspond to the volume of the sample, to get the free energy. We choose the usual normalization for ψ

$$|\psi|^2 \equiv n_s^*, \tag{3.4}$$

where n_s^* defines an effective superelectron density. Following our discussion in the previous chapter we can promptly recognize that $m^* = 2m$ and $e^* = 2e$ (with m and e the mass and charge of an electron) because the supercurrent is formed by composite bosons (Cooper pairs) made of two bound electrons. To obtain the so-called *Ginzburg-Landau equations*, we need to use variational derivatives and minimize the free energy with respect to the order parameter, which gives the equation for the order parameter, and with respect to the vector potential, which yields a complimentary equation for the supercurrent.

3.1.2 Variation with respect to the order parameter - the first Ginzburg-Landau equation

We introduce the variation of $\psi^*(\mathbf{r})$ given by $\delta\psi^*(\mathbf{r})$. The corresponding variation of the free energy is therefore

$$\delta F = \int d\mathbf{r}\left[\left(a\psi + b|\psi|^2\psi\right)\delta\psi^* + \frac{\hbar^2}{2m^*}\left(\boldsymbol{\nabla}\psi - \frac{ie^*}{\hbar c}\mathbf{A}\psi\right)\cdot\left(\boldsymbol{\nabla}\delta\psi^* + \frac{ie^*}{\hbar c}\mathbf{A}\delta\psi^*\right).\right] \tag{3.5}$$

Now, the last term is integrated by parts, using the divergence theorem and nullifying the obtained integral over the superconductor surface, as follows

$$\left(\boldsymbol{\nabla}\psi - \frac{ie^*}{\hbar c}\mathbf{A}\psi\right)\cdot\left(\boldsymbol{\nabla}\delta\psi^* + \frac{ie^*}{\hbar c}\mathbf{A}\delta\psi^*\right)$$

$$= \boldsymbol{\nabla}\psi\cdot\boldsymbol{\nabla}\delta\psi^* + \left(\frac{e^*\mathbf{A}}{\hbar c}\right)^2\psi\delta\psi^* + \delta\psi^*\frac{ie^*}{\hbar c}\mathbf{A}\cdot\boldsymbol{\nabla}\psi - \psi\frac{ie^*}{\hbar c}\mathbf{A}\cdot\boldsymbol{\nabla}\delta\psi^*. \tag{3.6}$$

Consider that

$$\boldsymbol{\nabla}\psi\cdot\boldsymbol{\nabla}\delta\psi^* = \boldsymbol{\nabla}\cdot\left(\boldsymbol{\nabla}\psi\delta\psi^*\right) - \delta\psi^*\boldsymbol{\nabla}^2\psi, \tag{3.7}$$

and that

$$\begin{aligned}\delta\psi^*\frac{ie^*}{\hbar c}\mathbf{A}\cdot\boldsymbol{\nabla}\psi-\psi\frac{ie^*}{\hbar c}\mathbf{A}\cdot\boldsymbol{\nabla}\delta\psi^* &= \frac{ie^*}{\hbar c}\mathbf{A}\cdot(\delta\psi^*\boldsymbol{\nabla}\psi-\psi\boldsymbol{\nabla}\delta\psi^*)\\ &= \frac{ie^*}{\hbar c}\mathbf{A}\cdot\big[\delta\psi^*\boldsymbol{\nabla}\psi-(\boldsymbol{\nabla}(\delta\psi^*\psi)-\delta\psi^*\boldsymbol{\nabla}\psi)\big]\\ &= \frac{ie^*}{\hbar c}\mathbf{A}\cdot\big[2\delta\psi^*\boldsymbol{\nabla}\psi-\boldsymbol{\nabla}(\delta\psi^*\psi)\big].\end{aligned}$$

Therefore

$$\begin{aligned}&\Big(\boldsymbol{\nabla}\psi-\frac{ie^*}{\hbar c}\mathbf{A}\psi\Big)\cdot\Big(\boldsymbol{\nabla}\delta\psi^*+\frac{ie^*}{\hbar c}\mathbf{A}\delta\psi^*\Big)\\ &=\boldsymbol{\nabla}\cdot(\boldsymbol{\nabla}\psi\delta\psi^*)-\delta\psi^*\boldsymbol{\nabla}^2\psi+\frac{ie^*}{\hbar c}\mathbf{A}\cdot\big[2\delta\psi^*\boldsymbol{\nabla}\psi-\boldsymbol{\nabla}(\delta\psi^*\psi)\big]+\Big(\frac{e^*\mathbf{A}}{\hbar c}\Big)^2\psi\delta\psi^*\\ &=\boldsymbol{\nabla}\bigg(\psi\delta\psi^*-\frac{ie^*\mathbf{A}}{\hbar c}(\delta\psi^*\psi)\bigg)-\Big(\boldsymbol{\nabla}^2\psi-\frac{2ie^*}{\hbar c}\mathbf{A}\cdot\boldsymbol{\nabla}\psi-\Big(\frac{e^*\mathbf{A}}{\hbar c}\Big)^2\psi\Big)\delta\psi^*,\end{aligned}$$

where the Coulomb gauge($\boldsymbol{\nabla}\cdot\mathbf{A}=0$) is used. Finally we get

$$\begin{aligned}\delta F=&\int_V d\mathbf{r}\Big[a\psi+b|\psi|^2\psi-\frac{\hbar^2}{2m^*}\Big(\boldsymbol{\nabla}-\frac{ie^*}{\hbar c}\mathbf{A}\Big)^2\psi\Big]\delta\psi^*\\ &+\oint_{\partial V}dS\frac{\hbar^2}{2m^*}\Big(\boldsymbol{\nabla}\psi-\frac{ie^*}{\hbar c}\mathbf{A}\psi\Big)\cdot\hat{\mathbf{n}}.\end{aligned}\tag{3.8}$$

Where we have integrated over the volume V enclosed by the surface ∂V. To get $\delta F=0$ for any value of $\delta\psi^*$, it is necessary that

$$a\psi+b|\psi|^2\psi-\frac{\hbar^2}{2m^*}\Big(\boldsymbol{\nabla}-\frac{ie^*}{\hbar c}\mathbf{A}\Big)^2\psi=0,\tag{3.9}$$

with the boundary condition

$$\Big(\boldsymbol{\nabla}\psi-\frac{ie^*}{\hbar c}\mathbf{A}\psi\Big)\cdot\hat{\mathbf{n}}\Big|_{\partial V}=0.\tag{3.10}$$

Equation (3.9) is called **First Ginzburg-Landau Equation** which describes the behavior of the order parameter near the critical temperature.

3.1.3 Variation with respect to the vector potential - the second Ginzburg-Landau equation

Now we introduce the variation of the vector potential $\delta\mathbf{A}$. The corresponding variation of the free energy reads

$$\begin{aligned}\delta F=&\int d\mathbf{r}\frac{\hbar^2}{2m^*}\bigg[-\frac{ie^*}{\hbar c}\psi\delta\mathbf{A}\cdot\Big(\boldsymbol{\nabla}+\frac{ie^*}{\hbar c}\mathbf{A}\Big)\psi^*+\frac{ie^*}{\hbar c}\psi^*\delta\mathbf{A}\cdot\Big(\boldsymbol{\nabla}-\frac{ie^*}{\hbar c}\mathbf{A}\Big)\psi\bigg]\\ &+\int d\mathbf{r}\frac{1}{4\pi}\mathbf{B}\cdot(\boldsymbol{\nabla}\times\delta\mathbf{A}),\end{aligned}$$

which can be rearranged as

$$\delta F = \int d\mathbf{r}\Big[\frac{\hbar^2}{2m^*}(\psi^*\boldsymbol{\nabla}\psi - \psi\boldsymbol{\nabla}\psi^*)\frac{ie^*}{\hbar c} + \frac{e^{*2}}{m^*c^2}|\psi|^2\mathbf{A}\Big]\cdot\delta\mathbf{A} + \int d\mathbf{r}\frac{1}{4\pi}\mathbf{B}\cdot\big(\boldsymbol{\nabla}\times\delta\mathbf{A}\big). \tag{3.11}$$

Where, by virtue of the standard definition, $\mathbf{B} = \boldsymbol{\nabla}\times\mathbf{A}$. Using the vector calculus identities, we get

$$\mathbf{B}\cdot\big(\boldsymbol{\nabla}\times\delta\mathbf{A}\big) = \boldsymbol{\nabla}\cdot(\delta\mathbf{A}\times\mathbf{B}) + \delta\mathbf{A}\cdot(\boldsymbol{\nabla}\times\mathbf{B})$$

and, invoking Ampère's law, we obtain

$$\delta F = \int d\mathbf{r}\Big[\frac{\hbar^2}{2m^*}(\psi^*\boldsymbol{\nabla}\psi - \psi\boldsymbol{\nabla}\psi^*)\frac{ie^*}{\hbar c} + \frac{e^{*2}}{m^*c^2}|\psi|^2\mathbf{A})\Big]\cdot\delta\mathbf{A} + \int d\mathbf{r}\frac{1}{4\pi}\Big(\boldsymbol{\nabla}\cdot(\delta\mathbf{A}\times\mathbf{B}) + \frac{4\pi}{c}\mathbf{j}_s\cdot\delta\mathbf{A}\Big), \tag{3.12}$$

with $\mathbf{j}_s$ the supercurrent density. Applying the divergence theorem, one separates the integration over the sufficiently large volume V_∞ (including the superconductor sample, $V < V_\infty$) and its surface ∂V_∞. So, we have

$$\delta F = \int_V d\mathbf{r}\left[\frac{\hbar^2}{2m^*}(\psi^*\boldsymbol{\nabla}\psi - \psi\boldsymbol{\nabla}\psi^*)\frac{ie^*}{\hbar c} + \frac{e^{*2}}{m^*c^2}|\psi|^2\mathbf{A}) + \frac{1}{c}\mathbf{j}_s\right]\cdot\delta\mathbf{A} + \frac{1}{4\pi}\oint_{\partial V_\infty} dS\Big(\delta\mathbf{A}\times\mathbf{B}\Big)\cdot\hat{\mathbf{n}}. \tag{3.13}$$

The last integral is zero because we suppose that the magnetic field decays at infinity . The first integral is over the volume V because the related integrand is zero beyond the superconducting sample. To get $\delta F = 0$ for an arbitrary variation of the vector potential, we need to have

$$\mathbf{j}_s = \frac{ie^*\hbar}{2m^*}(\psi\boldsymbol{\nabla}\psi^* - \psi^*\boldsymbol{\nabla}\psi) - \frac{e^{*2}}{m^*c}|\psi|^2\mathbf{A}. \tag{3.14}$$

Equation (3.14) is known as **Second Ginzburg-Landau Equation**. It determines the supercurrent $\mathbf{j}_s$.

3.1.4 Solutions in simple cases

Even though a solution to the Ginzburg-Landau equations (3.9) and (3.14) cannot be obtained in the general case, we can get some insight by examining limiting cases. We will see that another important length will appear in the theory, in addition to the London penetration depth.

In the absence of a magnetic field the first Ginzburg-Landau equation reads

$$a\psi + b|\psi|^2\psi = 0. \tag{3.15}$$

This equation admits two spatially uniform solutions

$$\psi = 0 \tag{3.16}$$

and

$$|\psi|^2 = -\frac{a}{b}. \tag{3.17}$$

The first solution corresponds to the normal state and appears both for $T > T_c$ and $T \leq T_c$. The second one is valid only for $T \leq T_c$, as the parameter a is negative below T_c and positive above.

As a second example, we consider the one-dimension geometry where ψ is not spatially uniform but the magnetic field is still zero. The Ginzburg-Landau equation becomes

$$-\frac{\hbar^2}{2m^*}\frac{\mathrm{d}^2\psi(z)}{\mathrm{d}z^2} + a\psi(z) + b|\psi(z)|^2\psi = 0. \tag{3.18}$$

We introduce a change of variables to achieve a dimensionless order parameter: $f(z) = \frac{\psi(z)}{|\psi_\infty|}$, where $|\psi_\infty| \equiv \sqrt{\frac{|a|}{b}}$. Thus, we arrive at

$$-\frac{\hbar^2}{2m^*|a|}\frac{\mathrm{d}^2 f(z)}{\mathrm{d}z^2} - f(z) + f^3(z) = 0, \tag{3.19}$$

which defines a natural scale for spatial variations of the order parameter. We define

$$\xi(T) \equiv \sqrt{\frac{\hbar^2}{2m^*(T_c - T)\alpha}}. \tag{3.20}$$

The quantity $\xi = \xi(T)$ is known as the Ginzburg-Landau coherence length.

Let us see how f behaves. By hypothesis, the field doesn't penetrate in the region where the order parameter is non-zero. So, we can use the following boundary conditions to solve this differential equation

$$f(0) = 0$$
$$f(z \to \infty) \to 1.$$

By multiplying this differential equation by $\frac{\mathrm{d}f}{\mathrm{d}x}$ and integrating we obtain

$$-\xi(T)^2\left(\frac{\mathrm{d}f}{\mathrm{d}z}\right)^2 - f^2 + \frac{1}{2}f^4 = cte.$$

Using the boundary condition in the infinity we have that

$$\xi(T)^2\left(\frac{\mathrm{d}f}{\mathrm{d}z}\right)^2 = \frac{1}{2}(1 - f^2)^2.$$

If f increases with z we take the positive square root and thus

$$\frac{\mathrm{d}f}{\mathrm{d}z} = \frac{1 - f^2}{\sqrt{2}\xi},$$

which we easily integrate and obtain

$$f = \tanh \frac{z}{\sqrt{2}\xi}.$$

Now we plot this function and can clearly see that the Ginzburg Landau coherence lenght is a natural scale of the variation of the order parameter.

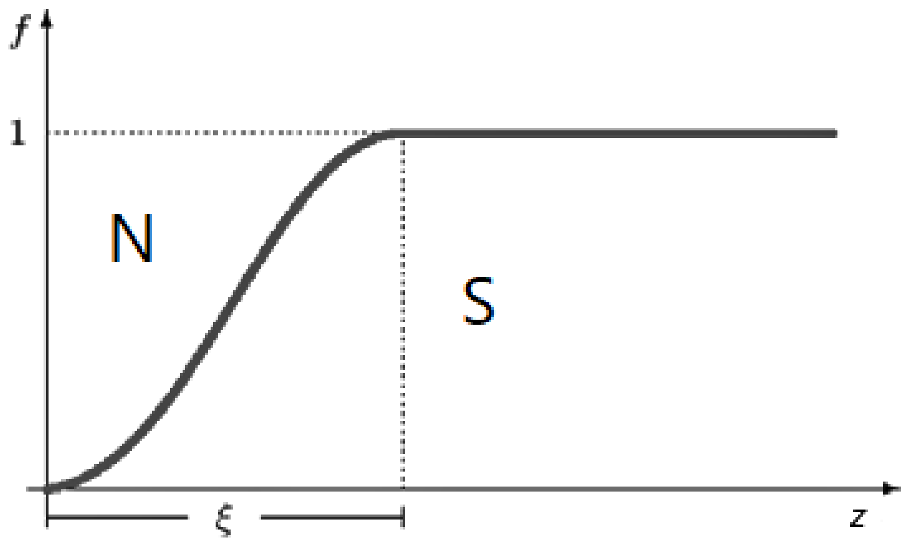


Figure 6: Behavior of the order parameter near the interface between superconducting and normal states.

As a final example, consider an applied magnetic field with an essentially uniform order parameter. The expression for the super-current then reduces to

$$\mathbf{j}(\mathbf{r}) = -\frac{e^{*2}}{m^* c}|\psi|^2 \mathbf{A}(\mathbf{r}). \tag{3.21}$$

Using this current in Ampere's law and taking the curl of both sides of the equation we get

$$\nabla^2 \mathbf{B} = \frac{4\pi|\psi|^2 e^{*2}}{m^* c^2}\mathbf{B}. \tag{3.22}$$

Solving this equation, we get the length at which the magnetic field is screened out inside the material. Following the usual normalization of the order parameter $|\psi|^2 = n_s^*$, we can clearly see that the obtained expression for the magnetic length recovers the London penetration depth considered in Chapter 1, $\lambda = \lambda(T)$. We write

$$\lambda(T) = \sqrt{\frac{m^* c^2}{4\pi n_s e^{*2}}}. \tag{3.23}$$

Therefore, we were able to get two important parameters, the Ginzburg-Landau coherence length and the London penetration depth just by consider simple limiting cases.

3.1.5 Ginzburg-Landau parameter and classification of superconductors

The importance of the coherence length and the London penetration depth can be seen by considering their ratio, i.e., the Ginzburg-Landau parameter

$$\kappa(T) \equiv \frac{\lambda(T)}{\xi(T)}. \tag{3.24}$$

By using the Ginzburg-Landau theory one can distinguish two types of superconductors. In Type I superconductors, superconductivity is abruptly destroyed when the applied field amplitude exceeds the thermodynamic critical value H_c. In Type II superconductors when a strong enough magnetic field is applied (exceeding the lower critical field), the superconductor can lower its free energy by creating regions of normal state in its interior, allowing penetration of magnetic field in these regions. In this case we have a coexistence of normal and superconducting phases which is called the mixed state. The difference between these two types is quantified via the Ginzburg-Landau parameter. When $\kappa < \frac{1}{\sqrt{2}}$, we have a type I superconductor. When $\kappa > \frac{1}{\sqrt{2}}$, we have a type II superconductor. One can see a relevant illustration below.

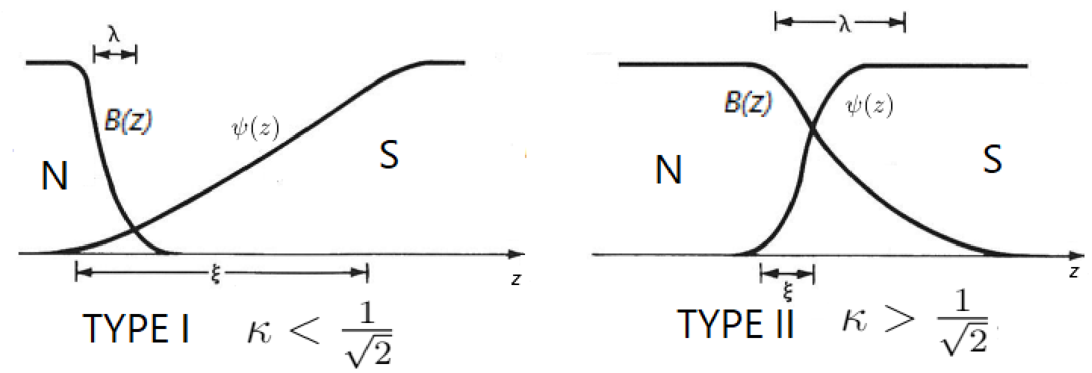


Figure 7: Spatial variation of the magnetic field $B(z)$ and the order parameter $\psi(z)$ in type I and type II superconductor.

3.2 BCS microscopic theory

Unlike phenomenological theories, the BCS microscopic theory of superconductivity can connect properties of superconductors with the material structure and related microscopic parameters. It has been developed in the 50's and published in 1957 by John Bardeen, Leon Cooper, and John Robert Schrieffer [6](BCS are initials of the last names of the physicists). This theory is able to explain superconductivity via the condensation of

Cooper pairs, being composite bosons. The focus of the present chapter is to find the BCS hamiltonian (this Hamiltonian was introduced by Nikolay Bogoliubov and coauthors) and diagonalize it to find the quasi-particle spectrum.

3.2.1 BCS-Bogoliubov Hamiltonian

We start our consideration by writing the Hamiltonian in term of the field operators

$$\hat{H} = \sum_a \int d\mathbf{r} \hat{\psi}_a^\dagger(\mathbf{r}) \xi_\mathbf{r} \hat{\psi}_a(\mathbf{r}) + \frac{1}{2} \sum_{a,b} \int d\mathbf{r} d\mathbf{r}' \hat{\psi}_a^\dagger(\mathbf{r}) \hat{\psi}_b^\dagger(\mathbf{r}') V(\mathbf{r}, \mathbf{r}') \hat{\psi}_b(\mathbf{r}') \hat{\psi}_a(\mathbf{r}), \tag{3.25}$$

where a and b are spin projection variables, $V(\mathbf{r}, \mathbf{r}')$ is the pair interaction potential, and $\xi_\mathbf{r} = -\frac{\hbar^2}{2m} \left(\boldsymbol{\nabla} - \frac{ie}{\hbar c} \mathbf{A}(\mathbf{r}) \right)^2 - \mu$ is the single-electron Hamiltonian (absorbing the chemical potential due to the grand canonical formalism, as it is usual for $U(1)$ symmetry breaking). For simplicity, the inter-particle potential is approximated as $V(\mathbf{r}, \mathbf{r}') = -g\delta(\mathbf{r} - \mathbf{r}')$, where $g > 0$ is the Gor'kov coupling (after Lev Gor'kov who first derived the Ginzburg-Landau theory from the BCS microscopic equations). Then, the Hamiltonian reads

$$\hat{H} = \int d\mathbf{r} \sum_a \hat{\psi}_a^\dagger(\mathbf{r}) \xi_\mathbf{r} \hat{\psi}_a(\mathbf{r}) - \frac{g}{2} \int d\mathbf{r} \sum_{a,b} \hat{\psi}_a^\dagger(\mathbf{r}) \hat{\psi}_b^\dagger(\mathbf{r}) \hat{\psi}_b(\mathbf{r}) \hat{\psi}_a(\mathbf{r}). \tag{3.26}$$

Now we are going to solve the problem, following seminal mean-field prescriptions by Bogoliubov with coauthors. Within the Bogoliubov mean-field approximation, the four operator product is written as

$$\hat{\psi}_a^\dagger(\mathbf{r}) \hat{\psi}_b^\dagger(\mathbf{r}) \hat{\psi}_b(\mathbf{r}) \hat{\psi}_a(\mathbf{r}) \simeq \hat{\psi}_a^\dagger(\mathbf{r}) \hat{\psi}_b^\dagger(\mathbf{r}) \langle \hat{\psi}_b(\mathbf{r}) \hat{\psi}_a(\mathbf{r}) \rangle + \tag{3.27}$$

$$+ \langle \hat{\psi}_a^\dagger(\mathbf{r}) \hat{\psi}_b^\dagger(\mathbf{r}) \rangle \hat{\psi}_b(\mathbf{r}) \hat{\psi}_a(\mathbf{r}) - \langle \hat{\psi}_a^\dagger(\mathbf{r}) \hat{\psi}_b^\dagger(\mathbf{r}) \rangle \langle \hat{\psi}_b(\mathbf{r}) \hat{\psi}_a(\mathbf{r}) \rangle.$$

Here we introduce the anomalous averages (anomalous Green functions)

$$\langle \hat{\psi}_a^\dagger(\mathbf{r}) \hat{\psi}_b^\dagger(\mathbf{r}) \rangle, \langle \hat{\psi}_b(\mathbf{r}) \hat{\psi}_a(\mathbf{r}) \rangle, \tag{3.28}$$

and such averages are given by

$$\langle \hat{\psi}_a^\dagger(\mathbf{r}) \hat{\psi}_b^\dagger(\mathbf{r}) \rangle = \frac{1}{\mathrm{Tr}\, e^{-\beta \hat{H}}} \mathrm{Tr} \left(e^{-\beta \hat{H}} \hat{\psi}_a^\dagger(\mathbf{r}) \hat{\psi}_b^\dagger(\mathbf{r}) \right), \tag{3.29}$$

where we recall that $\hat{H}$ is the grand canonical Hamiltonian. Notice that the Hartree-Fock contribution is suppressed here. The interaction energy is given by

$$\langle H_{BCS,int} \rangle \simeq -\frac{g}{2} \sum_{a,b} \int d\mathbf{r} \langle \hat{\psi}_a^\dagger(\mathbf{r}) \hat{\psi}_b^\dagger(\mathbf{r}) \rangle \langle \hat{\psi}_b(\mathbf{r}) \hat{\psi}_a(\mathbf{r}) \rangle. \tag{3.30}$$

The physical meaning of $\langle \hat{\psi}_b(\mathbf{r}) \hat{\psi}_a(\mathbf{r}) \rangle$ will be explained later but here we can simply accept that it is the *(center-of-mass) pair wave function* of two bound electrons, i.e., the *pair wave function of the composite boson or the Cooper pair.* The standard picture of superconductivity implies the *spin singlet pairing.* This means that the total spin of the Cooper pair is zero. We can, therefore only have the following combinations: $a =\uparrow, b =\downarrow$ and $a =\downarrow, b =\uparrow$. Carrying out the summation over the spin projections and using the anti-commutation rules for fermionic field operators, $[\hat{\psi}_a(\mathbf{r}), \hat{\psi}_b^\dagger(\mathbf{r}')]_+ = \delta_{ab}\delta(\mathbf{r}-\mathbf{r}')$ and $[\hat{\psi}_a(\mathbf{r}), \hat{\psi}_b(\mathbf{r}')]_+ = [\hat{\psi}_a^\dagger(\mathbf{r}), \hat{\psi}_b^\dagger(\mathbf{r}')]_+ = 0$, where $[\ ]_+$ is the anti-commutator backets, we obtain the BCS approximation of the interaction part of the Hamiltonian as

$$\langle H_{BCS,int}\rangle = -g\int d\mathbf{r}\langle\hat{\psi}_\uparrow^\dagger(\mathbf{r})\hat{\psi}_\downarrow^\dagger(\mathbf{r})\rangle\langle\hat{\psi}_\downarrow(\mathbf{r})\hat{\psi}_\uparrow(\mathbf{r})\rangle = -\int d\mathbf{r}\frac{|\Delta(\mathbf{r})|^2}{g},$$

where we introduce the order parameter $\Delta(\mathbf{r})$ as

$$\Delta(\mathbf{r}) \equiv g\langle\hat{\psi}_\uparrow(\mathbf{r})\hat{\psi}_\downarrow(\mathbf{r})\rangle. \tag{3.31}$$

The order parameter is also called the gap function because it is defined such that it yields the energy gap in the excitation spectrum of a uniform superconductor. Using the definition for the order parameter and Bogoilubov's prescriptions, we can write the BCS-model Hamiltonian as

$$\begin{aligned} H_{BCS} = &\int d\mathbf{r}\Big(\psi_\uparrow^\dagger(\mathbf{r})\xi_\mathbf{r}\psi_\uparrow(\mathbf{r}) + \psi_\downarrow^\dagger(\mathbf{r})\xi_\mathbf{r}\psi_\downarrow(\mathbf{r})\Big) \\ &+ \int d\mathbf{r}\Big(\psi_\uparrow^\dagger(\mathbf{r})\psi_\downarrow^\dagger(\mathbf{r})\Delta(\mathbf{r}) + \Delta^*(\mathbf{r})\psi_\downarrow(\mathbf{r})\psi_\uparrow(\mathbf{r})\Big) + C, \end{aligned} \tag{3.32}$$

where $C = \int d\mathbf{r}\frac{|\Delta(\mathbf{r})|^2}{g}$. But now we encounter a problem because this Hamiltonian is not diagonal. To work with the Hamiltonian in this form will be incredibly time consuming. We will now diagonalize it because it will be at the center of all our calculations.

3.2.2 Diagonalization of the BCS Hamiltonian

To start our calculations consider the BCS hamiltonian in the Heisenberg representation. The fermionic field operators in the Heisenber formalism are

$$\begin{aligned} \psi_\uparrow(\mathbf{r}, t) &= e^{iH_{BCS}}\psi_\uparrow(\mathbf{r})e^{-iH_{BCS}}, \\ \psi_\downarrow(\mathbf{r}, t) &= e^{iH_{BCS}}\psi_\downarrow(\mathbf{r})e^{-iH_{BCS}}. \end{aligned}$$

The equation of motion for these field operators is

$$\begin{aligned} i\hbar\partial_t\psi_\uparrow(\mathbf{r}, t) =& [\psi_\uparrow(\mathbf{r}, t), H_{BCS}] = e^{iH_{BCS}\frac{t}{\hbar}}[\psi_\uparrow(\mathbf{r}), H_{BCS}]e^{-iH_{BCS}\frac{t}{\hbar}}. \\ i\hbar\partial_t\psi_\downarrow^\dagger(\mathbf{r}, t) =& [\psi_\downarrow^\dagger(\mathbf{r}, t), H_{BCS}] = e^{iH_{BCS}\frac{t}{\hbar}}[\psi_\downarrow^\dagger(\mathbf{r}), H_{BCS}]e^{-iH_{BCS}\frac{t}{\hbar}}. \end{aligned}$$

Simple calculations yields

$$\begin{aligned} [\psi_\uparrow(\mathbf{r}), \hat{H}_{BCS}] =& \xi_\mathbf{r}\psi_\uparrow(\mathbf{r}) + \Delta(\mathbf{r})\psi_\downarrow^\dagger(\mathbf{r}) \\ [\psi_\downarrow(\mathbf{r}), \hat{H}_{BCS}] =& \xi_\mathbf{r}\psi_\downarrow(\mathbf{r}) - \Delta(\mathbf{r})\psi_\uparrow^\dagger(\mathbf{r}). \end{aligned} \tag{3.33}$$

And we can write

$$-[\psi_\downarrow^\dagger(\mathbf{r}), H_{BCS}] = \xi_\mathbf{r}^* \psi_\downarrow^\dagger(\mathbf{r}) - \Delta^*(\mathbf{r})\psi_\uparrow(\mathbf{r}). \tag{3.34}$$

So the equations of motion are

$$i\hbar\partial_t \begin{pmatrix} \psi_\uparrow(\mathbf{r},t) \\ \psi_\downarrow^\dagger(\mathbf{r},t) \end{pmatrix} = \underbrace{\begin{pmatrix} \xi_\mathbf{r} & \Delta(\mathbf{r}) \\ \Delta^*(\mathbf{r}) & -\xi_\mathbf{r}^* \end{pmatrix}}_{\mathbb{H}_{BdG}} \begin{pmatrix} \psi_\uparrow(\mathbf{r},t) \\ \psi_\downarrow^\dagger(\mathbf{r},t) \end{pmatrix} \tag{3.35}$$

$\mathbb{H}_{BdG}$ is called Bogoliubov-deGennes matrix. The eigenvalues and eigenstates of $\mathbb{H}_{BdG}$ are given by

$$\begin{pmatrix} \xi_\mathbf{r} & \Delta(\mathbf{r}) \\ \Delta^*(\mathbf{r}) & -\xi_\mathbf{r}^* \end{pmatrix} \begin{pmatrix} u_\lambda(\mathbf{r}) \\ v_\lambda(\mathbf{r}) \end{pmatrix} = \epsilon_\lambda \begin{pmatrix} u_\lambda(\mathbf{r}) \\ v_\lambda(\mathbf{r}) \end{pmatrix}. \tag{3.36}$$

These equations are commonly known as the Bogoliubov-de Gennes equations.

We can, also,express the field operators $\psi(\mathbf{r},t)$ and $\psi^\dagger(\mathbf{r},t)$ in terms of $u_\lambda(\mathbf{r})$ and $v_\lambda(\mathbf{r})$ as

$$\begin{pmatrix} \psi_\uparrow(\mathbf{r},t) \\ \psi_\downarrow^\dagger(\mathbf{r},t) \end{pmatrix} = \sum_\lambda \Gamma_\lambda(t) \begin{pmatrix} u_\lambda(\mathbf{r}) \\ v_\lambda(\mathbf{r}) \end{pmatrix}$$

Let us now substitute this expression in the equation of motion for the field operators. We obtain

$$i\hbar\partial_t \sum_\lambda \Gamma_\lambda(t) \begin{pmatrix} u_\lambda(\mathbf{r}) \\ v_\lambda(\mathbf{r}) \end{pmatrix} = \mathbb{H}_{BdG} \sum_\lambda \Gamma_\lambda(t) \begin{pmatrix} u_\lambda(\mathbf{r}) \\ v_\lambda(\mathbf{r}) \end{pmatrix}.$$

Using the eigenvalue equation we can write

$$i\hbar\partial_t \sum_\lambda \Gamma_\lambda(t) \begin{pmatrix} u_\lambda(\mathbf{r}) \\ v_\lambda(\mathbf{r}) \end{pmatrix} = \sum_\lambda \epsilon_\lambda \Gamma_\lambda(t) \begin{pmatrix} u_\lambda(\mathbf{r}) \\ v_\lambda(\mathbf{r}) \end{pmatrix}.$$

Now we multiply by the complex conjugated eigenstates of the BdG matrix and integrate over all space, as follows

$$\int d\mathbf{r} \begin{pmatrix} u_{\lambda'}^*(\mathbf{r}) & v_{\lambda'}^*(\mathbf{r}) \end{pmatrix} i\hbar\partial_t \sum_\lambda \Gamma_\lambda(t) \begin{pmatrix} u_\lambda(\mathbf{r}) \\ v_\lambda(\mathbf{r}) \end{pmatrix}$$
$$= \int d\mathbf{r} \begin{pmatrix} u_{\lambda'}^*(\mathbf{r}) & v_{\lambda'}^*(\mathbf{r}) \end{pmatrix} \sum_\lambda \epsilon_\lambda \Gamma_\lambda(t) \begin{pmatrix} u_\lambda(\mathbf{r}) \\ v_\lambda(\mathbf{r}) \end{pmatrix}.$$

From the Bogoliubov-de Gennes equations one obtains

$$\text{Completeness}: \begin{cases} \sum_\lambda u_\lambda(\mathbf{r}) u_\lambda^*(\mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}'), \\ \sum_\lambda v_\lambda(\mathbf{r}) u_\lambda^*(\mathbf{r}') = 0. \end{cases} \tag{3.37}$$

$$\text{Orthogonality}: \int d\mathbf{r} \begin{pmatrix} u_\lambda^*(\mathbf{r}) & v_\lambda^*(\mathbf{r}) \end{pmatrix} \begin{pmatrix} u_{\lambda'}(\mathbf{r}) \\ v_{\lambda'}(\mathbf{r}) \end{pmatrix} = \delta_{\lambda,\lambda'}, \tag{3.38}$$

(from this relation we can prove that the γ-operators obey the fermionic anti-commutation relations) and so

$$i\hbar\partial_\tau \Gamma_\lambda(t) = \epsilon_\lambda \Gamma_\lambda(t). \tag{3.39}$$

This is not the end of the story. In fact, there are two branches of the solution to the BdG equations that we specify as $\lambda = \nu, \pm$. One can check that they obey the relation

$$u_{\nu,-} = -v^*_{\nu,+},\; v_{\nu,-} = u^*_{\nu,+},\; \epsilon_{\nu,-} = -\epsilon_{\nu,+} = E_\nu, \tag{3.40}$$

where $*$ means the complex conjugate operation and $\epsilon_{\nu,+}$ is normally positive (except of the depairing regime). Defining $u_\nu \equiv u_{\nu,+}$, $v_\nu \equiv v_{\nu,+}$, and $E_\nu \equiv \epsilon_{\nu,+}$, we introduce new Heisenberg fermionic operators $\gamma_{\nu\uparrow}(t)$ and $\gamma_{\nu\downarrow}(t)$ in the following way:

$$\begin{pmatrix} \psi_\uparrow(\mathbf{r},t) \\ \psi^\dagger_\downarrow(\mathbf{r},t) \end{pmatrix} = \sum_\nu \begin{pmatrix} u_\nu(\mathbf{r}) & -v^*_\nu(\mathbf{r}) \\ v_\nu(\mathbf{r}) & u^*_\nu(\mathbf{r}) \end{pmatrix} \begin{pmatrix} \gamma_{\nu\uparrow}(t) \\ \gamma^\dagger_{\nu\downarrow}(t) \end{pmatrix}. \tag{3.41}$$

Where $\Gamma_{\nu,+}(t) = \gamma_{\nu,\uparrow}(t), \Gamma_{\nu,-}(t) = \gamma^\dagger_{\nu,\downarrow}(t)$. This is the Bogoliubov-Valatin canonical transformation. As we can see, the Bogoliubov-Valatin transformation mixes electron and hole operators with opposite spins - this is the only way to get rid of nondiagonal pairing terms. The physical significance of this is that the quasi-particles in the superconductor are rather like centaurs: "partly electrons, partly holes." For obvious reasons they are called bogolons.

We can also calculate the inverse Bogoliubov-Valatin transformation. Multiplying this expression to the left by the inverse matrix

$$\begin{pmatrix} u^*_\nu(\mathbf{r}) & v^*_\nu(\mathbf{r}) \\ -v_\nu(\mathbf{r}) & u_\nu(\mathbf{r}) \end{pmatrix}$$

and integrating over all $\mathbf{r}$, one obtains

$$\begin{pmatrix} \gamma_{\nu\uparrow}(t) \\ \gamma^\dagger_{\nu\downarrow}(t) \end{pmatrix} = \int d\mathbf{r} \begin{pmatrix} u^*_\nu(\mathbf{r}) & v^*_\nu(\mathbf{r}) \\ -v_\nu(\mathbf{r}) & u_\nu(\mathbf{r}) \end{pmatrix} \begin{pmatrix} \psi_\uparrow(\mathbf{r},t) \\ \psi^\dagger_\downarrow(\mathbf{r},t) \end{pmatrix} \tag{3.42}$$

Does the transformation of equation (3.41) diagonalizes the Hamiltonian? Let us apply it in the equation of motion for the fermionic operators. We will obtain

$$i\hbar\partial_t \sum_\nu \begin{pmatrix} u_\nu(\mathbf{r}) & -v^*_\nu(\mathbf{r}) \\ v_\nu(\mathbf{r}) & u^*_\nu(\mathbf{r}) \end{pmatrix} \begin{pmatrix} \gamma_{\nu\uparrow}(t) \\ \gamma^\dagger_{\nu\downarrow}(t) \end{pmatrix} = \mathbb{H}_{BdG} \sum_\nu \begin{pmatrix} u_\nu(\mathbf{r}) & -v^*_\nu(\mathbf{r}) \\ v_\nu(\mathbf{r}) & u^*_\nu(\mathbf{r}) \end{pmatrix} \begin{pmatrix} \gamma_{\nu\uparrow}(t) \\ \gamma^\dagger_{\nu\downarrow}(t) \end{pmatrix}.$$

From the eigenvector equation we find that

$$\begin{aligned} i\hbar\partial_t \sum_\nu & \begin{pmatrix} u_\nu(\mathbf{r}) & -v^*_\nu(\mathbf{r}) \\ v_\nu(\mathbf{r}) & u^*_\nu(\mathbf{r}) \end{pmatrix} \begin{pmatrix} \gamma_{\nu\uparrow}(t) \\ \gamma^\dagger_{\nu\downarrow}(t) \end{pmatrix} \\ = \sum_\nu & \begin{pmatrix} u_\nu(\mathbf{r}) & -v^*_\nu(\mathbf{r}) \\ v_\nu(\mathbf{r}) & u^*_\nu(\mathbf{r}) \end{pmatrix} \begin{pmatrix} E_\nu & 0 \\ 0 & -E_\nu \end{pmatrix} \begin{pmatrix} \gamma_{\nu\uparrow}(t) \\ \gamma^\dagger_{\nu\downarrow}(t) \end{pmatrix}. \end{aligned}$$

And so

$$i\hbar\partial_t \begin{pmatrix} \gamma_{\nu,\uparrow} \\ \gamma^\dagger_{\nu,\downarrow} \end{pmatrix} = \begin{pmatrix} E_\nu & 0 \\ 0 & -E_\nu \end{pmatrix} \begin{pmatrix} \gamma_{\nu,\uparrow} \\ \gamma^\dagger_{\nu,\downarrow} \end{pmatrix}.$$

Therefore, the γ operators diagonalize the hamiltonian with E_ν as the eigenvalue.

The anticommutation rules for the quasiparticle operators are derived using the Bogoliubov-Valatin transformation. We will derive them as follows

$$\begin{aligned}
&\gamma_{\nu,\uparrow}\gamma^\dagger_{\nu',\uparrow}+\gamma^\dagger_{\nu',\uparrow}\gamma_{\nu,\uparrow} \\
&= \int d\mathbf{r}d\mathbf{r}'\Big\{\left[u^*_\nu(\mathbf{r})\psi_\uparrow(\mathbf{r}) + v^*_\nu\psi^\dagger_\downarrow(\mathbf{r})\right]\left[u_{\nu'}(\mathbf{r}')\psi^\dagger_\uparrow(\mathbf{r}') + v_{\nu'}(\mathbf{r}')\psi_\downarrow(\mathbf{r}')\right] \\
&+ \int d\mathbf{r}d\mathbf{r}'\Big\{\left[u_{\nu'}(\mathbf{r}')\psi^\dagger_\uparrow(\mathbf{r}') + v_{\nu'}(\mathbf{r}')\psi_\downarrow(\mathbf{r}')\right]\left[u^*_\nu(\mathbf{r})\psi_\uparrow(\mathbf{r}) + v^*_\nu(\mathbf{r})\psi^\dagger_\downarrow(\mathbf{r})\right]\Big\} \\
&= \int d\mathbf{r}d\mathbf{r}'\Big\{\big[\underbrace{\psi_\uparrow(\mathbf{r})\psi^\dagger_\uparrow(\mathbf{r}') + \psi^\dagger_\uparrow(\mathbf{r}')\psi_\uparrow(\mathbf{r})}_{\delta(\mathbf{r}-\mathbf{r}')}\big]u^*_\nu(\mathbf{r})u_{\nu'}(\mathbf{r}') \\
&\qquad + \big[\underbrace{\psi^\dagger_\downarrow(\mathbf{r})\psi^\dagger_\uparrow(\mathbf{r}') + \psi^\dagger_\uparrow(\mathbf{r}')\psi^\dagger_\downarrow(\mathbf{r})}_{0}\big]v^*_\nu(\mathbf{r})u_{\nu'}(\mathbf{r}') \\
&\qquad + \big[\underbrace{\psi_\uparrow(\mathbf{r})\psi_\downarrow(\mathbf{r}') + \psi_\downarrow(\mathbf{r}')\psi_\uparrow(\mathbf{r})}_{0}\big]u^*_\nu(\mathbf{r})v_{\nu'}(\mathbf{r}') \\
&\qquad + \big[\underbrace{\psi^\dagger_\downarrow(\mathbf{r})\psi_\downarrow(\mathbf{r}') + \psi_\downarrow(\mathbf{r}')\psi^\dagger_\downarrow(\mathbf{r})}_{\delta(\mathbf{r}-\mathbf{r}')}\big]v^*_\nu(\mathbf{r})v_{\nu'}(\mathbf{r}')\Big\}.
\end{aligned}$$

Therefore, we obtain

$$\gamma_{\nu,\uparrow}\gamma^\dagger_{\nu',\uparrow}+\gamma^\dagger_{\nu',\uparrow}\gamma_{\nu,\uparrow} = \int d\mathbf{r}\Big(u^*_\nu(\mathbf{r})u_{\nu'}(\mathbf{r}) + v^*_\nu(\mathbf{r})v_{\nu'}(\mathbf{r})\Big) = \delta_{\nu,\nu'}$$

For the general case we can write

$$\gamma^\dagger_{\sigma,\nu}\gamma_{\sigma',\nu'} + \gamma_{\sigma',\nu'}\gamma^\dagger_{\sigma,\nu} = \delta_{\sigma,\sigma'}\delta_{\nu,\nu'}, \tag{3.43}$$

$$\gamma_{\sigma,\nu}\gamma_{\sigma',\nu'} + \gamma_{\sigma',\nu'}\gamma_{\sigma,\nu} = 0, \tag{3.44}$$

where σ is the spin projection. Now, let us use the Bogoliubov-Valatin transformation in order to obtain the diagonalized Hamiltonian. The field operators are written as

$$\psi_\uparrow(\mathbf{r},t) = \sum_\nu u_\nu(\mathbf{r})\gamma_{\nu,\uparrow}(t) - v^*_\nu(\mathbf{r})\gamma^\dagger_{\nu,\downarrow}(t),$$

$$\psi^\dagger_\downarrow(\mathbf{r},t) = \sum_\nu v_\nu(\mathbf{r})\gamma_{\nu,\uparrow}(t) + u^*_\nu(\mathbf{r})\gamma^\dagger_{\nu,\downarrow}(t).$$

Let us write the BCS Hamiltonian as $H_{BCS} = H_0 + H_\Delta + H_{\Delta^*} + C$ and calculate step by step. The first term is

$$H_0 = \int d\mathbf{r}\Bigg\{ \sum_{\nu,\nu'} \Big(u_\nu^*(\mathbf{r})\gamma_{\nu,\uparrow}^\dagger(t) - v_\nu(\mathbf{r})\gamma_{\nu,\downarrow}(t)\Big)\xi_\mathbf{r}\Big(u_{\nu'}(\mathbf{r})\gamma_{\nu',\uparrow}(t) - v_{\nu'}^*(\mathbf{r})\gamma_{\nu',\downarrow}^\dagger(t)\Big)$$
$$+ \sum_{\nu,\nu'} \Big(v_\nu(\mathbf{r})\gamma_{\nu,\uparrow}(t) + u_\nu^*(\mathbf{r})\gamma_{\nu,\downarrow}^\dagger(t)\Big)\xi_\mathbf{r}\Big(v_{\nu'}^*(\mathbf{r})\gamma_{\nu',\uparrow}^\dagger(t) + u_{\nu'}(\mathbf{r})\gamma_{\nu',\downarrow}(t)\Big)\Bigg\}$$
$$= \int d\mathbf{r}\Bigg\{ \sum_{\nu,\nu'} u_\nu^*(\mathbf{r})\xi_\mathbf{r}u_{\nu'}(\mathbf{r})\gamma_{\nu,\uparrow}^\dagger(t)\gamma_{\nu',\uparrow}(t) + \sum_{\nu,\nu'} v_\nu(\mathbf{r})\xi_\mathbf{r}v_{\nu'}^*(\mathbf{r})\gamma_{\nu,\downarrow}(t)\gamma_{\nu',\downarrow}^\dagger(t)$$
$$- \sum_{\nu,\nu'} u_\nu^*(\mathbf{r})\xi_\mathbf{r}v_{\nu'}^*(\mathbf{r})\gamma_{\nu,\uparrow}^\dagger(t)\gamma_{\nu',\downarrow}^\dagger(t) - \sum_{\nu,\nu'} v_\nu(\mathbf{r})\xi_\mathbf{r}u_{\nu'}(\mathbf{r})\gamma_{\nu,\downarrow}(t)\gamma_{\nu',\uparrow}(t)$$
$$+ \sum_{\nu,\nu'} v_\nu(\mathbf{r})\xi_\mathbf{r}v_{\nu'}^*(\mathbf{r})\gamma_{\nu,\uparrow}(t)\gamma_{\nu',\uparrow}^\dagger(t) + \sum_{\nu,\nu'} u_\nu^*(\mathbf{r})\xi_\mathbf{r}u_{\nu'}(\mathbf{r})\gamma_{\nu,\downarrow}^\dagger(t)\gamma_{\nu',\downarrow}(t)$$
$$+ \sum_{\nu,\nu'} u_\nu^*(\mathbf{r})\xi_\mathbf{r}v_{\nu'}^*(\mathbf{r})\gamma_{\nu,\downarrow}^\dagger(t)\gamma_{\nu',\uparrow}^\dagger(t) + \sum_{\nu,\nu'} v_\nu(\mathbf{r})\xi_\mathbf{r}u_{\nu'}(\mathbf{r})\gamma_{\nu,\uparrow}(t)\gamma_{\nu',\downarrow}(t)\Bigg\}.$$

The second term has the form

$$H_\Delta = \int d\mathbf{r}\sum_{\nu,\nu'} \Delta(\mathbf{r})\Big(u_\nu^*(\mathbf{r})\gamma_{\nu,\uparrow}^\dagger(t) - v_\nu(\mathbf{r})\gamma_{\nu,\downarrow}(t)\Big)\Big(v_{\nu'}(\mathbf{r})\gamma_{\nu',\uparrow}(t) + u_{\nu'}^*(\mathbf{r})\gamma_{\nu',\downarrow}^\dagger(t)\Big)$$
$$= \int d\mathbf{r}\Bigg\{ \sum_{\nu,\nu'} \Delta(\mathbf{r})\Big[u_\nu^*(\mathbf{r})v_{\nu'}(\mathbf{r})\gamma_{\nu,\uparrow}^\dagger(t)\gamma_{\nu',\uparrow}(t) - v_\nu(\mathbf{r})v_{\nu'}(\mathbf{r})\gamma_{\nu,\downarrow}(t)\gamma_{\nu',\uparrow}(t)\Big]$$
$$+ \sum_{\nu,\nu'} \Delta(\mathbf{r})\Big[u_\nu^*(\mathbf{r})u_{\nu'}^*(\mathbf{r})\gamma_{\nu,\uparrow}^\dagger(t)\gamma_{\nu',\downarrow}^\dagger(t) - v_\nu(\mathbf{r})u_{\nu'}^*(\mathbf{r})\gamma_{\nu,\downarrow}(t)\gamma_{\nu',\downarrow}^\dagger(t)\Big]\Bigg\}.$$

And H_{Δ^*} is

$$H_{\Delta^*} = \int d\mathbf{r}\sum_{\nu,\nu'} \Delta^*(\mathbf{r})\Big(v_\nu^*(\mathbf{r})\gamma_{\nu,\uparrow}^\dagger(t) + u_\nu(\mathbf{r})\gamma_{\nu,\downarrow}(t)\Big)\Big(u_{\nu'}(\mathbf{r})\gamma_{\nu',\uparrow}(t) - v_{\nu'}^*(\mathbf{r})\gamma_{\nu',\downarrow}^\dagger(t)\Big)$$
$$= \int d\mathbf{r}\Bigg\{ \sum_{\nu,\nu'} \Delta^*(\mathbf{r})\Big[v_\nu^*(\mathbf{r})u_{\nu'}(\mathbf{r})\gamma_{\nu,\uparrow}^\dagger(t)\gamma_{\nu',\uparrow}(t) - v_\nu^*(\mathbf{r})v_{\nu'}^*(\mathbf{r})\gamma_{\nu,\uparrow}^\dagger(t)\gamma_{\nu',\downarrow}^\dagger(t)\Big]$$
$$+ \sum_{\nu,\nu'} \Delta^*(\mathbf{r})\Big[u_\nu(\mathbf{r})u_{\nu'}(\mathbf{r})\gamma_{\nu,\downarrow}(t)\gamma_{\nu',\uparrow}(t) - u_\nu(\mathbf{r})v_{\nu'}^*(\mathbf{r})\gamma_{\nu,\downarrow}(t)\gamma_{\nu',\downarrow}^\dagger(t)\Big]\Bigg\}.$$

We collect terms proportional to $\gamma^\dagger_{\nu,\uparrow}(t)\gamma_{\nu',\uparrow}(t)$ and $\gamma_{\nu,\uparrow}(t)\gamma^\dagger_{\nu',\uparrow}(t)$ as follows

$$\begin{aligned}
I_{11} =& \int d\mathbf{r} \sum_{\nu,\nu'} \Big[u^*_\nu(\mathbf{r})\xi_\mathbf{r} u_{\nu'}(\mathbf{r}) + \Delta(\mathbf{r})u^*_\nu(\mathbf{r})v_{\nu'}(\mathbf{r})\Big]\gamma^\dagger_{\nu,\uparrow}(t)\gamma_{\nu',\uparrow}(t) \\
&+ \int d\mathbf{r} \sum_{\nu,\nu'} \Big\{v_\nu(\mathbf{r})\xi_\mathbf{r} v^*_{\nu'}(\mathbf{r})\gamma_{\nu,\uparrow}(t)\gamma^\dagger_{\nu',\uparrow}(t) + \Delta^*(\mathbf{r})v^*_\nu(\mathbf{r})u_{\nu'}(\mathbf{r})\gamma^\dagger_{\nu,\uparrow}(t)\gamma_{\nu',\uparrow}(t)\Big\} \\
=& \int d\mathbf{r} \sum_{\nu,\nu'} \Big[u^*_\nu(\mathbf{r})\xi_\mathbf{r} u_{\nu'}(\mathbf{r}) + \Delta(\mathbf{r})u^*_\nu(\mathbf{r})v_{\nu'}(\mathbf{r})\Big]\gamma^\dagger_{\nu,\uparrow}(t)\gamma_{\nu',\uparrow}(t) \\
&+ \int d\mathbf{r} \sum_{\nu,\nu'} \Big[-v_\nu(\mathbf{r})\xi_\mathbf{r} v^*_{\nu'}(\mathbf{r}) + \Delta^*(\mathbf{r})v^*_\nu(\mathbf{r})u_{\nu'}(\mathbf{r})\Big]\gamma^\dagger_{\nu,\uparrow}(t)\gamma_{\nu',\uparrow}(t)\Big\} \\
&+ \int d\mathbf{r} \sum_{\nu} v_\nu(\mathbf{r})\xi_\mathbf{r} v^*_\nu(\mathbf{r}).
\end{aligned}$$

We can write the second term as

$$\begin{aligned}
&\int d\mathbf{r} \sum_{\nu,\nu'} \Big[-v_\nu(\mathbf{r})\xi_\mathbf{r} v^*_{\nu'}(\mathbf{r}) + \Delta^*(\mathbf{r})v^*_\nu(\mathbf{r})u_{\nu'}(\mathbf{r})\Big]\gamma^\dagger_{\nu,\uparrow}(t)\gamma_{\nu',\uparrow}(t)\Big\} \\
&= \int d\mathbf{r} \sum_{\nu,\nu'} v^*(\mathbf{r})_\nu \Big[-\xi^*_\mathbf{r} v_{\nu'}(\mathbf{r}) + \Delta^*(\mathbf{r})u_{\nu'}(\mathbf{r})\Big]\gamma^\dagger_{\nu,\uparrow}(t)\gamma_{\nu',\uparrow}(t)\Big\},
\end{aligned}$$

where we have used the integration by parts and the zero boundary conditions for u and v at infinity. We take the Bogoliubov-de Gennes equations (3.36) and the completeness relation (3.37) and obtain

$$\begin{aligned}
I_{11} =& \int d\mathbf{r} \sum_{\nu,\nu'} E_{\nu'}\Big[u^*_\nu(\mathbf{r})u_{\nu'}(\mathbf{r}) + v^*_\nu(\mathbf{r})v_{\nu'}(\mathbf{r})\Big]\gamma^\dagger_{\nu,\uparrow}(t)\gamma_{\nu',\uparrow}(t) + \int d\mathbf{r} \sum_{\nu} v_\nu(\mathbf{r})\xi_\mathbf{r} v^*_\nu(\mathbf{r}) \\
=& \sum_{\nu,\nu'} E_{\nu'}\delta_{\nu',\nu}\gamma^\dagger_{\nu,\uparrow}(t)\gamma_{\nu',\uparrow}(t) + \int d\mathbf{r} \sum_{\nu} v_\nu(\mathbf{r})\xi_\mathbf{r} v^*_\nu(\mathbf{r}) \\
=& \sum_{\nu} E_{\nu}\gamma^\dagger_{\nu,\uparrow}(t)\gamma_{\nu,\uparrow}(t) + \int d\mathbf{r} \sum_{\nu} v_\nu(\mathbf{r})\xi_\mathbf{r} v^*_\nu(\mathbf{r}).
\end{aligned}$$

Let us now gather terms proportional to $\gamma^\dagger_{\nu,\downarrow}(t)\gamma_{\nu',\downarrow}(t)$ and to $\gamma_{\nu,\downarrow}(t)\gamma^\dagger_{\nu',\downarrow}(t)$.

$$\begin{aligned}
I_{22} =& \int d\mathbf{r} \sum_{\nu,\nu'} \Big[v_\nu(\mathbf{r})\xi_\mathbf{r} v^*_{\nu'}(\mathbf{r}) - \Delta(\mathbf{r})v_\nu(\mathbf{r})u^*_{\nu'}(\mathbf{r})\Big]\gamma_{\nu,\downarrow}(t)\gamma^\dagger_{\nu',\downarrow}(t) \\
&+ \int d\mathbf{r} \sum_{\nu,\nu'} u^*_\nu(\mathbf{r})\xi_\mathbf{r} u_{\nu'}(\mathbf{r})\gamma^\dagger_{\nu,\downarrow}(t)\gamma_{\nu',\downarrow}(t) - \Delta^*(\mathbf{r})u_\nu(\mathbf{r})v^*_{\nu'}(\mathbf{r})\gamma_{\nu,\downarrow}(t)\gamma^\dagger_{\nu',\downarrow}(t) \\
=& \int d\mathbf{r} \sum_{\nu,\nu'} \Big[v_\nu(\mathbf{r})\xi_\mathbf{r} v^*_{\nu'}(\mathbf{r}) - \Delta(\mathbf{r})v_\nu(\mathbf{r})u^*_{\nu'}(\mathbf{r})\Big]\gamma_{\nu,\downarrow}(t)\gamma^\dagger_{\nu',\downarrow}(t) \\
&- \int d\mathbf{r} \sum_{\nu,\nu'} \Big[u^*_\nu(\mathbf{r})\xi_\mathbf{r} u_{\nu'}(\mathbf{r}) + \Delta^*(\mathbf{r})u_\nu(\mathbf{r})v^*_{\nu'}(\mathbf{r})\Big]\gamma_{\nu,\downarrow}(t)\gamma^\dagger_{\nu',\downarrow}(t) \\
&+ \int d\mathbf{r} \sum_{\nu,\nu'} u^*_\nu(\mathbf{r})\xi_\mathbf{r} u_\nu(\mathbf{r}).
\end{aligned}$$

The second term can be written as

$$\int d\mathbf{r} \sum_{\nu,\nu'} \Big[u_\nu^*(\mathbf{r})\xi_\mathbf{r} u_{\nu'}(\mathbf{r}) + \Delta^*(\mathbf{r})u_\nu(\mathbf{r})v_{\nu'}^*(\mathbf{r})\Big]\gamma_{\nu,\downarrow}(t)\gamma_{\nu',\downarrow}^\dagger(t)$$
$$= \int d\mathbf{r} \sum_{\nu,\nu'} u_\nu(\mathbf{r})\Big[\xi_\mathbf{r}^* u_{\nu'}^*(\mathbf{r}) + \Delta^*(\mathbf{r})v_{\nu'}^*(\mathbf{r})\Big]\gamma_{\nu,\downarrow}(t)\gamma_{\nu',\downarrow}^\dagger(t).$$

Then

$$\begin{aligned}
I_{22} =& \int d\mathbf{r} \sum_{\nu,\nu'} \Big[v_\nu(\mathbf{r})\xi_\mathbf{r} v_{\nu'}^*(\mathbf{r}) - \Delta(\mathbf{r})v_\nu(\mathbf{r})u_{\nu'}^*(\mathbf{r})\Big]\gamma_{\nu,\downarrow}(t)\gamma_{\nu',\downarrow}^\dagger(t)\\
&- \int d\mathbf{r} \sum_{\nu,\nu'} u_\nu(\mathbf{r})\Big[\xi_\mathbf{r}^* u_{\nu'}^*(\mathbf{r}) + \Delta^*(\mathbf{r})v_{\nu'}^*(\mathbf{r})\Big]\gamma_{\nu,\downarrow}(t)\gamma_{\nu',\downarrow}^\dagger(t) + \int d\mathbf{r} \sum_{\nu,\nu'} u_\nu^*(\mathbf{r})\xi_\mathbf{r} u_\nu(\mathbf{r})\\
=& - \int d\mathbf{r} \sum_{\nu,\nu'} E_{\nu'}\Big[u_\nu^*(\mathbf{r})u_{\nu'}(\mathbf{r}) + v_\nu^*(\mathbf{r})v_{\nu'}(\mathbf{r})\Big]\gamma_{\nu,\downarrow}(t)\gamma_{\nu',\downarrow}^\dagger(t) + \int d\mathbf{r} \sum_{\nu} u_\nu^*(\mathbf{r})\xi_\mathbf{r} u_\nu(\mathbf{r})\\
=& - \sum_{\nu,\nu'} E_{\nu'}\delta_{\nu,\nu'}\gamma_{\nu,\downarrow}(t)\gamma_{\nu',\downarrow}^\dagger(t) + \int d\mathbf{r} \sum_{\nu} u_\nu^*(\mathbf{r})\xi_\mathbf{r} u_\nu(\mathbf{r})\\
=& - \sum_{\nu} E_{\nu}\gamma_{\nu,\downarrow}(t)\gamma_{\nu',\downarrow}^\dagger(t) + \int d\mathbf{r} \sum_{\nu} u_\nu^*(\mathbf{r})\xi_\mathbf{r} u_\nu(\mathbf{r}).
\end{aligned}$$

Now we gather the off-diagonal terms.

$$\begin{aligned}
I_{12} =& - \int d\mathbf{r} \sum_{\nu,\nu'} \Big[u_\nu^*(\mathbf{r})\xi_\mathbf{r} v_{\nu'}^*(\mathbf{r}) + \Delta^*(\mathbf{r})v_\nu^*(\mathbf{r})v_{\nu'}^*(\mathbf{r})\Big]\gamma_{\nu,\uparrow}^\dagger(t)\gamma_{\nu',\downarrow}^\dagger(t)\\
&+ \int d\mathbf{r} \sum_{\nu,\nu'} \Big\{u_\nu^*(\mathbf{r})\xi_\mathbf{r} v_{\nu'}^*(\mathbf{r})\gamma_{\nu,\downarrow}^\dagger(t)\gamma_{\nu',\uparrow}^\dagger(t) + \Delta(\mathbf{r})u_\nu^*(\mathbf{r})u_{\nu'}^*(\mathbf{r})\gamma_{\nu,\uparrow}^\dagger(t)\gamma_{\nu',\downarrow}^\dagger(t)\Big\}\\
=& - \int d\mathbf{r} \sum_{\nu,\nu'} v_\nu^*(\mathbf{r})\Big[\xi_\mathbf{r}^* u_{\nu'}^*(\mathbf{r}) + \Delta^*(\mathbf{r})v_{\nu'}^*(\mathbf{r})\Big]\gamma_{\nu,\uparrow}^\dagger(t)\gamma_{\nu',\downarrow}^\dagger(t)\\
&+ \int d\mathbf{r} \sum_{\nu,\nu'} u_\nu^*(\mathbf{r})\Big[-\xi_\mathbf{r} v_{\nu'}^*(\mathbf{r}) + \Delta(\mathbf{r})u_{\nu'}^*(\mathbf{r})\Big]\gamma_{\nu,\uparrow}^\dagger(t)\gamma_{\nu',\downarrow}^\dagger(t)\\
=& \sum_{\nu,\nu'} E_{\nu'}\gamma_{\nu,\uparrow}^\dagger(t)\gamma_{\nu',\downarrow}^\dagger(t) \int d\mathbf{r}\Big[u_\nu^*(\mathbf{r})v_{\nu'}^*(\mathbf{r}) - v_\nu^*(\mathbf{r})u_{\nu'}^*(\mathbf{r})\Big] = 0.
\end{aligned}$$

And

$$\begin{aligned}
I_{21} =& - \int d\mathbf{r} \sum_{\nu,\nu'} \Big[v_\nu(\mathbf{r})\xi_\mathbf{r} u_{\nu'}(\mathbf{r}) + \Delta(\mathbf{r})v_\nu(\mathbf{r})v_{\nu'}(\mathbf{r})\Big]\gamma_{\nu,\downarrow}(t)\gamma_{\nu',\uparrow}(t)\\
&+ \int d\mathbf{r} \sum_{\nu,\nu'} \Big\{v_\nu(\mathbf{r})\xi_\mathbf{r} u_{\nu'}(\mathbf{r})\gamma_{\nu,\uparrow}(t)\gamma_{\nu',\downarrow}(t) + \Delta^*(\mathbf{r})u_\nu(\mathbf{r})u_{\nu'}(\mathbf{r})\gamma_{\nu,\downarrow}(t)\gamma_{\nu',\uparrow}(t)\Big\}\\
=& - \int d\mathbf{r} \sum_{\nu,\nu'} v_\nu(\mathbf{r})\Big[\xi_\mathbf{r} u_{\nu'}(\mathbf{r}) + \Delta(\mathbf{r})v_{\nu'}(\mathbf{r})\Big]\gamma_{\nu,\downarrow}(t)\gamma_{\nu',\uparrow}(t)\\
&+ \int d\mathbf{r} \sum_{\nu,\nu'} u_{\nu'}(\mathbf{r})\Big[-\xi_\mathbf{r}^* v_\nu(\mathbf{r}) + \Delta^*(\mathbf{r})u_\nu(\mathbf{r})\Big]\gamma_{\nu,\downarrow}(t)\gamma_{\nu',\uparrow}(t)\\
=& \sum_{\nu,\nu'} E_{\nu'}\gamma_{\nu,\downarrow}(t)\gamma_{\nu',\uparrow}(t) \int d\mathbf{r}\Big[u_\nu(\mathbf{r})v_{\nu'}(\mathbf{r}) - v_\nu(\mathbf{r})u_{\nu'}(\mathbf{r})\Big] = 0.
\end{aligned}$$

Finally we have

$$H_{BCS} = U_0 + \sum_{\nu} E_\nu(\gamma^\dagger_{\nu\uparrow}\gamma_{\nu\uparrow} + \gamma^\dagger_{\nu\downarrow}\gamma_{\nu\downarrow}), \tag{3.45}$$

where

$$U_0 = \int d\mathbf{r}\frac{|\Delta|^2}{g} + \sum_{\nu} u^*_\nu(\mathbf{r})\xi_{\mathbf{r}}u_\nu(\mathbf{r}) + v^*_\nu(\mathbf{r})\xi_{\mathbf{r}}v_\nu(\mathbf{r}) - E_\nu,$$

is the ground state energy of the superconductor. The second term is the quasi-particle term,which describes the elementary excitations above the ground state

3.2.3 Application to a simple situation

To get a feeling of the validity of this theory, let's consider an example of a uniform superconductor in zero magnetic field. For this case we can use the plane wave approximation and the BdG equation becomes

$$\begin{pmatrix} \xi_{\mathbf{r}} & \Delta \\ \Delta^* & -\xi^*_{\mathbf{r}} \end{pmatrix} \begin{pmatrix} u_{\mathbf{k}}\frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{\sqrt{V}} \\ v_{\mathbf{k}}\frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{\sqrt{V}} \end{pmatrix} = E_{\mathbf{k}} \begin{pmatrix} u_{\mathbf{k}}\frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{\sqrt{V}} \\ v_{\mathbf{k}}\frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{\sqrt{V}} \end{pmatrix},$$

and we can write

$$\begin{pmatrix} \xi_{\mathbf{k}} & \Delta \\ \Delta^* & -\xi_{\mathbf{k}} \end{pmatrix} \begin{pmatrix} u_{\mathbf{k}} \\ v_{\mathbf{k}} \end{pmatrix} = E_{\mathbf{k}} \begin{pmatrix} u_{\mathbf{k}} \\ v_{\mathbf{k}} \end{pmatrix}.$$

Where $\xi_{\mathbf{k}} = \frac{\hbar^2 k^2}{2m} - \mu$. The nontrivial solution exists only when

$$\det \begin{pmatrix} \xi_{\mathbf{k}} - E_{\mathbf{k}} & \Delta \\ \Delta^* & -\xi_{\mathbf{k}} - E_{\mathbf{k}} \end{pmatrix} = 0,$$

we should, of course, choose the positive sign which yields

$$E_{\mathbf{k}} = \sqrt{\xi^2_{\mathbf{k}} + |\Delta|^2}. \tag{3.46}$$

And, as expected, the excitation energy spectrum has a energy gap. Plotting this expression we can clearly see this result.

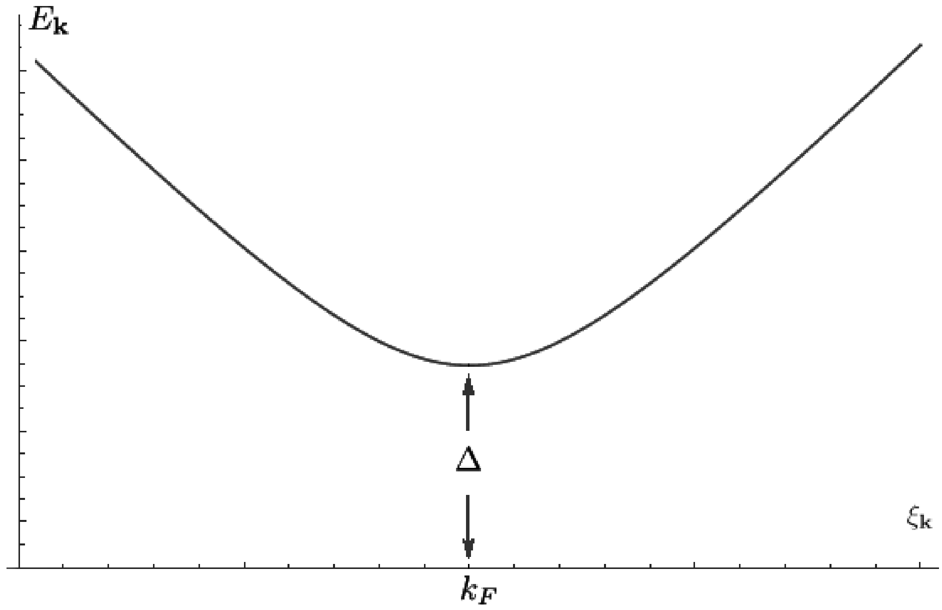


Figure 8: Quasi-particle dispersion

3.3 Microscopic derivation of GL equations

We have seen that BCS theory can explain superconductivity on microscopic arguments, i.e., the formation of the Cooper pair in the presence of the Fermi sea. Lev Gor'kov [7] has showed that the Ginzburg-Landau equations, that were initially introduced on the phenomenological basis, can be derived from the microscopic BCS theory via the Green function formalism. Now, we will show how one can get the Ginzburg-Landau equation for the order parameter from the BCS theory by using the Gor'kov equations (we will consider zero field case, for illustration). In our consideration we will follow closely the Gor'kov original development but we will work with the anomalous averages introduced by Bogoliubov.

3.3.1 Equations of motion for field operators

Basically, the Gor'kov equations are directly related to the equations of motion for the finite temperature Heisenberg field operators. However, instead of working directly with them we will introduce Green functions for these equations of motion. To start we will introduce the Heisenberg formalism for imaginary time

$$\hbar\partial_\tau \hat{A}(\tau) = [\hat{H}, \hat{A}(\tau)].$$

The Heisenberg operators are defined as

$$\hat{A}(\tau) = e^{\frac{\hat{H}\tau}{\hbar}} \hat{A} e^{\frac{-\hat{H}\tau}{\hbar}},$$
$$\hat{\bar{A}}(\tau) = e^{\frac{\hat{H}\tau}{\hbar}} \hat{A}^{\dagger} e^{\frac{-\hat{H}\tau}{\hbar}}.$$

So, the fermionic field operators on this representation obey the following equation of motion

$$\begin{aligned} \hbar\partial_\tau \hat{\psi}_\uparrow(\mathbf{r},\tau) &= [\hat{H}_{BCS}, \hat{\psi}_\uparrow(\mathbf{r},\tau)], \\ \hbar\partial_\tau \hat{\psi}_\downarrow^\dagger(\mathbf{r},\tau) &= [\hat{H}_{BCS}, \hat{\psi}_\downarrow^\dagger(\mathbf{r},\tau)]. \end{aligned} \tag{3.47}$$

Knowing that $[\hat{H}, \hat{A}] = -[\hat{A}, \hat{H}]$ and using equations (3.33) and (3.34) these equations of motion become

$$\hbar\partial_\tau \begin{pmatrix} \psi_\uparrow(\mathbf{r},\tau) \\ \psi_\downarrow^\dagger(\mathbf{r},\tau) \end{pmatrix} = \begin{pmatrix} -\xi_\mathbf{r} & -\Delta(\mathbf{r}) \\ -\Delta^*(\mathbf{r}) & \xi_\mathbf{r}^* \end{pmatrix} \begin{pmatrix} \psi_\uparrow(\mathbf{r},\tau) \\ \psi_\downarrow^\dagger(\mathbf{r},\tau) \end{pmatrix}, \tag{3.48}$$

where the Bogoliubov-de Gennes matrix is clearly seen.

3.3.2 Green functions formalism

Now, we introduce the corresponding Green function for the differential equation above. It is

$$\mathcal{G}(\mathbf{r}\tau_1, \mathbf{r}\tau_2) \equiv -\frac{1}{\hbar}\langle T_\tau[\psi_\uparrow(\mathbf{r}\tau_1)\psi_\uparrow^\dagger(\mathbf{r}'\tau_2)]\rangle. \tag{3.49}$$

Where T_τ is the time ordering operator for the imaginary time. It works as

$$T_\tau[A(\tau_1)B(\tau_2)] = \begin{cases} A(\tau_1)B(\tau_2) \text{ , if } \tau_1 > \tau_2, \\ -B(\tau_2)A(\tau_1) \text{ , if } \tau_2 > \tau_1. \end{cases} \tag{3.50}$$

We can use the Heaviside step function θ to express the Green function using

$$T_\tau[\psi_\uparrow(\mathbf{r}\tau_1)\psi_\uparrow^\dagger(\mathbf{r}'\tau_2)] = \theta(\tau_1-\tau_2)\psi_\uparrow(\mathbf{r}\tau_1)\psi_\uparrow^\dagger(\mathbf{r}'\tau_2) - \theta(\tau_2-\tau_1)\psi_\uparrow^\dagger(\mathbf{r}'\tau_2)\psi_\uparrow(\mathbf{r}\tau_1).$$

We can see that this is true because when $\tau_1 > \tau_2$ then $\theta(\tau_1-\tau_2) = 1$ and $\theta(\tau_2-\tau_1) = 0$ and when $\tau_1 < \tau_2$ then $\theta(\tau_1-\tau_2) = 0$ and $\theta(\tau_2-\tau_1) = 1$. We do this because we know the derivative of the Heaviside step function which is

$$\frac{\mathrm{d}\theta(x)}{\mathrm{d}x} = \delta(x). \tag{3.51}$$

Differentiating $\mathcal{G}$ with respect to τ_1 we get

$$\begin{aligned} \hbar\partial_{\tau_1}\mathcal{G} = &-\delta(\tau_1-\tau_2)\langle\psi_\uparrow(\mathbf{r}\tau_1)\psi_\uparrow^\dagger(\mathbf{r}'\tau_2)\rangle \\ &+\frac{1}{\hbar}\theta(\tau_1-\tau_2)\langle\hbar\partial_{\tau_1}\psi_\uparrow(\mathbf{r}\tau_1)\psi_\uparrow^\dagger(\mathbf{r}'\tau_2)\rangle \\ &-\delta(\tau_2-\tau_1)\langle\psi_\uparrow^\dagger(\mathbf{r}'\tau_2)\psi_\uparrow(\mathbf{r}\tau_1)\rangle \\ &-\frac{1}{\hbar}\theta(\tau_2-\tau_1)\langle\hbar\psi_\uparrow^\dagger(\mathbf{r}'\tau_2)\partial_{\tau_1}\psi_\uparrow(\mathbf{r}\tau_1)\rangle. \end{aligned}$$

We can see that this expression can be written as

$$\hbar\partial_{\tau_1}\mathcal{G}(\mathbf{r}\tau_1,\mathbf{r}'\tau_2) = -\delta(\tau_1-\tau_2)\langle\Big[\psi_\uparrow(\mathbf{r}\tau_1)\psi_\uparrow^\dagger(\mathbf{r}'\tau_2)\Big]_+\rangle$$
$$-\frac{1}{\hbar}\langle T_\tau[\hbar\partial_{\tau_1}(\psi_\uparrow(\mathbf{r}\tau_1)\psi_\uparrow^\dagger(\mathbf{r}'\tau_2)]\rangle.$$

From the anti-commutation rules for fermionic field operators we know that

$$\Big[\psi_\sigma(\mathbf{r}\tau_1)\psi_{\sigma'}^\dagger(\mathbf{r}'\tau_2)\Big]_+ = \delta(\tau_1-\tau_2)\delta(\mathbf{r}-\mathbf{r}')\delta_{\sigma,\sigma'}. \tag{3.52}$$

Then we can write

$$\hbar\partial_{\tau_1}\mathcal{G}(\mathbf{r}\tau_1,\mathbf{r}'\tau_2) = -\delta(\tau_1-\tau_2)\delta(\mathbf{r}-\mathbf{r}')$$
$$-\frac{1}{\hbar}\langle T_\tau[\hbar\partial_{\tau_1}(\psi_\uparrow(\mathbf{r}\tau_1)\psi_\uparrow^\dagger(\mathbf{r}'\tau_2)]\rangle.$$

From the Heisenberg equations of motions for the fermionic field operators we know that

$$\hbar\partial_\tau\psi_\uparrow(\mathbf{r}\tau) = -\xi_\mathbf{r}\psi_\uparrow(\mathbf{r}\tau) - \Delta(\mathbf{r})\psi_\downarrow^\dagger(\mathbf{r}\tau). \tag{3.53}$$

Putting everything together we have that

$$\hbar\partial_{\tau_1}\mathcal{G}(\mathbf{r}\tau_1,\mathbf{r}'\tau_2) = \frac{1}{\hbar}\xi_\mathbf{r}\langle T_\tau[\psi_\uparrow(\mathbf{r}\tau_1)\psi_\uparrow^\dagger(\mathbf{r}'\tau_2)]\rangle$$
$$+\frac{1}{\hbar}\Delta(\mathbf{r})\langle T_\tau[\psi_\downarrow^\dagger(\mathbf{r}\tau_1)\psi_\uparrow^\dagger(\mathbf{r}'\tau_2)]\rangle$$
$$-\delta(\mathbf{r}-\mathbf{r}')\delta(\tau_1-\tau_2).$$

Now we are led to introduce a new Green Function

$$\widetilde{\mathcal{F}}(\mathbf{r}\tau_1,\mathbf{r}'\tau_2) \equiv -\frac{1}{\hbar}\langle T_\tau[\psi_\downarrow^\dagger(\mathbf{r}\tau_1)\psi_\uparrow^\dagger(\mathbf{r}'\tau_2)]\rangle, \tag{3.54}$$

such that

$$\hbar\partial_{\tau_1}\mathcal{G}(\mathbf{r}\tau_1,\mathbf{r}'\tau_2) = -\xi_\mathbf{r}\mathcal{G}(\mathbf{r}\tau_1,\mathbf{r}'\tau_2) - \Delta(\mathbf{r})\widetilde{\mathcal{F}}(\mathbf{r}\tau_1,\mathbf{r}'\tau_2)$$
$$-\delta(\mathbf{r}-\mathbf{r}')\delta(\tau_1-\tau_2),$$

or

$$(\hbar\partial_{\tau_1}+\xi_\mathbf{r})\mathcal{G}(\mathbf{r}\tau_1,\mathbf{r}'\tau_2) + \Delta(\mathbf{r})\widetilde{\mathcal{F}}(\mathbf{r}\tau_1,\mathbf{r}'\tau_2) = -\delta(\mathbf{r}-\mathbf{r}')\delta(\tau_1-\tau_2). \tag{3.55}$$

We use the same procedure and differentiate $\widetilde{\mathcal{F}}(\mathbf{r}\tau_1,\mathbf{r}'\tau_2)$ with respect to imaginary time. We obtain

$$\hbar\partial_{\tau_1}\widetilde{\mathcal{F}}(\mathbf{r}\tau_1,\mathbf{r}'\tau_2) = \xi_\mathbf{r}^*\widetilde{\mathcal{F}}(\mathbf{r}\tau_1,\mathbf{r}'\tau_2) - \Delta^*(\mathbf{r})\mathcal{G}(\mathbf{r}\tau_1,\mathbf{r}'\tau_2),$$

or

$$(\hbar\partial_{\tau_1}-\xi_\mathbf{r}^*)\widetilde{\mathcal{F}}(\mathbf{r}\tau_1,\mathbf{r}'\tau_2) + \Delta^*(\mathbf{r})\mathcal{G}(\mathbf{r}\tau_1,\mathbf{r}'\tau_2) = 0. \tag{3.56}$$

It is convenient to introduce two more Green functions

$$\widetilde{\mathcal{G}}(\mathbf{r}\tau_1, \mathbf{r}'\tau_2) \equiv -\frac{1}{\hbar}\langle T_\tau[\psi_\downarrow^\dagger(\mathbf{r}\tau_1)\psi_\downarrow(\mathbf{r}'\tau_2)]\rangle, \tag{3.57}$$

and

$$\mathcal{F}(\mathbf{r}\tau_1, \mathbf{r}'\tau_2) \equiv -\frac{1}{\hbar}\langle T_\tau[\psi_\uparrow(\mathbf{r}\tau_1)\psi_\downarrow(\mathbf{r}'\tau_2)]\rangle. \tag{3.58}$$

The equation of motion for these Green functions are simply

$$\begin{aligned}\hbar\partial_{\tau_1}\widetilde{\mathcal{G}}(\mathbf{r}\tau_1, \mathbf{r}'\tau_2) &= -\delta(\mathbf{r}-\mathbf{r}')\delta(\tau_1-\tau_2)\\ &\quad+\xi_\mathbf{r}^*\widetilde{\mathcal{G}}(\mathbf{r}\tau_1, \mathbf{r}'\tau_2)\\ &\quad-\Delta^*(\mathbf{r})\mathcal{F}(\mathbf{r}\tau_1, \mathbf{r}'\tau_2),\end{aligned}$$

we organize this equation as

$$(\hbar\partial_{\tau_1}-\xi_\mathbf{r}^*)\widetilde{\mathcal{G}}(\mathbf{r}\tau_1, \mathbf{r}'\tau_2)+\Delta^*(\mathbf{r})\mathcal{F}(\mathbf{r}\tau_1, \mathbf{r}'\tau_2) = -\hbar\delta(\mathbf{r}-\mathbf{r}')\delta(\tau_1-\tau_2).$$

And

$$\hbar\partial_{\tau_1}\widetilde{\mathcal{F}}(\mathbf{r}\tau_1, \mathbf{r}'\tau_2) = -\xi_\mathbf{r}\widetilde{\mathcal{F}}(\mathbf{r}\tau_1, \mathbf{r}'\tau_2) - \Delta(\mathbf{r})\widetilde{\mathcal{G}}(\mathbf{r}\tau_1, \mathbf{r}'\tau_2),$$

or

$$(\hbar\partial_{\tau_1}+\xi_\mathbf{r})\widetilde{\mathcal{F}}(\mathbf{r}\tau_1, \mathbf{r}'\tau_2)+\Delta(\mathbf{r})\widetilde{\mathcal{G}}(\mathbf{r}\tau_1, \mathbf{r}'\tau_2) = 0. \tag{3.59}$$

Let us organize these 4 equations in a more visible pleasing way as

$$\begin{cases}(\hbar\partial_{\tau_1}+\xi_\mathbf{r})\mathcal{G}(\mathbf{r}\tau_1, \mathbf{r}'\tau_2)+\Delta(\mathbf{r})\widetilde{\mathcal{F}}(\mathbf{r}\tau_1, \mathbf{r}'\tau_2) = -\delta(\mathbf{r}-\mathbf{r}')\delta(\tau_1-\tau_2),\\ (\hbar\partial_{\tau_1}-\xi_\mathbf{r}^*)\widetilde{\mathcal{G}}(\mathbf{r}\tau_1, \mathbf{r}'\tau_2)+\Delta^*(\mathbf{r})\mathcal{F}(\mathbf{r}\tau_1, \mathbf{r}'\tau_2) = -\delta(\mathbf{r}-\mathbf{r}')\delta(\tau_1-\tau_2),\end{cases} \tag{3.60}$$

$$\begin{cases}(\hbar\partial_{\tau_1}-\xi_\mathbf{r}^*)\widetilde{\mathcal{F}}(\mathbf{r}\tau_1, \mathbf{r}'\tau_2)+\Delta^*(\mathbf{r})\mathcal{G}(\mathbf{r}\tau_1, \mathbf{r}'\tau_2) = 0,\\ (\hbar\partial_{\tau_1}+\xi_\mathbf{r})\mathcal{F}(\mathbf{r}\tau_1, \mathbf{r}'\tau_2)+\Delta(\mathbf{r})\widetilde{\mathcal{G}}(\mathbf{r}\tau_1, \mathbf{r}'\tau_2) = 0.\end{cases} \tag{3.61}$$

These however are not the final format of these equations that we want to use. We will perform a Fourier transform from imaginary time to frequency.

3.3.3 Some properties of finite temperature Green functions

Consider the imaginary-time boundary condition for the Green functions. We will see that they have a period of $2\beta\hbar$. To get this result, first we will demonstrate that the Green function will depend only on the difference $\tau_1 - \tau_2$ as follows

$$\mathcal{G}(\mathbf{r}\tau_1, \mathbf{r}'\tau_2) = -\frac{1}{\hbar\,\mathrm{Tr}\,e^{-\beta\hat{H}_{BCS}}}\,\mathrm{Tr}\left(e^{-\beta\hat{H}_{BCS}}T_\tau[\psi_\uparrow(\mathbf{r}\tau_1)\psi_\uparrow^\dagger(\mathbf{r}'\tau_2)]\right).$$

Supose that $\tau_1 > \tau_2$ (below $\hat{K} = \hat{H}_{BCS}$) and so

$$\begin{aligned}\mathcal{G}(\mathbf{r}\tau_1, \mathbf{r}'\tau_2) &= -\frac{1}{\hbar\,\mathrm{Tr}\,e^{-\beta\hat{K}}}\,\mathrm{Tr}\left(e^{-\beta\hat{K}}\psi_\uparrow(\mathbf{r}\tau_1)\psi_\uparrow^\dagger(\mathbf{r}'\tau_2)\right)\\ &= -\frac{1}{\hbar\,\mathrm{Tr}\,e^{-\beta\hat{K}}}\,\mathrm{Tr}\left(e^{-\beta\hat{K}}e^{\hat{K}\frac{\tau_1}{\hbar}}\psi_\uparrow(\mathbf{r})e^{-\hat{K}\frac{\tau_1}{\hbar}}e^{\hat{K}\frac{\tau_2}{\hbar}}\psi_\uparrow^\dagger(\mathbf{r}')e^{-\hat{K}\frac{\tau_2}{\hbar}}\right).\end{aligned}$$

Under the trace we can rearrange these operators.

$$\begin{aligned}\mathcal{G}(\mathbf{r}\tau_1,\mathbf{r}'\tau_2) &= -\frac{1}{\hbar\,\mathrm{Tr}\,e^{-\beta\hat{K}}}\,\mathrm{Tr}\left(e^{-\beta\hat{K}}e^{\hat{K}\frac{\tau_1-\tau_2}{\hbar}}\psi_\uparrow(\mathbf{r})e^{-\hat{K}\frac{\tau_1-\tau_2}{\hbar}}\psi^\dagger_\uparrow(\mathbf{r}')\right)\\ &= -\frac{1}{\hbar\,\mathrm{Tr}\,e^{-\beta\hat{K}}}\,\mathrm{Tr}\left(e^{-\beta\hat{K}}\psi_\uparrow(\mathbf{r}\tau)\psi^\dagger_\uparrow(\mathbf{r}')\right)\end{aligned}$$

Therefore

$$\mathcal{G}(\mathbf{r}\tau_1,\mathbf{r}'\tau_2) = \mathcal{G}(\mathbf{r},\mathbf{r}',\tau), \tag{3.62}$$

where $\tau = \tau_1 - \tau_2$. Now let us demonstrate the periodicity of the Green functions. First we explicitly write

$$\mathcal{G}(\mathbf{r},\mathbf{r}',\tau>0) = -\frac{1}{\hbar\,\mathrm{Tr}\,e^{-\beta\hat{K}}}\,\mathrm{Tr}\left(e^{-\beta\hat{K}}\psi_\uparrow(\mathbf{r}\tau)\psi^\dagger_\uparrow(\mathbf{r}')\right).$$

We will show that

$$\mathcal{G}(\mathbf{r},\mathbf{r}',\tau<0) = -\mathcal{G}(\mathbf{r},\mathbf{r}',\tau+\beta\hbar), \tag{3.63}$$

and by the same procedure we will get

$$\mathcal{G}(\mathbf{r},\mathbf{r}',\tau>0) = -\mathcal{G}(\mathbf{r},\mathbf{r}',\tau-\beta\hbar). \tag{3.64}$$

Suppose that $-\beta\hbar < \tau < 0$ and we do the following

$$\begin{aligned}\mathcal{G}(\mathbf{r},\mathbf{r}',\tau<0) =& -\frac{1}{\hbar\,\mathrm{Tr}\,e^{-\beta\hat{K}}}\,\mathrm{Tr}\left(e^{-\beta\hat{K}}T_\tau[\psi_\uparrow(\mathbf{r}\tau)\psi^\dagger_\uparrow(\mathbf{r}')]\right).\\ =&\frac{1}{\hbar\,\mathrm{Tr}\,e^{-\beta\hat{K}}}\,\mathrm{Tr}\left(e^{-\beta\hat{K}}\psi^\dagger_\uparrow(\mathbf{r}')\psi_\uparrow(\mathbf{r}\tau)\right).\\ =&\frac{1}{\hbar\,\mathrm{Tr}\,e^{-\beta\hat{K}}}\,\mathrm{Tr}\left(e^{-\beta\hat{K}}\psi^\dagger_\uparrow(\mathbf{r}')e^{\hat{K}\frac{\tau}{\hbar}}\psi_\uparrow(\mathbf{r})e^{-\hat{K}\frac{\tau}{\hbar}}\right),\\ =&\frac{1}{\hbar\,\mathrm{Tr}\,e^{-\beta\hat{K}}}\,\mathrm{Tr}\left(e^{-\beta\hat{K}}e^{-\beta\hat{K}}e^{\beta\hat{K}}\psi^\dagger_\uparrow(\mathbf{r}')e^{\hat{K}\frac{\tau}{\hbar}}\psi_\uparrow(\mathbf{r})e^{-\hat{K}\frac{\tau}{\hbar}}\right),\\ =&\frac{1}{\hbar\,\mathrm{Tr}\,e^{-\beta\hat{K}}}\,\mathrm{Tr}\left(e^{-\beta\hat{K}}\psi^\dagger_\uparrow(\mathbf{r}')e^{\hat{K}\frac{\tau+\hbar\beta}{\hbar}}\psi_\uparrow(\mathbf{r})e^{-\hat{K}\frac{\tau+\beta\hbar}{\hbar}}\right)\\ =&\frac{1}{\hbar\,\mathrm{Tr}\,e^{-\beta\hat{K}}}\,\mathrm{Tr}\left(e^{-\beta\hat{K}}\psi^\dagger_\uparrow(\mathbf{r}')\psi_\uparrow(\mathbf{r},\tau+\beta\hbar)\right).\\ =&\frac{1}{\hbar\,\mathrm{Tr}\,e^{-\beta\hat{K}}}\,\mathrm{Tr}\left(e^{-\beta\hat{K}}\psi_\uparrow(\mathbf{r},\tau+\beta\hbar)\psi^\dagger_\uparrow(\mathbf{r}')\right)\\ =&-\mathcal{G}(\mathbf{r},\mathbf{r}',\tau+\beta\hbar). \qquad\qquad \tau+\beta\hbar>0\end{aligned}$$

So, we can see that the Temperature Green functions with imaginary time are define for $-\beta\hbar < \tau < \beta\hbar$. This finite range for the imaginary time has a important consequence. To see this let us make a Fourier transformation in τ

$$\mathcal{G}(\mathbf{r},\mathbf{r}',\tau) = \frac{1}{\beta\hbar}\sum_\omega e^{-i\omega\tau}\mathcal{G}_\omega(\mathbf{r},\mathbf{r}'), \tag{3.65}$$

The inverse transformation is

$$\mathcal{G}_\omega(\mathbf{r},\mathbf{r}') = \frac{1}{2}\int_{-\beta\hbar}^{\beta\hbar} e^{i\omega_n\tau}\mathcal{G}(\mathbf{r},\mathbf{r}',\tau)d\tau \tag{3.66}$$

Let us prove that ω only takes discrete values and that they are different based on the statistics of the particle we are dealing with. Consider that

$$\begin{aligned}\mathcal{G}_\omega(\mathbf{r},\mathbf{r}') =&\frac{1}{2}\int_0^{\beta\hbar} e^{i\omega\tau}\mathcal{G}(\mathbf{r},\mathbf{r}',\tau)d\tau + \frac{1}{2}\int_{-\beta\hbar}^{0} e^{i\omega_n\tau}\mathcal{G}(\mathbf{r},\mathbf{r}',\tau)d\tau,\\ =&\frac{1}{2}\int_0^{\beta\hbar} e^{i\omega\tau}\mathcal{G}(\mathbf{r},\mathbf{r}',\tau)d\tau - \frac{1}{2}\int_{-\beta\hbar}^{0} e^{i\omega_n\tau}\mathcal{G}(\mathbf{r},\mathbf{r}'\tau+\beta\hbar)d\tau.\end{aligned}$$

We make the following change of variables: $\tau \to \tau + \beta\hbar$ and we get

$$\mathcal{G}_\omega(\mathbf{r},\mathbf{r}') = \frac{1}{2}\int_0^{\beta\hbar} e^{i\omega\tau}\mathcal{G}(\mathbf{r},\mathbf{r}',\tau)d\tau - \frac{1}{2}\int_0^{\beta\hbar} e^{i\omega(\tau-\beta\hbar)}\mathcal{G}(\mathbf{r},\mathbf{r}'\tau)d\tau,$$

$$\mathcal{G}_\omega(\mathbf{r},\mathbf{r}') = \frac{1}{2}\Big(1 \mp e^{i\omega\beta\hbar}\Big)\int_0^{\beta\hbar} e^{i\omega\tau}\mathcal{G}(\mathbf{r},\mathbf{r}'\tau)d\tau. \tag{3.67}$$

To have a nonzero solution we need that

$$\omega = \frac{(2n+1)\pi}{\beta\hbar}.$$

Therefore, we can clearly see that this frequency only takes discrete values as a direct consequence of the limited range of the imaginary time to which the Green functions are defined. We called it Matsubara frequency.

3.3.4 Matsubara Green Functions

The Green function in terms of the Matsubara frequency is just called Matsubara Green function. We will work with these functions. Performing a Fourier transformation on equations (3.60) and (3.61) we will get

$$\begin{cases}(-i\hbar\omega+\xi_{\mathbf{r}})\mathcal{G}_\omega(\mathbf{r},\mathbf{r}') + \Delta(\mathbf{r})\widetilde{\mathcal{F}}_\omega(\mathbf{r},\mathbf{r}') = -\delta(\mathbf{r}-\mathbf{r}'),\\ (-i\hbar\omega-\xi^*_{\mathbf{r}})\widetilde{\mathcal{G}}_\omega(\mathbf{r},\mathbf{r}') + \Delta^*(\mathbf{r})\mathcal{F}_\omega(\mathbf{r},\mathbf{r}') = -\delta(\mathbf{r}-\mathbf{r}'),\end{cases} \tag{3.68}$$

$$\begin{cases}(-i\hbar\omega-\xi^*_{\mathbf{r}})\widetilde{\mathcal{F}}_\omega(\mathbf{r},\mathbf{r}') + \Delta^*(\mathbf{r})\mathcal{G}_\omega(\mathbf{r},\mathbf{r}') = 0,\\ (-i\hbar\omega+\xi_{\mathbf{r}})\mathcal{F}_\omega(\mathbf{r},\mathbf{r}') + \Delta(\mathbf{r})\widetilde{\mathcal{G}}_\omega(\mathbf{r},\mathbf{r}') = 0.\end{cases} \tag{3.69}$$

We can express them in a more elegant way. It is

$$\left\{\begin{pmatrix} i\hbar\omega & 0\\ 0 & i\hbar\omega\end{pmatrix} - \begin{pmatrix}\xi_{\mathbf{r}} & \Delta(\mathbf{r})\\ \Delta^*(\mathbf{r}) & -\xi^*_{\mathbf{r}}\end{pmatrix}\right\}\begin{pmatrix}\mathcal{G}_\omega(\mathbf{r},\mathbf{r}') & \mathcal{F}_\omega(\mathbf{r},\mathbf{r}')\\ \widetilde{\mathcal{F}}_\omega(\mathbf{r},\mathbf{r}') & \widetilde{\mathcal{G}}\omega(\mathbf{r},\mathbf{r}')\end{pmatrix} = \delta(\mathbf{r}-\mathbf{r}')\check{1}_2. \tag{3.70}$$

Where, $\check{1}_2$ is the 2x2 unit matrix.

Using the matrix notations, we can further rewrite the Green function equations, called Gor'kov-Nambu equations:

$$i\hbar\omega\check{\mathcal{G}}_\omega = \check{1}_2 + \check{\xi}\check{\mathcal{G}}_\omega + \check{\Delta}\check{\mathcal{G}}_\omega, \tag{3.71}$$

with

$$\check{\xi} = \begin{pmatrix} \hat{\xi} & 0 \\ 0 & -\hat{\xi}^* \end{pmatrix}, \quad \check{\Delta} = \begin{pmatrix} 0 & \hat{\Delta} \\ \hat{\Delta}^* & 0 \end{pmatrix}. \tag{3.72}$$

The matrix elements of the operators $\hat{\xi}$ and $\hat{\Delta}$ in the single-particle Hilbert space are given by

$$\hat{\xi} = \langle \mathbf{r} | \, \hat{\xi} \, | \mathbf{r}' \rangle = \delta(\mathbf{r} - \mathbf{r}')\xi_{\mathbf{r}} \quad \hat{\Delta} = \langle \mathbf{r} | \, \hat{\Delta} \, | \mathbf{r}' \rangle = \Delta(\mathbf{r})\delta(\mathbf{r} - \mathbf{r}').$$

We also introduce

$$\check{\mathcal{G}}_\omega = \begin{pmatrix} \hat{\mathcal{G}}_\omega & \hat{\mathcal{F}}_\omega \\ \hat{\widetilde{\mathcal{F}}}_\omega & \hat{\widetilde{\mathcal{G}}}_\omega \end{pmatrix}, \tag{3.73}$$

with the operators $\hat{\mathcal{G}}_\omega, \hat{\widetilde{\mathcal{G}}}_\omega, \hat{\mathcal{F}}_\omega$, and $\hat{\widetilde{\mathcal{F}}}_\omega$ defined as

$$\begin{aligned} \langle \mathbf{r} | \, \hat{\mathcal{G}}_\omega \, | \mathbf{r}' \rangle &= \mathcal{G}_\omega(\mathbf{r}, \mathbf{r}'), \langle \mathbf{r} | \, \hat{\widetilde{\mathcal{G}}}_\omega \, | \mathbf{r}' \rangle = \widetilde{\mathcal{F}}_\omega(\mathbf{r}, \mathbf{r}'), \\ \langle \mathbf{r} | \, \hat{\mathcal{F}}_\omega \, | \mathbf{r}' \rangle &= \mathcal{F}_\omega(\mathbf{r}, \mathbf{r}'), \langle \mathbf{r} | \, \hat{\widetilde{\mathcal{F}}}_\omega \, | \mathbf{r}' \rangle = \widetilde{\mathcal{F}}_\omega(\mathbf{r}, \mathbf{r}'). \end{aligned} \tag{3.74}$$

To solve equation (3.71) we introduce $\mathcal{G}_\omega^{(0)}(\mathbf{r}, \mathbf{r}')$, the Green function for the normal state in the same magnetic field. The corresponding equation reads

$$(i\hbar\omega - \check{\xi})\check{\mathcal{G}}_\omega^{(0)} = \check{1}_2, \tag{3.75}$$

where

$$\check{\mathcal{G}}_\omega^{(0)} = \begin{pmatrix} \hat{\mathcal{G}}_\omega^{(0)} & 0 \\ 0 & \hat{\widetilde{\mathcal{G}}}_\omega^{(0)} \end{pmatrix}.$$

We can, therefore, write

$$\check{\mathcal{G}}_\omega^{(0)} = (i\hbar\omega - \check{\xi})^{-1}. \tag{3.76}$$

Then equation (3.71) can be written as

$$\check{\mathcal{G}}_\omega = \check{\mathcal{G}}_\omega^{(0)} + \check{\mathcal{G}}_\omega^{(0)} \check{\Delta} \check{\mathcal{G}}_\omega. \tag{3.77}$$

From this equation in the matrix form we can get the relations

$$\begin{aligned} \mathcal{F}_\omega &= \mathcal{G}_\omega^{(0)} \Delta^* \widetilde{\mathcal{G}}_\omega \\ \widetilde{\mathcal{G}}_\omega &= \widetilde{\mathcal{G}}_\omega^{(0)} + \widetilde{\mathcal{G}}_\omega^{(0)} \Delta^* \mathcal{F}_\omega \end{aligned} \tag{3.78}$$

Using this couple equations we can get the following expression

$$\widetilde{\mathcal{G}}_\omega = \widetilde{\mathcal{G}}_\omega^{(0)} + \widetilde{\mathcal{G}}_\omega^{(0)} \Delta^* \mathcal{G}_\omega^{(0)} \Delta \widetilde{\mathcal{G}}_\omega \tag{3.79}$$

Now we take this and substitute on the equation for $\widetilde{\mathcal{F}}_\omega$ as follows

$$\mathcal{F}_\omega = \mathcal{G}_\omega^{(0)} \Delta \widetilde{\mathcal{G}}_\omega^{(0)} + \mathcal{G}_\omega^{(0)} \Delta \widetilde{\mathcal{G}}_\omega^{(0)} \Delta^* \mathcal{G}_\omega^{(0)} \Delta \widetilde{\mathcal{G}}_\omega \tag{3.80}$$

Repeating this procedure we obtain

$$\mathcal{F}_\omega = \mathcal{G}^{(0)}_\omega \Delta \widetilde{\mathcal{G}}^{(0)}_\omega + \mathcal{G}^{(0)}_\omega \Delta \widetilde{\mathcal{G}}^{(0)}_\omega \Delta^* \mathcal{G}^{(0)}_\omega \Delta \widetilde{\mathcal{G}}^{(0)}_\omega + \mathcal{G}^{(0)}_\omega \Delta \widetilde{\mathcal{G}}^{(0)}_\omega \Delta^* \mathcal{G}^{(0)}_\omega \Delta \widetilde{\mathcal{G}}^{(0)}_\omega \Delta^* \mathcal{G}^{(0)}_\omega \Delta \widetilde{\mathcal{G}}_\omega.$$

This equation can be truncated to a desired order, which yields a nonlinear integral equation. For our present purposes we will only keep the first two terms. In integral form we have the following equation(pay attention to the rather complicated dependence of the Green functions inside the integral)

$$\mathcal{F}_\omega(\mathbf{r},\mathbf{r}') = \int d\mathbf{y} \mathcal{G}^{(0)}_\omega(\mathbf{r},\mathbf{y})\Delta(\mathbf{y})\widetilde{\mathcal{G}}^{(0)}_\omega(\mathbf{y},\mathbf{r}) \tag{3.81}$$

$$+ \int d\mathbf{y}_1 d\mathbf{y}_2 d\mathbf{y}_3 \mathcal{G}^{(0)}_\omega(\mathbf{r},\mathbf{y}_1)\Delta(\mathbf{y}_1)\widetilde{\mathcal{G}}^{(0)}_\omega(\mathbf{y}_1,\mathbf{y}_2)\Delta^*(\mathbf{y}_2)\mathcal{G}^{(0)}_\omega(\mathbf{y}_2,\mathbf{y}_3)\Delta(\mathbf{y}_3)\widetilde{\mathcal{G}}^{(0)}_\omega(\mathbf{y}_3,\mathbf{r}).$$

The last step before calculating the Ginzburg-Landau equation is to express the order parameter in terms of the Green function. Remember that

$$\Delta(\mathbf{r}) = g\langle \hat{\psi}_\uparrow(\mathbf{r})\hat{\psi}_\downarrow(\mathbf{r})\rangle, \tag{3.82}$$

and that

$$\mathcal{F}(\mathbf{r},\mathbf{r}',\tau) = -\frac{1}{\hbar}\langle T_\tau[\psi_\uparrow(\mathbf{r}\tau)\psi_\downarrow(\mathbf{r}'0)]\rangle. \tag{3.83}$$

To express the order parameter we do the following

$$\Delta(\mathbf{r}) = -g\hbar \lim_{\tau\to 0^+} \mathcal{F}(\mathbf{r},\mathbf{r},\tau) \tag{3.84}$$

Observe that the limit is τ going to zero from the positive side. This ensures that $\tau_1 > \tau_2$ and we get the correct relation. Now we wish to use Matsubara Green functions. The order parameters is expressed by

$$\Delta(\mathbf{r}) = -\frac{g}{\beta} \lim_{\tau\to 0^+} \sum_\omega e^{-i\omega\tau}\mathcal{F}_\omega(\mathbf{r},\mathbf{r}) \tag{3.85}$$

From here onward we will use $k_B = 1$ Taking the expression for $\mathcal{F}_\omega$ we get

$$\begin{aligned}\Delta(\mathbf{r}) &= \int d\mathbf{y} K_a(\mathbf{r},\mathbf{y})\Delta(\mathbf{y}) \\ &+ \int d\mathbf{y}_1 d\mathbf{y}_2 d\mathbf{y}_3 K_b(\mathbf{r},\mathbf{y}_1,\mathbf{y}_2,\mathbf{y}_3)\Delta(\mathbf{y}_1)\Delta(\mathbf{y}_2)^*\Delta(\mathbf{y}_3).\end{aligned} \tag{3.86}$$

The kernels of the integrals are

$$K_a(\mathbf{r},\mathbf{y}) = -gT \lim_{\tau\to 0^+} \sum_\omega e^{-i\omega\tau}\mathcal{G}^{(0)}_\omega(\mathbf{r},\mathbf{y})\widetilde{\mathcal{G}}^{(0)}_\omega(\mathbf{y},\mathbf{r}),$$

and,

$$K_b = -gT \lim_{\tau\to 0^+} \sum_\omega e^{-i\omega\tau}\mathcal{G}^{(0)}_\omega(\mathbf{r},\mathbf{y}_1)\widetilde{\mathcal{G}}^{(0)}_\omega(\mathbf{y}_1,\mathbf{y}_2)\mathcal{G}^{(0)}_\omega(\mathbf{y}_2,\mathbf{y}_3)\widetilde{\mathcal{G}}^{(0)}_\omega(\mathbf{y}_3,\mathbf{r}).$$

The equation for the order parameter can be converted into a nonlinear partial differential equation by (odd powers of the gradient don't contribute in the final calculation)

$$\Delta(\mathbf{y}) = \Delta(\mathbf{r}) + \frac{1}{2}\big((\mathbf{r}-\mathbf{y})\cdot\boldsymbol{\nabla}\big)^2\Delta(\mathbf{r}) + \cdots \tag{3.87}$$

if we assume that we are close to the critical temperature. This makes sense because the order parameter becomes smaller the close we get to the critical temperature. Therefore, the gap equation will be

$$\begin{aligned}\Delta(\mathbf{r}) =&\Delta(\mathbf{r})\int d\mathbf{y}K_a(\mathbf{r},\mathbf{y}) + \frac{1}{2}\boldsymbol{\nabla}^2\Delta(\mathbf{r})\int d\mathbf{y}K_a(\mathbf{r},\mathbf{y})(\mathbf{r}-\mathbf{y})^2+ \\ &+|\Delta|^2\Delta(\mathbf{r})\int d\mathbf{y}_1 d\mathbf{y}_2 d\mathbf{y}_3 K_b(\mathbf{r},\mathbf{y}_1,\mathbf{y}_2,\mathbf{y}_3).\end{aligned} \tag{3.88}$$

Let us use the following notation

$$\frac{\Delta(\mathbf{r})}{g} = a_1\Delta(\mathbf{r}) + a_2\boldsymbol{\nabla}^2\Delta + b_1|\Delta|^2\Delta(\mathbf{r}). \tag{3.89}$$

The terms a_i are related to the integrals with kernel K_a and the term b_1 are related to the integral with kernel K_b. We say that a_1 is the local term, a_2 is the term proportional to the square gradient and b_1 is the term proportional to Δ^3. Each one of the integrals will give the 3 Ginzburg-Landau coefficients that are present on equation (3.9). To calculate these integrals we need to know the form of the normal-state Green function. Here, we will only calculate for zero magnetic field with plane wave approximation so we can set the vector potential to zero. From equation (3.76) we have

$$\mathcal{G}^{(0)}_\omega(\mathbf{r},\mathbf{y}) = \int \frac{d\mathbf{k}}{(2\pi)^3}\frac{e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{y})}}{i\hbar\omega - \xi_\mathbf{k}}, \tag{3.90}$$

$$\widetilde{\mathcal{G}}^{(0)}_\omega(\mathbf{r},\mathbf{y}) = \int \frac{d\mathbf{k}}{(2\pi)^3}\frac{e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{y})}}{i\hbar\omega + \xi_\mathbf{k}}. \tag{3.91}$$

Here $\xi_\mathbf{k} = \frac{\hbar^2k^2}{2m} - \mu$ is the single particle energy measured from the chemical potential.

3.3.5 Systematic expansion in small deviation from the critical temperature

Before we dive into the calculation of each of the Ginzburg-Landau coefficient it is productive first to take a step back and look at the temperature dependence of these elements. Each integral kernel is directly dependent on temperature but they also depend on the Matsubara frequency which in turn is dependent on temperature. If we take this temperature and simply do the calculations we will run into complications. In fact, we don't need to perform the calculations for an arbitrary temperature. We already know that superconductivity starts at a very specific temperature called critical temperature.

We are interest in the system near this temperature. So, for the Standard Ginzburg-Landau equation we will introduce a parameter which becomes small near the critical temperature and can be used to produce a single-small-parameter series expansion of the gap equation[8]. It is

$$\tau = 1 - \frac{T}{T_c}. \tag{3.92}$$

When $T \to T_c$, the order parameter decays as $\Delta \propto \tau^{1/2}$ and $\boldsymbol{\nabla}\Delta \propto \tau^{1/2}$. By using this parameter we will be able to collect the relevant quantities for our present endeavor but it will also empower us to go beyond the Standard Ginzburg-Landau equations if needed. For now we will calculate first terms up to $\tau^{1/2}$ which will give us a equation for the critical temperature. After that we will collect terms up to $\tau^{3/2}$ which will give us the Standard Ginzburg-Landau equation. If we would go up to $\tau^{5/2}$ we will obtain the so called Extended Ginzburg Landau equation. This systematic expansion of the gap equation in τ can be facilitated by introducing the scaling transformation for the order parameter and the spatial derivatives as

$$\begin{aligned} \Delta &= \tau^{1/2}\bar{\Delta} \\ \boldsymbol{\nabla} &= \tau^{1/2}\bar{\boldsymbol{\nabla}} \end{aligned}.$$

We obtain

$$\tau^{1/2}\frac{\bar{\Delta}}{g} = a_1\tau^{1/2}\bar{\Delta} + a_2\tau^{3/2}\bar{\boldsymbol{\nabla}}^2\bar{\Delta} + b_1\tau^{3/2}|\bar{\Delta}|^2\bar{\Delta}. \tag{3.93}$$

The solution to the gap equation must also be sought in the form of a series expansion in τ .

$$\bar{\Delta} = \bar{\Delta}_0 + \tau\bar{\Delta}_1 + \cdots$$

Then we write

$$\begin{aligned} \frac{\tau^{1/2}}{g}(\bar{\Delta}_0 + \tau\bar{\Delta}_1) =& a_1(\bar{\Delta}_0 + \tau\bar{\Delta}_1)\tau^{1/2} \\ &+ a_2\bar{\boldsymbol{\nabla}}^2(\bar{\Delta}_0 + \tau\bar{\Delta}_1)\tau^{3/2} \\ &+ b_1|\bar{\Delta}_0 + \tau\bar{\Delta}_1|^2(\bar{\Delta}_0 + \tau\bar{\Delta}_1)\tau^{3/2}. \end{aligned} \tag{3.94}$$

We will keep this in mind because we are going to need this expression.

3.3.6 Calculation of the Ginzburg-Landau coefficients

Now we are going to explicitly calculate the integrals we found. Remember that for each term we have an integration over momenta and a summation over Matsubara frequencies.

TERM PROPORTIONAL TO Δ^3

Using the normal-state Green function we write

$$b_1 = -T \sum_{\omega} \int d\mathbf{y}_1 d\mathbf{y}_2 d\mathbf{y}_3 \frac{d\mathbf{k}}{(2\pi)^3} \frac{e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{y}_1)}}{(i\hbar\omega - \xi_{\mathbf{k}})} \frac{d\mathbf{k}_1}{(2\pi)^3} \frac{e^{i\mathbf{k}_1\cdot(\mathbf{y}_1-\mathbf{y}_2)}}{(i\hbar\omega + \xi_{\mathbf{k}_1})}$$
$$\times \frac{d\mathbf{k}_2}{(2\pi)^3} \frac{e^{i\mathbf{k}_2\cdot(\mathbf{y}_2-\mathbf{y}_3)}}{(i\hbar\omega - \xi_{\mathbf{k}_2})} \frac{d\mathbf{k}_3}{(2\pi)^3} \frac{e^{i\mathbf{k}_3\cdot(\mathbf{y}_3-\mathbf{r})}}{(i\hbar\omega + \xi_{\mathbf{k}_3})}.$$

The exponential doesn't play a part here because the integral converges without any more complications(unfortunately this cannot be said for all of the remaining terms). Some of these integrals will lead to delta functions as follows

$$\begin{aligned} b_1 =& -T \sum_{\omega} \int \frac{d\mathbf{k}}{(2\pi)^3} \frac{d\mathbf{k}_1 d\mathbf{k}_2 d\mathbf{k}_3 \delta(\mathbf{k}_1 - \mathbf{k})\delta(\mathbf{k}_2 - \mathbf{k}_1)\delta(\mathbf{k}_3 - \mathbf{k}_2) e^{i(\mathbf{k}-\mathbf{k}_3)\cdot\mathbf{r}}}{(2\pi)^9 (i\hbar\omega - \xi_{\mathbf{k}})(i\hbar\omega + \xi_{\mathbf{k}_1})(i\hbar\omega - \xi_{\mathbf{k}_2})(i\hbar\omega + \xi_{\mathbf{k}_3})}, \\ =& -T \sum_{\omega} \int \frac{d\mathbf{k}}{(2\pi)^3} \frac{1}{(i\hbar\omega - \xi_{\mathbf{k}})^2} \frac{1}{(i\hbar\omega + \xi_{\mathbf{k}})^2} \\ =& -T \sum_{\omega} \int \frac{d\mathbf{k}}{(2\pi)^3} \frac{1}{(\hbar^2\omega^2 + \xi_{\mathbf{k}})^2}. \end{aligned}$$

We introduce the following approximation consistently to evaluate integrals that are peaked near the Fermi surface. It is

$$\int \frac{d\mathbf{k}}{(2\pi)^3} \cdots \approx N(0) \int d\xi \cdots \tag{3.95}$$

Where, $N(0)$ is the Density of States per spin projection near the Fermi surface and its value is: $N(0) = \frac{mk_F}{2\pi^2\hbar^2}$ and k_F is the Fermi momentum. b_1 then becomes

$$b_1 = -N(0)T \sum_{\omega} \int d\xi \frac{1}{(\hbar^2\omega^2 + \xi^2)^2}. \tag{3.96}$$

By setting $x = \frac{\xi}{\hbar\omega}$ we find

$$b_1 = -N(0)T \sum_{\omega} \frac{dx}{|\hbar\omega|^3} \int_{-\infty}^{\infty} d\xi \frac{1}{(1+x^2)^2}.$$

Realizing that $\sum_{x} |f(x)| = 2 \sum_{x>0} f(x)$, we get

$$b_1 = -2N(0)T \sum_{\omega>0} \frac{1}{(\hbar\omega)^3} \frac{\pi}{2} = -N(0)\pi T \frac{1}{(2\pi T)^3} \sum_{n=0}^{\infty} \frac{1}{(n+1/2)^3},$$

Finally,

$$b_1 = -N(0) \frac{7\zeta(3)}{8\pi^2 T^2}. \tag{3.97}$$

Here ζ is the zeta function. Now, we applied the expansion of the small parameter τ

$$\frac{T_c^2}{T^2} = \frac{1}{(1-\tau)^2} \approx 1 + 2\tau + \mathcal{O}(\tau^2),$$

because τ is small. Since $\Delta^3 \propto \tau^{3/2}$ we need to get the zeroth power of this expansion in τ. We obtain

$$b_1 = -N(0)\frac{7\zeta(3)}{8\pi^2 T_c^2}. \tag{3.98}$$

TERM PROPORTIONAL TO THE SQUARED GRADIENT

This term is given by

$$\frac{1}{2}\int d\mathbf{y} K_a(\mathbf{r},\mathbf{y})(\mathbf{r}-\mathbf{y})^2 = -\frac{T}{2}\sum_{\omega}\int d\mathbf{z}\mathcal{G}_{\omega}^{(0)}(\mathbf{r},\mathbf{r}+\mathbf{z})\widetilde{\mathcal{G}}_{\omega}^{(0)}(\mathbf{r}+\mathbf{z},\mathbf{r})\mathbf{z}^2.$$

Where we made a change of variables: $\mathbf{r}-\mathbf{y}\to\mathbf{z}$. To calculate this integral we need to do a little trick. We take the normal-state Green function and perform a Fourier transform on the coordinates and get the following

$$\frac{1}{i\hbar\omega-\xi_{\mathbf{k}}} = \int d\mathbf{z}\mathcal{G}_{\omega}^{(0)}(\mathbf{r},\mathbf{r}+\mathbf{z})e^{-i\mathbf{k}\cdot\mathbf{z}}. \tag{3.99}$$

Now, we differentiate with respect to the momenta

$$\boldsymbol{\nabla}_{\mathbf{k}}\left(\frac{1}{i\hbar\omega-\xi_{\mathbf{k}}}\right) = \int d\mathbf{z}(-i\mathbf{z})\mathcal{G}_{\omega}^{(0)}(\mathbf{r},\mathbf{r}+\mathbf{z})e^{-i\mathbf{k}\cdot\mathbf{z}}. \tag{3.100}$$

And now we reverse the Fourier transform to obtain

$$\mathbf{z}\mathcal{G}_{\omega}^{(0)}(\mathbf{r},\mathbf{r}+\mathbf{z}) = \int\frac{d\mathbf{k}}{(2\pi)^3}\Big(-\frac{1}{i}\Big)\boldsymbol{\nabla}_{\mathbf{k}}\left(\frac{1}{i\hbar\omega-\xi_{\mathbf{k}}}\right)e^{i\mathbf{k}\cdot\mathbf{z}}. \tag{3.101}$$

In similar fashion for the hole Green function

$$-\mathbf{z}\widetilde{\mathcal{G}}_{\omega}^{(0)}(\mathbf{r}+\mathbf{z},\mathbf{r}) = \int\frac{d\mathbf{k}}{(2\pi)^3}\Big(-\frac{1}{i}\Big)\boldsymbol{\nabla}_{\mathbf{k}}\left(\frac{1}{i\hbar\omega+\xi_{\mathbf{k}}}\right)e^{-i\mathbf{k}\cdot\mathbf{z}}. \tag{3.102}$$

Now, we are able to express the term proportional to the square gradient as follows

$$\begin{aligned}
a_2 =& -\frac{T}{2}\sum_{\omega}\int d\mathbf{z}\mathcal{G}_{\omega}^{(0)}(\mathbf{r},\mathbf{r}+\mathbf{z})\widetilde{\mathcal{G}}_{\omega}^{(0)}(\mathbf{r}+\mathbf{z},\mathbf{r})\mathbf{z}^2\\
=&\frac{T}{2}\sum_{\omega}\int d\mathbf{z}\Big(\mathbf{z}\mathcal{G}_{\omega}^{(0)}(\mathbf{r},\mathbf{r}+\mathbf{z})\Big)\Big(-\mathbf{z}\widetilde{\mathcal{G}}_{\omega}^{(0)}(\mathbf{r}+\mathbf{z},\mathbf{r})\Big)\\
=&\frac{T}{2}\int d\mathbf{z}\frac{d\mathbf{k}}{(2\pi)^3}\frac{d\mathbf{k}'}{(2\pi)^3}\Big(-\frac{1}{i}\Big)\boldsymbol{\nabla}_{\mathbf{k}}\left(\frac{1}{i\hbar\omega-\xi_{\mathbf{k}}}\right)e^{i\mathbf{k}\cdot\mathbf{z}}\Big(-\frac{1}{i}\Big)\boldsymbol{\nabla}_{\mathbf{k}'}\left(\frac{1}{i\hbar\omega+\xi_{\mathbf{k}'}}\right)e^{-i\mathbf{k}'\cdot\mathbf{z}}\\
=&\frac{T}{2}\sum_{\omega}\int\frac{d\mathbf{k}}{(2\pi)^3}\frac{d\mathbf{k}'}{(2\pi)^3}\left(\frac{\mathbf{k}}{(i\hbar\omega-\xi_{\mathbf{k}})^2}\right)\left(\frac{\mathbf{k}'}{(i\hbar\omega+\xi_{\mathbf{k}'})^2}\right)\delta(\mathbf{k}-\mathbf{k}')\\
=&\frac{T}{2}\sum_{\omega}\int\frac{d\mathbf{k}}{(2\pi)^3}\left(\frac{\hbar^2}{m}\right)^2\frac{\mathbf{k^2}}{(\hbar^2\omega^2+\xi_{\mathbf{k}}^2)^2}.
\end{aligned}$$

Because we are considering a spherical Fermi surface $\frac{\mathbf{k}^2}{3} = k_x^2 = k_y^2 = k_z^2$. So, if we integrate $\int d\mathbf{k}\mathbf{k}^2$ over Cartesian coordinates we will have 3 times the contribution of the integration over spherical coordinates. Therefore, we write

$$a_2 = \frac{T}{6}\sum_{\omega}\int \frac{d\mathbf{k}}{2\pi^2}\left(\frac{\hbar^2}{m}\right)^2 \frac{k^2}{(\hbar^2\omega^2+\xi_{\mathbf{k}}^2)^2}. \tag{3.103}$$

Using the approximation for expressions peaked near the Fermi surface we obtain

$$\begin{aligned}\frac{T}{6}\left(\frac{\hbar^2}{m}\right)^2 k_F^2 N(0)\sum_{\omega}\int d\xi\frac{1}{(\hbar^2\omega^2+\xi^2)^2} =&\frac{TN(0)v_F^2\hbar^2\pi}{6}\sum_{\omega>0}\frac{1}{(\hbar\omega)^3}\\ =&\frac{N(0)v_F^2\hbar^2}{6}\frac{7\zeta(3)}{(8\pi^2T^2)},\end{aligned}$$

where, v_F is the fermi velocity. And, expanding in powers of τ and taking the term proportional to the zeroth power because $\nabla^2\Delta \propto \tau^{3/2}$ we finally get

$$a_2 = \frac{v_F^2\hbar^2N(0)}{48T_c^2\pi^2}7\zeta(3). \tag{3.104}$$

LOCAL TERM

The local term is obtained as

$$\begin{aligned}a_1 = \int d\mathbf{y}K_a(\mathbf{r},\mathbf{y}) &= -T\lim_{\tau\to 0+}\sum_{\omega}e^{i\omega\tau}\int d\mathbf{y}\mathcal{G}_{\omega}^{(0)}(\mathbf{r},\mathbf{y})\widetilde{\mathcal{G}}_{\omega}^{(0)}(\mathbf{y},\mathbf{r})\\ =&-T\lim_{\tau\to 0+}\sum_{\omega}e^{i\omega\tau}\int d\mathbf{y}\frac{d\mathbf{k}}{(2\pi)^3}\frac{d\mathbf{k}_1}{(2\pi)^3}\frac{e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{y})}}{(i\hbar\omega-\xi_{\mathbf{k}})}\frac{e^{i\mathbf{k}\cdot(\mathbf{y}-\mathbf{r})}}{(i\hbar\omega+\xi_{\mathbf{k}})}\\ =&-T\lim_{\tau\to 0+}\sum_{\omega}e^{i\omega\tau}\int\frac{d\mathbf{k}}{(2\pi)^3}\frac{d\mathbf{k}_1}{(2\pi)^3}\frac{\delta(\mathbf{k}_1-\mathbf{k})}{(i\hbar\omega-\xi_{\mathbf{k}})}\frac{e^{i\mathbf{r}\cdot(\mathbf{k}-\mathbf{k}_1)}}{(i\hbar\omega+\xi_{\mathbf{k}})}\\ =&-T\lim_{\tau\to 0+}\sum_{\omega}e^{i\omega\tau}\int\frac{d\mathbf{k}}{(2\pi)^3}\frac{1}{\hbar^2\omega^2+\xi_{\mathbf{k}}^2}\\ =&N(0)T\sum_{\omega}\int d\xi\frac{1}{\hbar^2\omega^2+\xi^2},\\ =&N(0)T\sum_{\omega}\frac{1}{\hbar\omega}\int_{-\infty}^{\infty}\frac{dx}{1+x^2}\\ =&2N(0)T\pi\sum_{\omega>0}\frac{1}{\hbar\omega}.\end{aligned}$$

This sum is divergent. How to deal with this? Let us go back a few steps.

$$a_1 = T\lim_{\tau\to 0+}\sum_{\omega}e^{i\omega\tau}\int\frac{d\mathbf{k}}{(2\pi)^3}\frac{1}{(\xi_{\mathbf{k}}-i\hbar\omega)}\frac{1}{(\xi_{\mathbf{k}}+i\hbar\omega)},$$

and we rewrite as

$$a_1 = T\lim_{\tau\to 0+}\sum_{\omega}\int\frac{d\mathbf{k}}{(2\pi)^3}\frac{1}{2\xi_{\mathbf{k}}}\left(\frac{e^{i\omega\tau}}{\xi_{\mathbf{k}}+i\hbar\omega}+\frac{e^{i\omega\tau}}{\xi_{\mathbf{k}}-i\hbar\omega}\right). \tag{3.105}$$

Let us evaluate

$$\lim_{\tau\to 0^+}\sum_{\omega}\frac{e^{i\omega\tau}}{i\hbar\omega+\xi_{\mathbf{k}}}.$$

This can be done with a contour integration as follows[9]. If C is a contour encircling the imaginary axis (Im$\{z\}$) we have the following relation (see fig.9)

$$\lim_{\tau\to 0^+}\sum_{\omega}\frac{e^{i\omega\tau}}{i\hbar\omega+\xi_{\mathbf{k}}}=-\frac{1}{2T\pi i}\int_C\frac{dz}{e^{z/T}+1}\frac{e^{z\tau/\hbar}}{z-\xi_{\mathbf{k}}}. \tag{3.106}$$

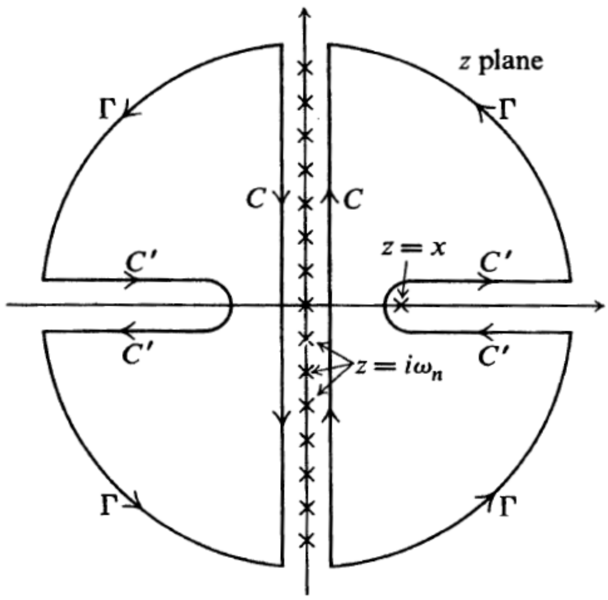


Figure 9: Contour for evaluation of the frequency sums.

This expression is true because the function $-\frac{1}{T}(e^{-z/T}-1)^{-1}$ has simple poles at $z=i\omega$. Deforming the contour to C' and Γ we are left with only one pole at $z=\xi_{\mathbf{k}}$ with unit residue. Taking the limit of τ we get

$$\lim_{\tau\to 0^+}\sum_{\omega}\frac{e^{i\omega\tau}}{i\hbar\omega+\xi_{\mathbf{k}}}=\frac{1}{T}\frac{1}{e^{-\hbar\xi_{\mathbf{k}}/T}+1}, \tag{3.107}$$

and

$$\lim_{\tau\to 0^+}\sum_{\omega}\frac{e^{i\omega\tau}}{i\hbar\omega-\xi_{\mathbf{k}}}=\frac{1}{T}\frac{1}{e^{\xi_{\mathbf{k}}/T}+1}. \tag{3.108}$$

Inserting these results in the expression for a_1 we obtain

$$a_1=\int\frac{d\mathbf{k}}{(2\pi)^3}\frac{1}{2\xi_{\mathbf{k}}}\Big(\frac{1}{e^{-\xi_{\mathbf{k}}/T}+1}-\frac{1}{e^{\xi_{\mathbf{k}}/T}+1}\Big).$$

Using the approximation for integrals peaked near the Fermi surface we write

$$a_1=N(0)\int d\xi\frac{1}{2\xi}\tanh\Big(\frac{\xi}{2T}\Big) \tag{3.109}$$

This integral is divergent. But, as we mention before in the case of temperature we are not dealing with a arbitrary range of energies. We can introduce cut-offs that comes from the limited range of scattering between two electrons above the Fermi surface. So, our integral very fittingly becomes

$$a_1 = N(0)\int_{-\hbar\omega_D}^{\hbar\omega_D} d\xi \frac{1}{2\xi}\tanh\left(\frac{\xi}{2T}\right) = N(0)\int_{0}^{\hbar\omega_D} d\xi \frac{1}{\xi}\tanh\left(\frac{\xi}{2T}\right)$$

Where ω_D is the Debye frequency. Now we solve this integral. To do that we perform a change of variables $z = \frac{\xi}{2T}$ we obtain

$$a_1 = N(0)\int_{0}^{\hbar\omega_D/2T} \frac{dz}{z}\tanh(z)$$

$$= \ln(z)\tanh(z)\Big|_0^{\hbar\omega_D/2T} - \int_0^{\hbar\omega_D/2T} dz\,\ln(z)\frac{1}{\cosh^2(z)}. \tag{3.110}$$

Here we use again the fact that we are not calculating for an arbitrary range of temperature. In fact we are working very closely to the critical temperature. As we are working with very small temperatures we can set $\hbar\omega_D/2T \to \infty$ and therefore

$$a_1 = N(0)\ln\left(\frac{\hbar\omega_D}{2T}\right) - \int_0^{\infty} dz\,\ln(z)\frac{1}{\cosh^2(z)} \tag{3.111}$$

The integral on the second term is easily found on textbooks[9]. Here we just quote the result. It is

$$\int_0^{\infty} dz\,\ln(z)\frac{1}{\cosh^2(z)} = -\ln\left(\frac{4e^{\gamma}}{\pi}\right), \tag{3.112}$$

where γ is the Euler–Mascheroni constant. Putting everything together we have

$$a_1 = N(0)\ln\left(\frac{2\hbar\omega_D e^{\gamma}}{\pi T}\right). \tag{3.113}$$

As we are considering the term $a_1\Delta(\mathbf{r})$ and $\Delta \propto \tau^{1/2}$ we have to collect terms up to $a_1 \propto \tau$. So, we do the following

$$a_1 = N(0)\ln\left(\frac{2\hbar\omega_D e^{\gamma}}{\pi T_c}\right) + N(0)\ln\left(\frac{T_c}{T}\right) = N(0)\ln\frac{2\hbar\omega_D e^{\gamma}}{\pi T_c} + N(0)\ln\left(\frac{1}{1-\tau}\right),$$

As τ is a small parameter we can do

$$a_1 = N(0)\ln\frac{2\hbar\omega_D e^{\gamma}}{\pi T_c} + N(0)(\tau + \mathcal{O}(\tau^2)). \tag{3.114}$$

Now we will use the following notation

$$a_1 = \mathcal{A}_T - a\tau. \tag{3.115}$$

We can readily identify this terms: $\mathcal{A}_T = N(0)\ln\frac{2\hbar\omega_D e^{\gamma}}{\pi T_c}$ and $a = -N(0)$.

3.3.7 Equation for the critical temperature

Now, we return to the expression 3.94. We truncated this equation up to $\tau^{3/2}$ order. But we can obtain another important equation if we truncate this expression up to $\tau^{1/2}$. We match all coefficients proportional to the main contribution to the order parameter Δ_0 up to the $\tau^{1/2}$. We will arrive at the following expression

$$\Delta_0(g^{-1} - \mathcal{A}_T) = 0. \tag{3.116}$$

The solution to this equation is

$$g\mathcal{A}_T = 1,$$

and will give us the expression of the critical temperature. It is

$$T_{c0} = \frac{2\hbar\omega_D e^{\gamma}}{\pi} e^{-1/gN(0)}. \tag{3.117}$$

This is referred to Mean-Field Critical temperature.

3.3.8 Ginzburg-Landau equation

At last we arrive at the goal of the second part of this chapter: the Ginzburg-Landau equation derived from BCS theory and as a consequence a connection between Ginzburg and Landau's theory of superconductivity and BCS theory. So, we go back now to the expression of the gap equation (3.94) and match coefficients proportional to Δ_0 but this time we take terms up to $\tau^{3/2}$. We will get the following equation

$$\tau^{1/2}\frac{\bar{\Delta}_0}{g} = a_1\tau^{1/2}\bar{\Delta}_0 + a_2\tau^{3/2}\bar{\boldsymbol{\nabla}}^2\bar{\Delta}_0 + b_1\tau^{3/2}|\bar{\Delta}_0|^2\bar{\Delta}_0. \tag{3.118}$$

But, from the critical temperature equation $g\mathcal{A}_T = 1$ we have that $a_1 = g^{-1} - a\tau$ so

$$\tau^{1/2}\frac{\bar{\Delta}_0}{g} = (g^{-1} - a\tau)\tau^{1/2}\bar{\Delta}_0 + a_2\tau^{3/2}\bar{\boldsymbol{\nabla}}^2\bar{\Delta}_0 + b_1\tau^{3/2}|\bar{\Delta}_0|^2\bar{\Delta}_0. \tag{3.119}$$

We rewrite it as

$$(-a\tau + g^{-1} - g^{-1})\tau^{1/2}\bar{\Delta}_0 + a_2\tau^{3/2}\bar{\boldsymbol{\nabla}}^2\bar{\Delta}_0 + b_1\tau^{3/2}|\bar{\Delta}_0|^2\bar{\Delta}_0 = 0, \tag{3.120}$$

and then

$$(-a\tau)\tau^{1/2}\bar{\Delta}_0 + a_2\tau^{3/2}\bar{\boldsymbol{\nabla}}^2\bar{\Delta}_0 + b_1\tau^{3/2}|\bar{\Delta}_0|^2\bar{\Delta}_0 = 0. \tag{3.121}$$

Multiplying this equation by $\tau^{3/2}$ we get

$$a\tau\Delta_0 - a_2\boldsymbol{\nabla}^2\Delta_0 - b_1|\Delta_0|^2\Delta_0 = 0. \tag{3.122}$$

We know that

$$a_2 = \frac{v_F^2\hbar^2 N(0)}{48T_c^2\pi^2}7\zeta(3) \qquad\qquad b_1 = -N(0)\frac{7\zeta(3)}{8\pi^2T_c^2}.$$

We define the terms $a_2 = \mathcal{K}$ and $b_1 = -b$. At last we write in a clear form the Ginzburg Landau equation for zero magnetic field

$$a\tau\Delta_0 + b|\Delta_0|^2\Delta_0 - \mathcal{K}\boldsymbol{\nabla}^2\Delta_0 = 0. \tag{3.123}$$

3.3.9 Determination of the Gap Function $\Delta(T)$

We have seen that indeed the Green Function formalism developed by Gor'kov recover the Ginzburg-Landau equations from BCS theory. But, do we have any experimental evidence that the BCS theory is valid? Well, now we will determine the gap function from Gor'kov equations. We take the coupled Gor'kov-Nambu equations

$$(-i\hbar\omega - \xi^*_{\mathbf{r}})\widetilde{\mathcal{F}}_\omega(\mathbf{r},\mathbf{r}') + \Delta^*(\mathbf{r})\mathcal{G}_\omega(\mathbf{r}',\mathbf{r}) = 0, \tag{3.124}$$

and

$$(-i\hbar\omega + \xi_{\mathbf{r}})\mathcal{G}_\omega(\mathbf{r},\mathbf{r}') + \Delta(\mathbf{r})\widetilde{\mathcal{F}}_\omega(\mathbf{r},\mathbf{r}') = -\delta(\mathbf{r}-\mathbf{r}'). \tag{3.125}$$

We make a Fourier transform to the momentum space and consider zero external magnetic field and therefore we can set the vector potential to zero. By doing this we are able to get a pair of algebraic equations

$$(-i\hbar\omega + \xi_{\mathbf{k}})\mathcal{G}_\omega(\mathbf{k}) + \Delta\widetilde{\mathcal{F}}_\omega(\mathbf{k}) = -1, \tag{3.126}$$

and

$$(-i\hbar\omega - \xi_{\mathbf{k}})\widetilde{\mathcal{F}}_\omega(\mathbf{k}) + \Delta^*\mathcal{G}_\omega(\mathbf{k}) = 0. \tag{3.127}$$

Solving this system of equations we are able to express the Green functions independent of one another as follows

$$\widetilde{\mathcal{F}}_\omega(\mathbf{k}) = -\frac{\Delta^*}{E^2_{\mathbf{k}} + \hbar^2\omega^2}, \tag{3.128}$$

and

$$\mathcal{G}_\omega(\mathbf{k}) = -\frac{(\xi_{\mathbf{k}} + i\hbar\omega)}{E^2_{\mathbf{k}} + \hbar^2\omega^2}. \tag{3.129}$$

$E^2_{\mathbf{k}} = \xi_{\mathbf{k}} + |\Delta|^2$ from equation (3.46) . Now we take the definition of the gap function in term of the Green function

$$\Delta(\mathbf{r}) = -gT\sum_\omega \lim_{\eta\to 0+} e^{i\omega\eta}\mathcal{F}_\omega(\mathbf{r},\mathbf{r}).$$

Then we get the following summation of integrals

$$-\Delta = gT\sum_\omega \lim_{\eta\to 0^+} e^{i\omega\eta}\int\frac{d\mathbf{k}}{(2\pi)^3}\frac{\Delta}{E^2_{\mathbf{k}} + \hbar^2\omega^2}.$$

Decomposing in fractions as we did before(see eq. 3.105 onward) we get the following expression

$$1 = g \int \frac{d\mathbf{k}}{(2\pi)^3} \frac{1}{2E_{\mathbf{k}}} \tanh\left(\frac{E_{\mathbf{k}}}{2T}\right).$$

For an integral peaked near the Fermi surface

$$1 = gN(0) \int d\xi \frac{1}{2\sqrt{\xi^2 + \Delta^2}} \tanh\left(\frac{\sqrt{\xi^2 + \Delta^2}}{2T}\right). \tag{3.130}$$

This reproduces the experimental data[10]. It is presented in fig. 10 where $\frac{\Delta(T)}{\Delta(0)}$ is plotted as a function of $\frac{T}{T_c}$

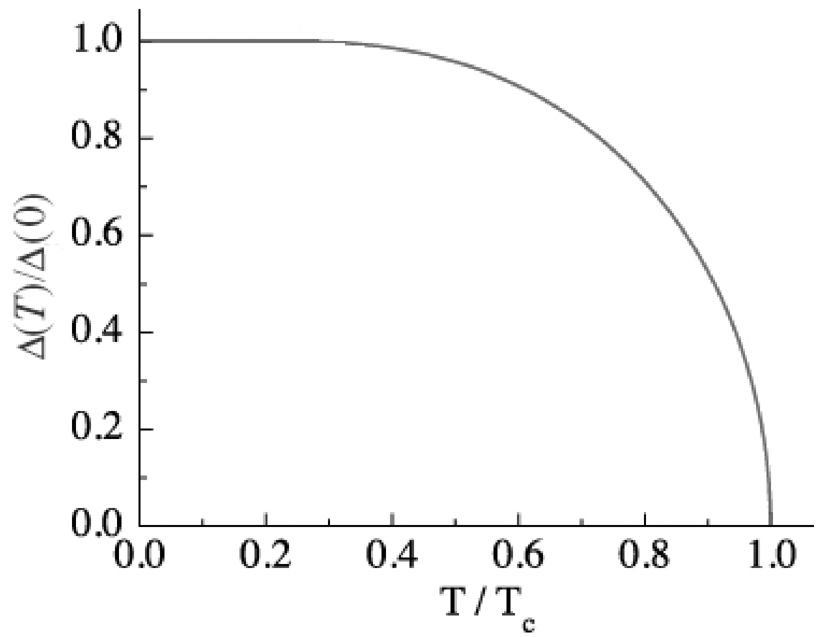


Figure 10: The Temperature-dependent gap in units of the zero-temperature order parameter calculated within the full BCS approach versus relative temperature.

3.3.10 Zero temperature energy gap

As our last calculation for this chapter we can get another important result. Let us calculate the gap function when the temperature drops to zero. As we do $T \to 0$ $\tanh\left(\frac{E_{\mathbf{k}}}{2T}\right) \to 1$ so we have

$$1 = gN(0) \int \frac{d\xi}{2\sqrt{\xi^2 + \Delta^2}} \tag{3.131}$$

This integral is divergent. As always we are not performing our calculations for an arbitrary quantity. The energy range that the electrons can scatter is proportional to the Debye energy.Therefore

$$1 = gN(0) \int_{-\hbar\omega_D}^{\hbar\omega_D} \frac{1}{2} \frac{d\xi}{\sqrt{\xi^2 + \Delta^2}} \tag{3.132}$$

We again used the approximation for integrals peaked near the Fermi surface. Solving this integral we get

$$1 = gN(0)\ln\left(\sqrt{1+\left(\frac{\hbar\omega_D}{\Delta}\right)^2} + \hbar\omega_D\right). \tag{3.133}$$

As $\frac{\hbar\omega_D}{\Delta} \gg 1$ we get finally:

$$\Delta(0) = 2\hbar\omega_D e^{-\frac{1}{gN(0)}}, \tag{3.134}$$

which is the zero temperature energy gap. We already know that

$$T_c = \frac{2\hbar\omega_D e^{\gamma}}{\pi} e^{-1/gN(0)}. \tag{3.135}$$

So, we have that

$$\frac{\Delta(0)}{T_c} \approx 1.76 \tag{3.136}$$

Within the used approach with the simplified form of effective interaction between electrons the ratio $\frac{\Delta(0)}{T_c}$ is universal, i.e. does not depend on the nature of superconductor. In fact the value of the fraction is slightly above 1.76. One of the early successes of BCS theory was the verification that this relationship is approximately satisfied in most of the known superconductors at the time.

4 APPLICATIONS OF MEAN FIELD THEORY

Until now we were focused on the case of *conventional* superconductors with only one contributing single-particle band and with no paramagnetic effects (no spin-magnetic interaction). In this chapter we are going to consider 2 cases that broaden the scope of our calculations: (1) superconductors in the paramagnetic limit and (2) superconductors with more than one contributing band.

4.1 Paramagnetic limit

While orbital effects lead to the formation of an Abrikosov vortex lattice bellow the orbital upper critical field in type-II superconductors, the spin-magnetic interaction promotes the tendency to Cooper pairing with non-zero momentum[11], the so-called Fulde-Ferrel-Larkin-Ovchinikov(FFLO) state[12] [13]. Now, our goal is to derive the Ginzburg-Landau equations with the spin-magnetic interaction taken into account. For the sake of illustration, we investigate a single-band (clean) superconductor with a spherical Fermi surface in the paramagnetic limit (orbital effects are neglected).

4.1.1 BCS Hamiltonian in the paramagnetic limit

Our starting point is the BCS Hamiltonian in the paramagnetic limit

$$H_{BCS} = \sum_a \int d\mathbf{r} \psi_a^\dagger(\mathbf{r}) \xi_{\mathbf{r},a} \psi_a(\mathbf{r}) + \int d\mathbf{r} \Big(\psi_\uparrow^\dagger(\mathbf{r}) \psi_\downarrow^\dagger(\mathbf{r}) \Delta(\mathbf{r}) + \Delta^*(\mathbf{r}) \psi_\downarrow(\mathbf{r}) \psi_\uparrow(\mathbf{r}) \Big) + C,$$

where the interaction part is considered within the Bogoliubov mean-field approximation. The single-electron energies now read

$$\xi_{\mathbf{r},\uparrow} = -\frac{\hbar^2 \boldsymbol{\nabla}_\mathbf{r}^2}{2m} + \mu_B B - \mu,\ \xi_{\mathbf{r},\downarrow} = -\frac{\hbar^2 \boldsymbol{\nabla}_\mathbf{r}^2}{2m} - \mu_B B - \mu,$$

where μ_B is the Bohr magneton, μ is the chemical potential, and the magnetic field is chosen in the z-direction.

The finite-temperature Heisenberg field operators obey the following equations of motion:

$$-\hbar\partial_\tau \begin{pmatrix} \psi_\uparrow(\mathbf{r},\tau) \\ \psi_\downarrow^\dagger(\mathbf{r},\tau) \end{pmatrix} = \mathbb{H}_{BdG} \begin{pmatrix} \psi_\uparrow(\mathbf{r},\tau) \\ \psi_\downarrow^\dagger(\mathbf{r},\tau) \end{pmatrix}, \tag{4.1}$$

where the Bogoliubov-de Gennes matrix in the paramagnetic limit reads

$$\mathbb{H}_{BdG} = \begin{pmatrix} \xi_{\mathbf{r},\uparrow} & \Delta(\mathbf{r}) \\ \Delta^*(\mathbf{r}) & -\xi^*_{\mathbf{r},\downarrow} \end{pmatrix}. \tag{4.2}$$

Now, as in the previous chapter, we are going to investigate the corresponding Green function formalism.

4.1.2 Green function formalism for paramagnetic limit

Similar to the previous chapter, we introduce the following Green functions:

$$\mathcal{G}(\mathbf{r}\tau_1,\mathbf{r}'\tau_2) = -\frac{1}{\hbar}\langle T_\tau[\psi_\uparrow(\mathbf{r}\tau_1)\psi_\uparrow^\dagger(\mathbf{r}'\tau_2)]\rangle, \tag{4.3}$$

$$\widetilde{\mathcal{F}}(\mathbf{r}\tau_1,\mathbf{r}'\tau_2) = -\frac{1}{\hbar}\langle T_\tau[\psi_\downarrow^\dagger(\mathbf{r}\tau_1)\psi_\uparrow^\dagger(\mathbf{r}'\tau_2)]\rangle, \tag{4.4}$$

$$\widetilde{\mathcal{G}}(\mathbf{r}\tau_1,\mathbf{r}'\tau_2) = -\frac{1}{\hbar}\langle T_\tau[\psi_\downarrow^\dagger(\mathbf{r}\tau_1)\psi_\downarrow(\mathbf{r}'\tau_2)]\rangle, \tag{4.5}$$

$$\mathcal{F}(\mathbf{r}\tau_1,\mathbf{r}'\tau_2) = -\frac{1}{\hbar}\langle T_\tau[\psi_\uparrow(\mathbf{r}\tau_1)\psi_\downarrow(\mathbf{r}'\tau_2)]\rangle. \tag{4.6}$$

Based on the above equations of motion for the Heisenberg field operators, one obtains the following equations of motion for the introduced Green functions:

$$\begin{cases} (\hbar\partial_{\tau_1} + \xi_{\mathbf{r},\uparrow})\mathcal{G}(\mathbf{r}\tau_1,\mathbf{r}'\tau_2) + \Delta(\mathbf{r})\widetilde{\mathcal{F}}(\mathbf{r}\tau_1,\mathbf{r}'\tau_2) = -\delta(\mathbf{r}-\mathbf{r}')\delta(\tau_1-\tau_2), \\ (\hbar\partial_{\tau_1} - \xi^*_{\mathbf{r},\downarrow})\widetilde{\mathcal{G}}(\mathbf{r}\tau_1,\mathbf{r}'\tau_2) + \Delta^*(\mathbf{r})\mathcal{F}(\mathbf{r}\tau_1,\mathbf{r}'\tau_2) = -\delta(\mathbf{r}-\mathbf{r}')\delta(\tau_1-\tau_2), \end{cases} \tag{4.7}$$

$$\begin{cases} (\hbar\partial_{\tau_1} - \xi^*_{\mathbf{r},\downarrow})\widetilde{\mathcal{F}}(\mathbf{r}\tau_1,\mathbf{r}'\tau_2) + \Delta^*(\mathbf{r})\mathcal{G}(\mathbf{r}\tau_1,\mathbf{r}'\tau_2) = 0, \\ (\hbar\partial_{\tau_1} + \xi_{\mathbf{r},\uparrow})\mathcal{F}(\mathbf{r}\tau_1,\mathbf{r}'\tau_2) + \Delta(\mathbf{r})\widetilde{\mathcal{G}}(\mathbf{r}\tau_1,\mathbf{r}'\tau_2) = 0. \end{cases} \tag{4.8}$$

Now, we invoke the Fourier representation with the fermionic Matsubara frequencies ω. The equation of motions for the Green functions becomes

$$\begin{cases} (-i\hbar\Omega + \xi_{\mathbf{r}})\mathcal{G}_\omega(\mathbf{r},\mathbf{r}') + \Delta(\mathbf{r})\widetilde{\mathcal{F}}_\omega(\mathbf{r},\mathbf{r}') = -\delta(\mathbf{r}-\mathbf{r}'), \\ (-i\hbar\Omega - \xi^*_{\mathbf{r}})\widetilde{\mathcal{G}}_\omega(\mathbf{r},\mathbf{r}') + \Delta^*(\mathbf{r})\mathcal{F}_\omega(\mathbf{r},\mathbf{r}') = -\delta(\mathbf{r}-\mathbf{r}'), \end{cases} \tag{4.9}$$

$$\begin{cases} (-i\hbar\Omega - \xi^*_{\mathbf{r}})\widetilde{\mathcal{F}}_\omega(\mathbf{r},\mathbf{r}') + \Delta^*(\mathbf{r})\mathcal{G}_\omega(\mathbf{r},\mathbf{r}') = 0, \\ (-i\hbar\Omega + \xi_{\mathbf{r}})\mathcal{F}_\omega(\mathbf{r},\mathbf{r}') + \Delta(\mathbf{r})\widetilde{\mathcal{G}}_\omega(\mathbf{r},\mathbf{r}') = 0, \end{cases} \tag{4.10}$$

where $\Omega = \omega + \frac{1}{\hbar} i\mu_B B$. Ω is called shifted Matsubara frequency. Following the matrix notations of the previous chapter we can write

$$i\hbar\Omega\check{\mathcal{G}}_\omega = \check{1}_2 + \check{\xi}\check{\mathcal{G}}_\omega + \check{\Delta}\check{\mathcal{G}}_\omega, \tag{4.11}$$

with

$$\check{\xi} = \begin{pmatrix} \hat{\xi} & 0 \\ 0 & -\hat{\xi}^* \end{pmatrix}, \quad \check{\Delta} = \begin{pmatrix} 0 & \hat{\Delta} \\ \hat{\Delta}^* & 0 \end{pmatrix}. \tag{4.12}$$

The matrix elements of the operators $\hat{\xi}$ and $\hat{\Delta}$ in the single-particle Hilbert space are given by

$$\hat{\xi} = \langle \mathbf{r} | \, \hat{\xi} \, | \mathbf{r}' \rangle = \delta(\mathbf{r} - \mathbf{r}')\xi_{\mathbf{r}}, \quad \hat{\Delta} = \langle \mathbf{r} | \, \hat{\Delta} \, | \mathbf{r}' \rangle = \Delta_{\mathbf{r}}\delta(\mathbf{r} - \mathbf{r}').$$

We also introduced

$$\check{\mathcal{G}}_\omega = \begin{pmatrix} \hat{\mathcal{G}}_\omega & \hat{\mathcal{F}}_\omega \\ \hat{\widetilde{\mathcal{F}}}_\omega & \hat{\widetilde{\mathcal{G}}}_\omega \end{pmatrix}, \tag{4.13}$$

with the operators $\hat{\mathcal{G}}_\omega, \hat{\widetilde{\mathcal{G}}}_\omega, \hat{\mathcal{F}}_\omega$, and $\hat{\widetilde{\mathcal{F}}}_\omega$ defined as

$$\begin{aligned} &\langle \mathbf{r} | \, \hat{\mathcal{G}}_\omega \, | \mathbf{r}' \rangle = \mathcal{G}_\omega(\mathbf{r}, \mathbf{r}'), \langle \mathbf{r} | \, \hat{\widetilde{\mathcal{G}}}_\omega \, | \mathbf{r}' \rangle = \widetilde{\mathcal{F}}_\omega(\mathbf{r}, \mathbf{r}'), \\ &\langle \mathbf{r} | \, \hat{\mathcal{F}}_\omega \, | \mathbf{r}' \rangle = \mathcal{F}_\omega(\mathbf{r}, \mathbf{r}'), \langle \mathbf{r} | \, \hat{\widetilde{\mathcal{F}}}_\omega \, | \mathbf{r}' \rangle = \widetilde{\mathcal{F}}_\omega(\mathbf{r}, \mathbf{r}'). \end{aligned} \tag{4.14}$$

The normal-state Green function matrix obeys the following equation of motion

$$(i\hbar\Omega - \check{\xi})\check{\mathcal{G}}^{(0)}_\omega = \check{1}_2, \tag{4.15}$$

where

$$\check{\mathcal{G}}^{(0)}_\omega = \begin{pmatrix} \hat{\mathcal{G}}^{(0)}_\omega & 0 \\ 0 & \hat{\widetilde{\mathcal{G}}}^{(0)}_\omega \end{pmatrix}.$$

We can, therefore, write

$$\check{\mathcal{G}}^{(0)}_\omega = (i\hbar\Omega - \check{\xi})^{-1}. \tag{4.16}$$

We can see that the only difference with our previous consideration is the appearance of the shifted Matsubara frequencies. We can therefore write the gap equation, based on our previous results, as

$$\Delta(\mathbf{r}) = \int d\mathbf{y} K_a(\mathbf{r}, \mathbf{y})\Delta(\mathbf{y}) + \int d\mathbf{y}_1 d\mathbf{y}_2 d\mathbf{y}_3 K_b(\mathbf{r}, \mathbf{y}_1, \mathbf{y}_2, \mathbf{y}_3)\Delta(\mathbf{y}_1)\Delta^*(\mathbf{y}_2)\Delta(\mathbf{y}_3).$$

The kernels of the integrals are

$$K_a(\mathbf{r}, \mathbf{y}) = -gT \lim_{\tau \to 0^+} \sum_\omega e^{i\omega\tau} \mathcal{G}^{(0)}_\omega(\mathbf{r}, \mathbf{y}) \widetilde{\mathcal{G}}^{(0)}_\omega(\mathbf{y}, \mathbf{r}),$$

and

$$K_b = -gT \lim_{\tau \to 0^+} \sum_\omega e^{i\omega\tau} \mathcal{G}^{(0)}_\omega(\mathbf{r}, \mathbf{y}_1) \widetilde{\mathcal{G}}^{(0)}_\omega(\mathbf{y}_1, \mathbf{y}_2) \mathcal{G}^{(0)}_\omega(\mathbf{y}_2, \mathbf{y}_3) \widetilde{\mathcal{G}}^{(0)}_\omega(\mathbf{y}_3, \mathbf{r}).$$

4.1.3 Calculations of the Ginzburg-Landau coefficients

Here the same formalism is applied to the calculation of the Ginzburg-Landau coefficients as previously. The only new feature is accounting for the shifted Matsubara frequency Ω.

TERM PROPORTIONAL TO Δ^3

$$b_1 = \int d\mathbf{y}_1 d\mathbf{y}_2 d\mathbf{y}_3 K_b(\mathbf{r}, \mathbf{y}_1, \mathbf{y}_2, \mathbf{y}_3) = \sum_{\omega} \int \frac{d\mathbf{k}}{(2\pi)^3} \frac{1}{(\hbar^2\Omega^2 + \xi_{\mathbf{k}}^2)^2}. \tag{4.17}$$

$$b_1 = TN(0)\pi \sum_{\omega>0} \frac{1}{(\hbar\Omega)^3} = \frac{N(0)}{8\pi^2 T^2} \operatorname{Re}\left(\sum_{n=0}^{\infty} \frac{1}{(n + \frac{1}{2} + i\frac{\mu_B B}{2\pi T})^3} \right). \tag{4.18}$$

Expanding around $\tau = 1 - \frac{T}{T_{c0}(B)}$ we have

$$i\frac{\mu_B B}{2\pi T} = i\frac{\mu_B B}{2\pi T_{c0}(B)} \frac{T_{c0}(B)}{T} = i\frac{\mu_B B}{2\pi T_{c0}(B)} \frac{1}{1-\tau} \approx i\frac{\mu_B B}{2\pi T_{c0}(B)}(1+\tau).$$

We only take the zeroth order of τ and we get

$$b_1 = \frac{N(0)}{8\pi^2 T_{c0}^2(B)} \operatorname{Re}\left(\sum_{n=0}^{\infty} \frac{1}{\left(n + \frac{1}{2} + i\frac{\mu_B B}{2\pi T_{c0}(B)}\right)^3} \right). \tag{4.19}$$

where $T_{c0}(B)$ is the mean-field critical temperature in the paramagnetic limit. a

TERM PROPORTIONAL TO THE SQUARED GRADIENT

We again have a similar term to the case without spin-magnetic interaction and we proceed in the exact same way. Therefore,

$$a_2 = \sum_{\omega} \int d\mathbf{y} K_a(\mathbf{r}, \mathbf{y})(\mathbf{r} - \mathbf{y})^2 = -\frac{T}{2} \int \frac{d\mathbf{k}^3}{(2\pi)^3} \left(\frac{\hbar^2}{m}\right)^2 \frac{\mathbf{k}^2}{(\hbar^2\Omega^2 + \xi_{\mathbf{k}}^2)^2}. \tag{4.20}$$

Expanding for τ small we get

$$a_2 = -\frac{v_F^2}{6} \frac{N(0)}{8\pi^2 T_{c0}^2(B)} \operatorname{Re}\left(\sum_{n=0}^{\infty} \frac{1}{(n + \frac{1}{2} + i\frac{\mu_B B}{2\pi T_{c0}(B)})^3} \right). \tag{4.21}$$

LOCAL LINEAR TERM

$$a_1 = \int d\mathbf{y} K_a(\mathbf{r}, \mathbf{y}) = T \sum_{\omega} \int \frac{d\mathbf{k}}{(2\pi)^3} \frac{1}{\hbar^2\Omega^2 + \xi_{\mathbf{k}}^2} = 2\pi T N(0) \operatorname{Re}\left(\sum_{\omega>0} \frac{1}{\hbar\Omega} \right). \tag{4.22}$$

Here, as before, we encounter a divergent sum. To deal with this we need to introduce cut-offs but for the paramagnetic limit. To avoid calculating new cut-offs we can use the cut-offs from the previous case we encounter in Chapter 3 but with some modifications. To do this consider the local term written in the following form

$$a_1 = 2\pi T N(0) \operatorname{Re}\left(\sum_{\omega>0} \left(\frac{1}{\hbar\Omega} - \frac{1}{\hbar\omega} \right) \right) + 2\pi T N(0) \sum_{\omega>0} \frac{1}{\hbar\omega}.$$

From our earlier calculations we know that

$$2\pi T N(0) \sum_{\omega>0} \frac{1}{\hbar\omega} = N(0) \ln \frac{2\hbar\omega_D e^{\gamma}}{\pi T}. \tag{4.23}$$

Therefore

$$a_1 = 2\pi T N(0) \operatorname{Re}\left(\sum_{\omega>0} \left(\frac{1}{\hbar\Omega} - \frac{1}{\hbar\omega} \right) \right) + N(0) \ln \frac{2\hbar\omega_D e^{\gamma}}{\pi T}, \tag{4.24}$$

We need to collect terms up to $\tau^{3/2}$ in the Ginzburg-Landau equation. Since the order parameter is proportional to $\tau^{1/2}$, a_1 has to include terms up to τ. So, the local-term coefficient becomes

$$a_1 = N(0) \left\{ \ln \frac{2\hbar\omega_D e^{\gamma}}{\pi T_{c0}(B)} + \ln \frac{T_{c0}(B)}{T} + \operatorname{Re}\left(\sum_{n=0}^{\infty} \frac{1}{n + \frac{1}{2} + i\frac{\mu_B B}{2\pi T_{c0}(B)}} - \sum_{n=0}^{\infty} \frac{1}{n + \frac{1}{2}} \right) \right\}.$$

We wish to express this term in the familiar form: $a_1 = \mathcal{A}_T - a(B)\tau$. If we do this, we have

$$\mathcal{A}_T = N(0) \left\{ \ln \frac{2\hbar\omega_D e^{\gamma}}{\pi T_{c0}(B)} + \operatorname{Re}\left(\sum_{n=0}^{\infty} \frac{1}{n + \frac{1}{2} + i\frac{\mu_B B}{2\pi T_{c0}(B)}} - \sum_{n=0}^{\infty} \frac{1}{n + \frac{1}{2}} \right) \right\},$$

In addition, $a(B)$ reads

$$a(B) = -\frac{N(0)}{T_{c0}(B)}, \tag{4.25}$$

where we use

$$\ln \frac{T_{c0}(B)}{T} = \ln \frac{1}{1-\tau} \approx \tau + \frac{\tau^2}{2}.$$

Finally, we have all three coefficients for the Ginzburg-Landau equation in the paramagnetic limit. Let us just summarize our calculations. The coefficients in the standard notations of the Ginzburg-Landau theory are given by

$$a(B) = -\frac{N(0)}{T_{c0}(B)},$$

$$b(B) = \frac{N(0)}{8\pi^2 T_{c0}^2(B)} \operatorname{Re}\left(\sum_{n=0}^{\infty} \frac{1}{\left(n + \frac{1}{2} + i\frac{\mu_B B}{2\pi T_{c0}(B)}\right)^3} \right),$$

and

$$\mathcal{K}(B) = -\frac{v_F^2}{6} \frac{N(0)}{8\pi^2 T_{c0}^2(B)} \operatorname{Re}\left(\sum_{n=0}^{\infty} \frac{1}{(n + \frac{1}{2} + i\frac{\mu_B B}{2\pi T_{c0}(B)})^3} \right).$$

4.1.4 Equation for critical temperature in the paramagnetic limit

Next step to get all the necessary formalism to work in the paramagnetic limit is to calculate the equation for the critical temperature. By the same reasons that we showed in

Chapter 3 the critical temperature equation is: $g\mathcal{A}_T = 1$, but know we have a dependence on the magnetic field. So, we write

$$gN(0)\Bigg\{ \ln\frac{2\omega_D e^\gamma}{\pi T_{c0}(B)} + \mathrm{Re}\left(\sum_{n=0}^{\infty}\frac{1}{n+\frac{1}{2}+i\frac{\mu_B B}{2\pi T_{c0}(B)}} - \sum_{n=0}^{\infty}\frac{1}{n+\frac{1}{2}}\right)\Bigg\} = 1.$$

The logarithm term can be evaluated as

$$\begin{aligned}\ln\frac{2\omega_D e^\gamma}{\pi T_{c0}(B)} &= \ln\left(\frac{2\omega_D e^\gamma}{\pi T_{c0}(B=0)}\frac{T_{c0}(B=0)}{T_{c0}(B)}\right),\\ &= \ln\frac{2\omega_D e^\gamma}{\pi T_{c0}(B=0)} + \ln\frac{T_{c0}(B=0)}{T_{c0}(B)},\\ &= \frac{1}{gN(0)} + \ln\frac{T_{c0}(B=0)}{T_{c0}(B)}.\end{aligned}$$

since

$$T_{c0}(B=0) = \frac{2\hbar\omega_D e^\gamma}{\pi}e^{-1/gN(0)}.$$

So, the critical temperature equation becomes

$$\frac{1}{gN(0)} + \ln\frac{T_{c0}(B=0)}{T_{c0}(B)} + \mathrm{Re}\left(\sum_{n=0}^{\infty}\frac{1}{n+\frac{1}{2}+i\frac{\mu_B B}{2\pi T_{c0}(B)}} - \sum_{n=0}^{\infty}\frac{1}{n+\frac{1}{2}}\right) = \frac{1}{gN(0)}.$$

Rearranging we obtain

$$\ln\frac{T_{c0}(B=0)}{T_{c0}(B)} = \mathrm{Re}\left(\sum_{n=0}^{\infty}\frac{1}{n+\frac{1}{2}} - \sum_{n=0}^{\infty}\frac{1}{n+\frac{1}{2}+i\frac{\mu_B B}{2\pi T_{c0}(B)}}\right).$$

In figure 11 we depic the critical temperature $T_{c0}(B)$ as function of $\mu_B B$.

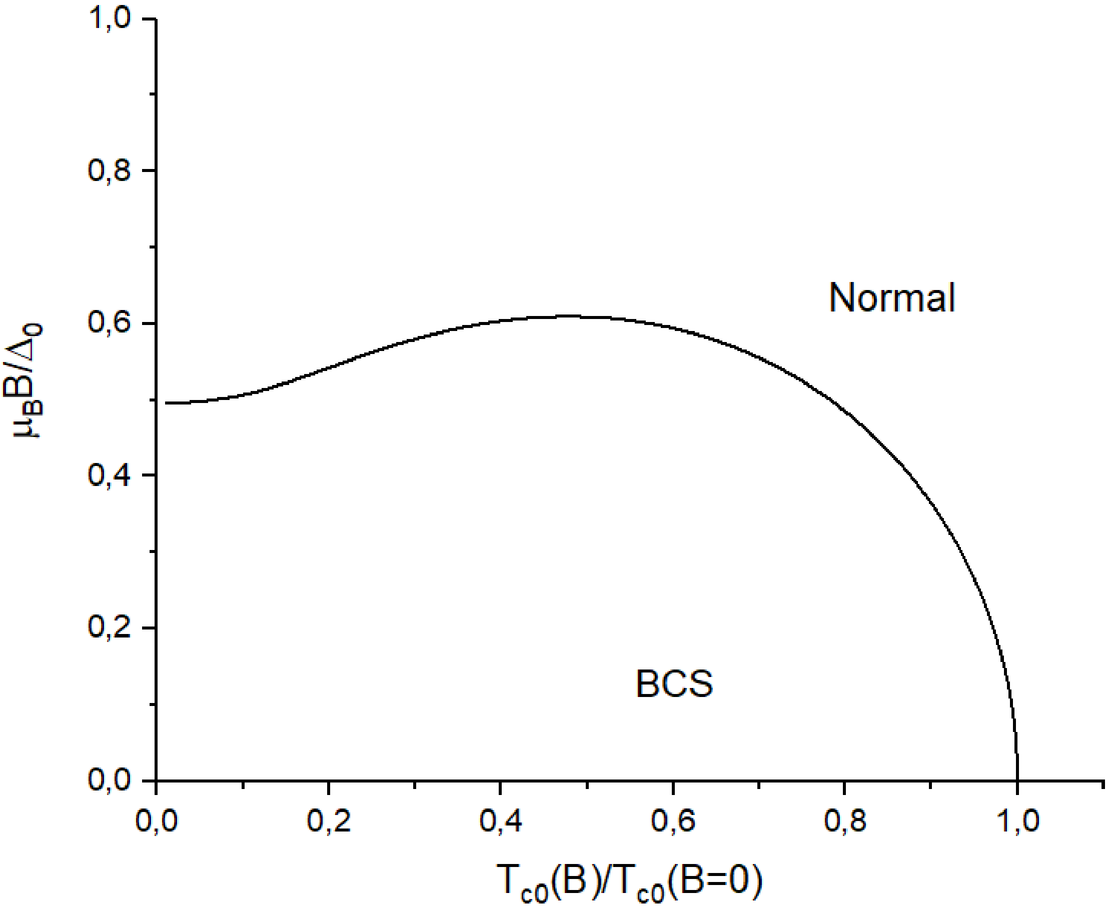


Figure 11: Critical temperature in the paramagnetic limit.

4.1.5 Ginzburg-Landau equation

In the paramagnetic limit the Ginzburg-Landau equation is the same as before with the only difference that the coefficients are magnetic field dependent. Here we just quote the previous result. It is

$$a(B)\Delta + b(B)|\Delta|^2\Delta - \mathcal{K}(B)\boldsymbol{\nabla}^2\Delta = 0. \tag{4.26}$$

4.1.6 Fulde-Ferrel-Larkin-Ovchinnikov phase

As it was shown long time ago by Larkin and Ovchinnikov and by Fulde and Ferrell[12][13], at low temperatures and when the magnetic field is acting on the spin of electrons only(paramagnetic limit), a transition from normal (N) to modulated superconducting state (FFLO state) must occur. The FFLO phase consists in a condensate of finite momentum Cooper pairs in contrast to the zero momenta pairs of the usual BCS state(as shown in chapter 2). Hence the FFLO superconducting order parameter acquires a spatial variation. A characteristic feature of the field-temperature phase diagram is the existence of a tricritical point (TCP) which is the meeting point of three transition lines separating the normal metal, the uniform superconductor and the FFLO state[11]. For clean s-wave superconductors the TCP is located at $T^* = 0.56T_{c0}$[14] and $B^* = 1.07T_{c0}$, T_{c0} being the zero field critical temperature. The FFLO state is only energetically favorable in a small part of the phase diagram, located at low temperatures $T < T^*$ and high fields,

Along the transition line define by $g\mathcal{A} = 1$ (see figure 11) the Ginzburg-Landau coefficient $b(B)$ changes sign and at the tri-critical point (T*, B*) where the BCS superconducting state, normal state and FFLO state meet, it becomes zero ($b = 0$). This means that

$$\mathrm{Re}\left(\sum_{n=0}^{\infty}\frac{1}{\left(n+\frac{1}{2}+i\frac{\mu_B B}{2\pi T_{c0}(B)}\right)^3}\right) = 0.$$

From this equation we get that

$$\frac{\mu_B B(T)}{2\pi T_{c0}(B)} \approx 0.3. \tag{4.27}$$

We also know that along the transition line $a_1(T) = 0$ because $\Delta = 0$ for the normal state. Taking the expression for this coefficient and calculating at which temperature $\frac{\mu_B B(T)}{2\pi T_{c0}(B)} = 0.3$ is true we obtain

$$\ln\frac{2\omega_D e^{\gamma}}{\pi T_{c0}(B)} + \mathrm{Re}\left(\sum_{n=0}^{\infty}\frac{1}{n+\frac{1}{2}+i0.3} - \sum_{n=0}^{\infty}\frac{1}{n+\frac{1}{2}}\right) = 0. \tag{4.28}$$

This is true when

$$\frac{T^*}{T_{c0}(B=0)} \approx 0.56. \tag{4.29}$$

and, therefore,

$$\frac{B^*(T^*)\mu_B}{T_{c0}(B=0)} \approx 1.07, \tag{4.30}$$

which give us the TCP on the field-temperature phase diagram.

Now, we will calculate the phase diagram for the modulated order parameter for a simple case to see that for low temperature and high magnetic field the system has a tendency to form Cooper pair with nonzero momenta. To do this we start with the following two Gor'kov equations in the paramagnetic limit

$$(-i\hbar\Omega - \xi^*_{\mathbf{r}})\widetilde{\mathcal{G}}_\omega(\mathbf{r}-\mathbf{r}') + \Delta^*(\mathbf{r})\mathcal{F}_\omega(\mathbf{r}-\mathbf{r}') = -\delta(\mathbf{r}-\mathbf{r}'),$$
$$(-i\hbar\Omega + \xi_{\mathbf{r}})\mathcal{F}_\omega(\mathbf{r}-\mathbf{r}') + \Delta(\mathbf{r})\widetilde{\mathcal{G}}_\omega(\mathbf{r}-\mathbf{r}') = 0.$$

We submit the following space dependence for the Green functions

$$\mathcal{F}_\omega(\mathbf{r}-\mathbf{r}') = \int \frac{d\mathbf{k}}{(2\pi)^3}\mathcal{F}_\omega(\mathbf{k})e^{i(\mathbf{k}+\mathbf{q}/\mathbf{2})\cdot(\mathbf{r}-\mathbf{r}')},$$
$$\widetilde{\mathcal{G}}_\omega(\mathbf{r}-\mathbf{r}') = \int \frac{d\mathbf{k}}{(2\pi)^3}\widetilde{\mathcal{G}}_\omega(\mathbf{k})e^{i(\mathbf{k}-\mathbf{q}/2)\cdot(\mathbf{r}-\mathbf{r}')},$$

where q is the centre of mass vector for the Cooper pair. We go to the fourier space and the Gor'kov equations become

$$\Big(-i\hbar\Omega - \Big[\frac{\hbar^2(\mathbf{k}-\mathbf{q}/2)^2}{2m} - \mu\Big]\Big)\widetilde{\mathcal{G}}_\omega(\mathbf{k}) + \Delta^*\mathcal{F}_\omega(\mathbf{k}) = -1,$$
$$\Big(-i\hbar\Omega + \Big[\frac{\hbar^2(\mathbf{k}+\mathbf{q}/2)^2}{2m} - \mu\Big]\Big)\mathcal{F}_\omega(\mathbf{k}) + \Delta\widetilde{\mathcal{G}}_\omega(\mathbf{k}) = 0.$$

Observe that

$$\frac{\hbar^2}{2m}(\mathbf{k}-\mathbf{q}/2)^2 - \mu = \frac{\hbar^2q^2}{8m} + \frac{\hbar^2k^2}{2m} - \frac{\hbar^2\mathbf{q}\cdot\mathbf{k}}{2m} - \mu \approx \xi_\mathbf{k} - \frac{\hbar^2\mathbf{q}\cdot\mathbf{k}}{2m}$$
$$\frac{\hbar^2}{2m}(\mathbf{k}+\mathbf{q}/2)^2 - \mu = \frac{\hbar^2q^2}{8m} + \frac{\hbar^2k^2}{2m} + \frac{\hbar^2\mathbf{q}\cdot\mathbf{k}}{2m} - \mu \approx \xi_\mathbf{k} + \frac{\hbar^2\mathbf{q}\cdot\mathbf{k}}{2m},$$

where $\xi_\mathbf{k} = \frac{\hbar^2k^2}{2m} - \mu$. Because the q-vector is of the order of the coherence length it is small when we compare with k_F in the regions of major interest , $q \ll k_F$, we need to keep only the first order terms of q. Then, the Gor'kov equation becomes

$$\Big(-i\hbar\Omega - \xi_\mathbf{k} + \frac{\hbar^2\mathbf{q}\cdot\mathbf{k}}{2m}\Big)\widetilde{\mathcal{G}}_\omega(\mathbf{k}) + \Delta^*\mathcal{F}_\omega(\mathbf{k}) = -1,$$
$$\Big(-i\hbar\Omega + \xi_\mathbf{k} + \frac{\hbar^2\mathbf{q}\cdot\mathbf{k}}{2m}\Big)\mathcal{F}_\omega(\mathbf{k}) + \Delta\widetilde{\mathcal{G}}_\omega(\mathbf{k}) = 0.$$

From this system of equations we obtain the following expression for the hole Green function

$$\mathcal{F}_\omega = -\frac{\Delta}{(i\hbar\Omega - \xi_\mathbf{k} - \frac{\hbar^2\mathbf{q}\cdot\mathbf{k}}{2m})(-i\hbar\Omega - \xi_\mathbf{k} + \frac{\hbar^2\mathbf{q}\cdot\mathbf{k}}{2m}) + |\Delta|^2},$$
$$\mathcal{F}_\omega = -\frac{\Delta}{(\hbar^2\Omega^2 + 2i\hbar^3\Omega\frac{\mathbf{q}\cdot\mathbf{k}}{2m} - \frac{\hbar^4q^2k^2}{4m^2} + \xi_\mathbf{k}^2) + |\Delta|^2},$$
$$\mathcal{F}_\omega = -\frac{\Delta}{(\hbar\Omega + i\frac{\hbar^2\mathbf{q}\cdot\mathbf{k}}{2m})^2 + \xi_\mathbf{k}^2 + |\Delta|^2}.$$

As we know, the order parameter is given by

$$\Delta = -gT\sum_n \lim_{\eta\to0^+} e^{i\omega\eta}\int\frac{d\mathbf{k}}{(2\pi)^3}\mathcal{F}_\omega(\mathbf{k}),$$

which means that

$$\Delta = gT\sum_n \lim_{\eta\to0^+} e^{i\omega\eta}\int\frac{d\mathbf{k}}{(2\pi)^3}\frac{\Delta}{(\hbar\Omega + i\frac{\hbar^2\mathbf{q}\cdot\mathbf{k}}{2m})^2 + \xi_\mathbf{k}^2 + |\Delta|^2}.$$

We then go to the critical point for the paramagnetic limit $T_{c0}(B)$, a point which we denote by T_{cp}. Because of this $|\Delta|^2 \to 0$ and we have

$$\Delta = gT_{c0}(B)\sum_n \lim_{\eta\to 0^+} e^{i\omega\eta}\int \frac{d\mathbf{k}}{(2\pi)^3}\frac{\Delta}{(\hbar\Omega + i\frac{\hbar^2\mathbf{q}\cdot\mathbf{k}}{2m})^2+\xi_{\mathbf{k}}^2}.$$

For the 1D case we obtain

$$\Delta = gT_{c0}(B)\sum_n \lim_{\eta\to 0^+} e^{i\omega\eta}\int \frac{dk}{2\pi}\frac{\Delta d(cos\theta)}{(\hbar\Omega + i\frac{\hbar^2 qk}{2m}cos\theta)^2+\xi_k^2}.$$

where for this case $cos\theta = \pm 1$. So,

$$\Delta = gT_{c0}(B)\sum_n \lim_{\eta\to 0^+} e^{i\omega\eta}\left[\int \frac{dk}{2\pi}\frac{\Delta}{(\hbar\Omega + i\frac{\hbar^2 qk}{2m})^2+\xi_k^2} + \int \frac{dk}{2\pi}\frac{\Delta}{(\hbar\Omega - i\frac{\hbar^2 qk}{2m})^2+\xi_k^2}\right].$$

We proceed with integration in the same way we did before (see eq. 4.22). We get

$$\begin{aligned}
\Delta =& gT_{c0}(B)\frac{m}{\hbar^2 2\pi k_F}\sum_n\sum_{\pm}\int_{-\infty}^{\infty} d\xi\frac{\Delta}{(\hbar\Omega \pm i\frac{\hbar^2 k_F}{2m})^2+\xi^2},\\
=& gT_{c0}(B)N_{1D}\frac{1}{2}\sum_n\sum_{\pm}\int_{-\infty}^{\infty} d\xi\frac{\Delta}{(\hbar\Omega \pm i\frac{\hbar q v_F}{2})^2+\xi^2},\\
=& gT_{c0}(B)N_{1D}\frac{1}{2}\sum_n\sum_{\pm}\frac{\Delta}{\hbar\Omega \pm i\frac{\hbar v_F q}{2}}\int_{-\infty}^{\infty} dx\frac{1}{1+x^2},\\
=& gT_{c0}(B)N_{1D}\pi\frac{1}{2}\sum_n\sum_{\pm}\frac{\Delta}{\hbar\Omega \pm i\frac{\hbar v_F q}{2}}.
\end{aligned}$$

This series is divergent. As before we do

$$\frac{1}{2}\sum_n\sum_{\pm}\frac{1}{(\hbar\Omega \pm i\frac{\hbar v_F q}{2})} = \sum_n\left(\frac{1}{2}\sum_{\pm}\frac{1}{(\hbar\Omega \pm i\frac{\hbar v_F q}{2})} - \frac{1}{\hbar\omega} + \frac{1}{\hbar\omega}\right),$$

with

$$\sum_n \frac{1}{\hbar\omega} = \frac{1}{\pi T}\ln\frac{2\hbar\omega_D e^{\gamma}}{\pi T}.$$

Finally we have that

$$\begin{aligned}
&\frac{1}{gN_{1D}} = \pi T_{c0}(B)\,\mathrm{Re}\left\{\sum_n\left(\frac{1}{2}\sum_{\pm}\frac{1}{(\hbar\Omega \pm i\frac{\hbar v_F q}{2})} - \frac{1}{\hbar\omega}\right)\right\} + \ln\frac{2\hbar\omega_D e^{\gamma}}{\pi T_{c0}(B)},\\
&\ln\frac{2\hbar\omega_D e^{\gamma}}{\pi T_{c0}(B)} - \frac{1}{gN_{1D}} = \pi T_{c0}(B)\,\mathrm{Re}\left\{\sum_n\left(\frac{1}{\hbar\omega} - \frac{1}{2}\sum_{\pm}\frac{1}{(\hbar\Omega \pm i\frac{\hbar v_F q}{2})}\right)\right\},\\
&\ln\frac{T_{c0}(B=0)}{T_{c0}(B)} + \ln\frac{2\hbar\omega_D e^{\gamma}}{T_{c0}(B=0)} - \frac{1}{gN_{1D}}\\
&= \pi T_{c0}(B)\,\mathrm{Re}\left\{\sum_n\left(\frac{1}{\hbar\omega} - \frac{1}{2}\sum_{\pm}\frac{1}{(\hbar\Omega \pm i\frac{\hbar v_F q}{2})}\right)\right\},\\
&\ln\frac{T_{c0}(B=0)}{T_{c0}(B)} = \pi T_{c0}(B)\,\mathrm{Re}\left\{\sum_n\left(\frac{1}{\hbar\omega} - \frac{1}{2}\sum_{\pm}\frac{1}{(\hbar\Omega \pm i\frac{\hbar v_F q}{2})}\right)\right\}.
\end{aligned}$$

The graph bellow shows this plot using the result for $q = 0$ as a reference. We can see the region of FFLO state for low temperatures and high magnetic fields.

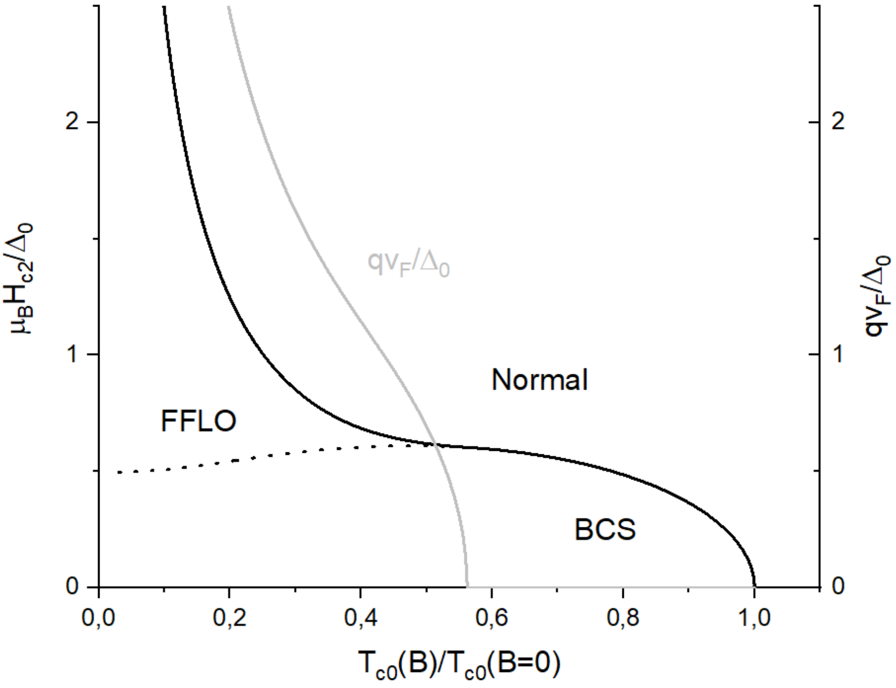


Figure 12: Phase diagram for $q \neq 0$ solid line and for $q = 0$ dashed line. The absolute value of the FFLO modulation vector q as a function of $T_{c0}(B)/T_{c0}(B = 0)$ gray line.

4.2 Multi-band superconductors

Multi-band and multi-gap superconductors have demonstrated a potential for realizing novel coherent quantum phenomena that can enhance their critical temperature. As we demonstrated in last chapter, $\tau = 1 - \frac{T}{T_c}$ controls all the relevant quantities and their spatial gradients. Within this approach, the Ginzburg-Landau theory follows from the systematic τ-expansion of the free energy and the gap equation. Here we find the series expansion in τ for the original system of the two equations for two band order parameters in the matrix form. While being more transparent and intuitively clear, this approach also significantly simplifies the technical aspects and also allows a generalization to the case of multiple contributing bands.

In this section first we will show a general expression for the free-energy functional of a two-band (clean) superconductor with s-wave pairing governed by the intra-band interaction strength $g_{\nu\nu}(\nu = 1, 2)$ and inter-band coupling $g_{12} = g_{21}$ of the Josephson type. Then we will investigate the τ expansion for the free energy and the corresponding τ-expansion for the matrix gap equation, which yields consequently the equation for the critical temperature and the standard Ginzburg-Landau formalism [15].

4.2.1 Free-energy functional density

The free-energy functional for a two-band s-wave superconductor with pairing between electrons in the same sub-band reads

$$F_s = F_{n,B=0} + \int d\mathbf{r}\Big\{\frac{\mathbf{B}^2(\mathbf{r})}{8\pi} + \vec{\mathbf{\Delta}}^\dagger \check{g}^{-1}\vec{\mathbf{\Delta}}\Big\} + \sum_{\nu=1,2}\mathcal{F}_\nu[\Delta_\nu], \tag{4.31}$$

where $\check{g}$ is the coupling matrix

$$\check{g} = \begin{pmatrix} g_{11} & g_{12} \\ g_{12} & g_{22}, \end{pmatrix}, \qquad \check{g}^{-1} = \frac{1}{G}\begin{pmatrix} g_{22} & g_{12} \\ -g_{12} & g_{11} \end{pmatrix}.$$

We also have that

$$\vec{\mathbf{\Delta}} = \begin{pmatrix} \Delta_1 \\ \Delta_2 \end{pmatrix}, \text{ and } G = g_{11}g_{22} - g_{12}^2.$$

The functional $\mathcal{F}_\nu[\Delta_\nu]$ can be represented as an infinite series in powers of Δ_ν as

$$\begin{aligned}\mathcal{F}_\nu = &-\int d\mathbf{r}d\mathbf{y}K_{\nu,a}(\mathbf{r},\mathbf{y})\Delta_\nu^*(\mathbf{r})\Delta_\nu(\mathbf{y}) \\ &-\frac{1}{2}\int d\mathbf{r}\prod_{j=1}^{3} d^3\mathbf{y}_j K_{\nu,b}(\mathbf{r},\{\mathbf{y}\}_3)\Delta_\nu^*(\mathbf{r})\Delta_\nu(\mathbf{y}_1)\Delta_\nu^*(\mathbf{y}_2)\Delta_\nu(\mathbf{y}_3) - \ldots.\end{aligned}$$

Where $\{\mathbf{y}\}_3 = \mathbf{y}_1, \mathbf{y}_2, \mathbf{y}_3$. In vicinity of the critical temperature this infinite series in powers of Δ_ν (and also Δ_ν^*) can be truncated. Keeping only the first two terms makes it possible to get the Ginzburg-Landau theory. The kernels of the integrals in the above expression are the same as those in the derivation of the Ginzburg-Landau equations in Chapter 3 (up to band index).

4.2.2 τ expansion

Applying the variational principle in this free-energy functional we can get the Ginzburg-Landau equation and the critical temperature equation. But, first we need to get the correct contributions to these equations. All relevant quantities of the problem, including the coherence length(s), are controlled by the same small parameter τ that we have discussed before. To get the explicit τ-dependence we introduce, as the first step, the scaling

$$\Delta_\nu = \tau^{1/2}\bar{\Delta}_\nu, \qquad \mathbf{r} = \tau^{-1/2}\bar{\mathbf{r}}, \qquad \mathbf{A} = \tau^{1/2}\bar{\mathbf{A}}, \qquad \mathbf{B} = \tau\bar{\mathbf{B}}. \tag{4.32}$$

One notes that the scaling of the spatial coordinates means $\mathbf{\nabla}_\mathbf{r} = \tau^{1/2}\bar{\mathbf{\nabla}}_\mathbf{r}$. The scaling of the free energy density is given by comparing with the single-band case. It is

$$f_s = f_{n,B=0} + \frac{1}{\tau}(g^{-1} - a_1)|\Delta|^2 + a_2|\mathbf{\nabla}\Delta|^2 + \frac{b_1}{2}|\Delta|^4,$$

because of the scaling of the order parameter and the magnetic field we have that

$$f = \bar{f}\tau^2$$

As the second step, we expand all the relevant quantities in τ, e.g.,

$$\begin{aligned}\bar{\Delta}_\nu =& \bar{\Delta}_\nu^{(0)} + \tau\bar{\Delta}_\nu^{(1)} + \cdots\,,\\ \bar{\mathbf{A}} =& \bar{\mathbf{A}}^{(0)} + \tau\bar{\mathbf{A}}^{(1)} + \cdots\,,\\ \bar{\mathbf{B}} =& \bar{\mathbf{B}}^{(0)} + \tau\bar{\mathbf{B}}^{(1)} + \cdots\,.\end{aligned}$$

By substituting these expressions in the free-energy expression and matching the same orders of magnitude, we get the τ-expansion for the free-energy functional.

We obtain

$$\bar{f}_s - \bar{f}_{n,B=0} = \tau^{-1}\bar{f}^{(-1)} + \tau^0\bar{f}^{(0)}. \tag{4.33}$$

Hereafter we omit bars over the scaled quantities unless it causes confusion. The lowest-order term in this expansion reads

$$f^{(-1)} = \vec{\mathbf{\Delta}}^{(0)\dagger}\check{L}\vec{\mathbf{\Delta}}^{(0)}, \tag{4.34}$$

where

$$\check{L} = \frac{1}{G}\begin{pmatrix} g_{22} - GN_1(0)\mathcal{A} & -g_{12} \\ -g_{12} & g_{11} - GN_2(0)\mathcal{A}\end{pmatrix}, \tag{4.35}$$

with

$$\mathcal{A} = \ln\frac{2e^\gamma\hbar\omega_D}{\pi T_{c0}} \tag{4.36}$$

T_{c0} the mean-field critical temperature and $N_i(0)$ is the DOS for the respective band. The leading-order term is

$$f^{(0)} = \frac{B^2}{8\pi} + \left(\vec{\mathbf{\Delta}}^{(0)\dagger}\check{L}\vec{\mathbf{\Delta}}^{(1)} + \text{c.c.}\right) + \sum_{\nu=1,2} f_\nu^{(0)}, \tag{4.37}$$

where

$$f_\nu^{(0)} = a_\nu|\Delta_\nu^{(0)}|^2 + \frac{b_\nu}{2}|\Delta_\nu^{(0)}|^4 + \mathcal{K}_\nu|\mathbf{D}\Delta_\nu^{(0)}|^2, \tag{4.38}$$

with $\mathbf{D} = \boldsymbol{\nabla} - i\frac{2e}{\hbar c}\mathbf{A}^{(0)}$. The coefficients of the expansion depend on the particular superconducting system.

4.2.3 Critical temperature equation

Taking the functional derivative of the free energy with the density $f^{(-1)}$ with respect to $\vec{\mathbf{\Delta}}^{(0)\dagger}$ and set it to zero we obtain

$$\check{L}\vec{\mathbf{\Delta}}^{(0)} = 0. \tag{4.39}$$

The condition to the existence of a nontrivial solution give us the critical temperature. This condition is

$$\det \check{L} = 0. \tag{4.40}$$

This means that

$$(g_{22} - N_1 G\mathcal{A})(g_{11} - N_2 G\mathcal{A}) - g_{12}^2 = 0. \tag{4.41}$$

This equation has two solutions but we have to choose the one with the largest critical temperature. To get a explicit expression for the critical temperature we will now calculate the solution to equation (4.39). If $\vec{\eta}$ is an eigenvector of the matrix $\check{L}$ and $\Psi(\mathbf{r})$ is, for now, an unknown function that we will specify later, we have that

$$\vec{\boldsymbol{\Delta}}^{(0)}(\mathbf{r}) = \Psi(\mathbf{r})\vec{\eta} \tag{4.42}$$

is a solution. Let us calculate $\vec{\eta}$. The characteristic equation of matrix $\check{L}$ is

$$(g_{22} - N_1 G\mathcal{A} - \lambda)(g_{11} - N_2 G\mathcal{A} - \lambda) = g_{12}^2,$$

where λ is the eigenvalue. However, the condition for a nontrivial solution that we have already considered means that we need to take the eigenvector associated with the $\lambda = 0$ eigenvalue. Therefore

$$\frac{1}{G}\begin{pmatrix} g_{22} - GN_1(0)\mathcal{A} & -g_{12} \\ -g_{12} & g_{11} - GN_2(0)\mathcal{A} \end{pmatrix}\vec{\eta} = 0,$$

$$\begin{pmatrix} g_{22} - GN_1(0)\mathcal{A} & -g_{12} \\ -g_{12} & g_{11} - GN_2(0)\mathcal{A} \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} = 0.$$

This system of equations has an infinite number of solutions different up to an arbitrary numerical factor. Choosing

$$\vec{\eta} = \begin{pmatrix} \sqrt{\frac{g_{12}}{g_{22} - GN_1\mathcal{A}}} \\ \sqrt{\frac{g_{22} - GN_1\mathcal{A}}{g_{12}}} \end{pmatrix}. \tag{4.43}$$

we can write

$$\vec{\boldsymbol{\Delta}}^{(0)} = \Psi(\mathbf{r})\begin{pmatrix} S^{-1/2} \\ S^{1/2} \end{pmatrix}, \tag{4.44}$$

with

$$S \equiv \frac{g_{22} - GN_1\mathcal{A}}{g_{12}}. \tag{4.45}$$

This result shows that the band order parameters are strictly proportional to one another with their position dependence governed by the $\psi(\mathbf{r})$ function.

We have calculated the eigenvector of $\check{L}$ because we need to use the value of S in our expression for the critical temperature. We can see that S is defined using $\mathcal{A}$ and the critical temperature is defined using $\mathcal{A}$. We wish to express the critical temperature in terms of the properties of the system only. To do this we will remove the dependence of S on $\mathcal{A}$. So, from the definition of S we have that

$$S = \frac{g_{22} - GN_1\mathcal{A}}{g_{12}},$$

or

$$\mathcal{A} = \frac{g_{22} - g_{12}S}{N_1 G}. \tag{4.46}$$

From the critical temperature equation

$$\frac{g_{12}}{g_{22} - GN_1\mathcal{A}} = \frac{g_{11} - GN_2\mathcal{A}}{g_{12}},$$

Since

$$\frac{1}{S} = \frac{g_{12}}{g_{22} - GN_1\mathcal{A}},$$

we can write

$$S^{-1} = \frac{g_{11} - GN_2\mathcal{A}}{g_{12}^2},$$

and we get

$$\mathcal{A} = \frac{g_{11} - g_{12}S^{-1}}{GN_2}. \tag{4.47}$$

Now, we can eliminate $\mathcal{A}$ from the equation and write

$$\frac{g_{12}S - g_{22}}{GN_1} = \frac{g_{12}S^{-1} - g_{11}}{GN_2}. \tag{4.48}$$

Introducing $\chi \equiv \frac{N_2}{N_1}$, this equation can be written as

$$\begin{aligned}
&\chi(g_{12}S - g_{22}) = g_{12}S^{-1} - g_{11},\\
&\chi g_{12}S^2 - g_{22}\chi S = g_{12} - g_{11}S,\\
&\chi g_{12}S^2 + S(g_{11} - g_{22}\chi) - g_{12} = 0,\\
&g_{12}S^2 + \Big(\frac{g_{11}}{\chi} - g_{22}\Big)S - \frac{g_{12}}{\chi} = 0.
\end{aligned}$$

Multiplying this equation by $(N_1 + N_2)$ we get

$$g_{12}(N_1 + N_2)S^2 + S\Big(\frac{g_{11}}{\chi} - g_{22}\Big)(N_1 + N_2) - \frac{g_{12}}{\chi}(N_1 + N_2) = 0.$$

We define $\lambda_{\mu\nu} \equiv g_{\mu\nu}(N_1 + N_2)$. So, we can write that

$$\lambda_{12}S^2 + \Big(\frac{\lambda_{11}}{\chi} - \lambda_{22}\Big)S - \frac{\lambda_{12}}{\chi} = 0. \tag{4.49}$$

Solving this quadratic equation we have two values of S. We take the one which gives the highest value for the critical temperature. It is

$$S = \frac{\Big(\lambda_{22} - \frac{\lambda_{11}}{\chi}\Big) + \sqrt{\Big(\lambda_{22} - \frac{\lambda_{11}}{\chi}\Big)^2 + 4\frac{\lambda_{12}^2}{\chi}}}{2\lambda_{12}} \tag{4.50}$$

Now, S is only given in terms of the system microscopic parameters χ and $\lambda_{\mu\nu}$. The last step in our calculation is to deal directly with the expression for the critical temperature and the value of $\mathcal{A}$. We got back to the following relation

$$\mathcal{A} = \frac{g_{22} - g_{12}S}{N_1 G}.$$

Now, let us write the following

$$\frac{N_1 + N_2}{1+\chi} = \frac{N_1 + N_2}{1 + \frac{N_2}{N_1}} = N_1\Big(\frac{N_1 + N_2}{N_1 + N_2}\Big) = N_1.$$

Then we substitute this expression in the relation for $\mathcal{A}$ as follows

$$\mathcal{A} = \frac{g_{22} - g_{12}}{\frac{N_1+N_2}{1+\chi}G} = (1+\chi)\frac{g_{22} - g_{12}S}{(N_1 + N_2)G} = (1+\chi)\frac{g_{22} - g_{12}S}{(N_1 + N_2)G}\left(\frac{N_1 + N_2}{N_1 + N_2}\right).$$

Following the definition of $\lambda_{\mu\nu}$, the above equation becomes

$$\mathcal{A} = (1+\chi)\frac{\lambda_{22} - \lambda_{11}S}{(N_1 + N_2)^2 G}.$$

The expression in the denominator can be written as

$$(N_1 + N_2)^2 G = (N_1 + N_2)^2(g_{11}g_{22} - g_{12}^2) = \lambda_{11}\lambda_{22} - \lambda_{12}^2$$

and so

$$\mathcal{A} = (1+\chi)\frac{\lambda_{22} - \lambda_{11}S}{\lambda_{11}\lambda_{22} - \lambda_{12}^2}. \tag{4.51}$$

Now, from equation (4.36) we find

$$T_{c0} = \frac{2e^{\gamma}\hbar\omega_D}{\pi}\exp\Big\{-(1+\chi)\frac{\lambda_{22} - \lambda_{11}S}{\lambda_{11}\lambda_{22} - \lambda_{12}^2}\Big\}. \tag{4.52}$$

For further illustration we use the fact that

$$T_{c0,1} = \frac{2e^{\gamma}\hbar\omega_D}{\pi}\exp\Big\{-\frac{1}{g_{11}N_1}\Big\},$$

where, $T_{c0,1}$ is the mean field critical temperature of band 1. The exponential function factor can be represented as

$$\exp\Big\{-\frac{1}{g_{11}N_1}\Big\} = \exp\left\{-\frac{1}{g_{11}\Big(\frac{N_1+N_2}{1+\chi}\Big)}\right\} = \exp\Big\{-\frac{1}{\frac{\lambda_{11}}{1+\chi}}\Big\},$$

and, finally, we get

$$\frac{T_{c0}}{T_{c0,1}} = \exp\Big\{(1+\chi)\Big(\frac{1}{\lambda_{11}} - \frac{\lambda_{22} - \lambda_{12}S}{\lambda_{11}\lambda_{22} - \lambda_{12}^2}\Big)\Big\}. \tag{4.53}$$

In the figure 13 we plot $\frac{T_{c0}}{T_{c0,1}}$ as function of the intra-band coupling λ_{12} for $\lambda_{22} = 0.3$ and $\lambda_{11} = 0.25$.

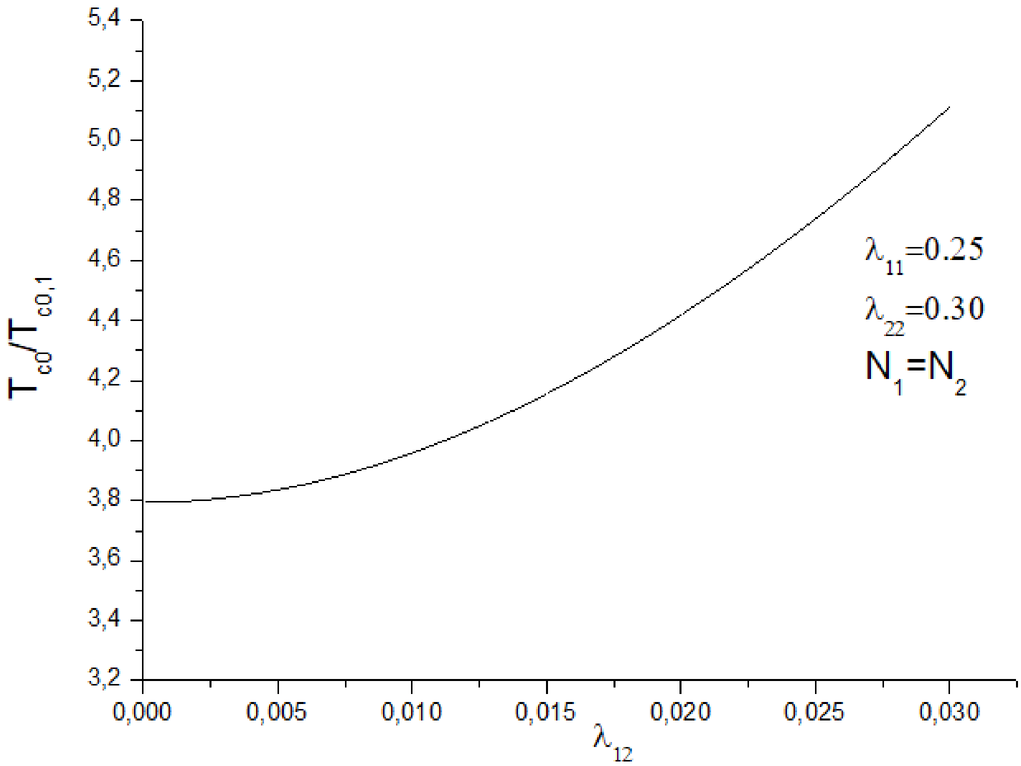


Figure 13: The mean-field critical temperature T_{c0} of the two-band superconductor versus λ_{12}.

4.2.4 Ginzburg-Landau equation for a two-band system

The free energy density contribution to the τ^0 order is

$$f^{(0)} = \frac{\mathbf{B}^2}{8\pi} + \vec{\mathbf{\Delta}}^{(0)\dagger}\check{L}\vec{\mathbf{\Delta}}^{(1)} + \vec{\mathbf{\Delta}}^{(0)}\check{L}\vec{\mathbf{\Delta}}^{(1)\dagger} + \sum_{\nu=1,2} f_\nu^{(0)}, \tag{4.54}$$

where

$$f_\nu^{(0)} = a_\nu|\Delta_\nu^{(0)}|^2 + \frac{b_\nu}{2}|\Delta_\nu^{(0)}|^4 - \mathcal{K}_\nu|\mathbf{D}\Delta_\nu^{(0)}|^2. \tag{4.55}$$

Taking the functional derivative of the free energy contribution corresponding to $f^{(0)}$ with respect to $\Delta_\nu^{(0)^\dagger}$, we obtain

$$\check{L}\vec{\mathbf{\Delta}^{(1)}} + \vec{\mathbf{W}}[\vec{\mathbf{\Delta}}^{(0)}] = 0, \tag{4.56}$$

where

$$\vec{\mathbf{W}} = \begin{pmatrix} W_1 \\ W_2 \end{pmatrix},$$

and $W_\nu = a_\nu \Delta_\nu^0 + b_\nu |\Delta_\nu^0|^2 \Delta_\nu^0 - \mathcal{K}_\nu \mathbf{D}^2 \Delta_\nu^0$. We can see that the stationary-point equation in this order for a two-band system mixes contributions from $\vec{\mathbf{\Delta}}^{(1)}$ and $\vec{\mathbf{\Delta}}^{(0)}$, unlike the single band case. However, despite this feature, we are still able to calculate $\Delta_\nu^{(0)}$ independently of $\Delta_\nu^{(1)}$. To do this, we express $\Delta^{(1)}$ as a linear combination of the following two linear independent vectors

$$\vec{\eta}_+ = \begin{pmatrix} S^{-1/2} \\ S^{1/2} \end{pmatrix}, \quad \vec{\eta}_- = \begin{pmatrix} S^{-1/2} \\ -S^{1/2} \end{pmatrix}, \tag{4.57}$$

i.e.,

$$\vec{\mathbf{\Delta}}^{(1)} = \phi_+(\mathbf{r})\vec{\eta}_+ + \phi_-(\mathbf{r})\vec{\eta}_-.$$

Substituting this expression in (4.56) we get

$$\phi_-(\mathbf{r})\check{L}\vec{\eta}_- + \vec{\mathbf{W}}[\vec{\mathbf{\Delta}}^0] = 0, \tag{4.58}$$

where we have taken into account the fact that $\vec{\eta}_+$ is an eigenvector of $\check{L}$ with zero eigenvalue. Projecting the obtained equation onto $\vec{\eta}_+$ we get

$$\vec{\eta}_+ \check{W}(\Delta^0) = 0, \tag{4.59}$$

as $\vec{\eta}_+ \check{L} = 0$. Now, let's write these matrices explicitly. They are

$$\left(S^{-1/2}, S^{1/2}\right) \begin{pmatrix} a_1\Psi(\mathbf{r})S^{-1/2} + b_1|\Psi(\mathbf{r})S^{-1/2}|^2\Psi(\mathbf{r})S^{-1/2} - \mathcal{K}_1\mathbf{D}^2\Psi(\mathbf{r})S^{-1/2} \\ a_1\Psi(\mathbf{r})S^{1/2} + b_1|\Psi(\mathbf{r})S^{1/2}|^2\Psi(\mathbf{r})S^{1/2} - \mathcal{K}_1\mathbf{D}^2\Psi(\mathbf{r})S^{1/2} \end{pmatrix},$$

which dictates

$$a\Psi(\mathbf{r}) + b|\Psi(\mathbf{r})|^2\Psi(\mathbf{r}) - \mathcal{K}\mathbf{D}^2\Psi(\mathbf{r}) = 0 \tag{4.60}$$

The relevant coefficients are averages over the contributing bands

$$a = a_1 S^{-1} + a_2 S, \tag{4.61}$$

$$b = b_1 S^{-2} + b_2 S^2, \tag{4.62}$$

$$\mathcal{K} = \mathcal{K}_1 S^{-1} + \mathcal{K}_2 S. \tag{4.63}$$

Thus, a consistent implementation of the two-band Ginzburg-Landau theory produces the effectively-single component Ginzburg-Landau formalism but with the parameters averaging over the both contributing bands. However, one should keep in mind that $\psi(\mathbf{r})$ can not be interpreted as an excitation gap but it is related to the band energy gaps through

$$\vec{\mathbf{\Delta}}^{(0)} = \Psi(\mathbf{r}) \begin{pmatrix} S^{-1/2} \\ S^{1/2} \end{pmatrix}. \tag{4.64}$$

5 FLUCTUATION THEORY

A major success in low temperature physics was achieved with the introduction of the notion of quasiparticles. According to this hypothesis the properties of many-body interacting system at low temperature are determined by the spectra of some low-energy, long-lived excitations. Another important milestone of many-body theory is the mean-field approximation. Phenomena which cannot be described by the quasiparticle method or by the mean field approximation are usually called fluctuation.

The BCS theory, as we saw in chapter 2, is a successful example of both quasiparticle and mean-field. However, BCS gives only good results for traditional superconductors. In the vicinity of transition, superconducting fluctuations influence different physical properties of a metal and lead to the appearance of small corrections to the corresponding physical characteristics in a wide range of temperatures. Our aim in this chapter is to consider how to deal with fluctuations and to demonstrate how to correct the critical temperature obtained from mean-field theory.

5.1 Fluctuation domain

The characteristics of high temperature and organic superconductors, low dimensional and amorphous superconducting systems studied nowadays strongly differ from those of the traditional superconductors discussed in Chapter 3. The phase transition turn out to be much more smeared out. The appearance of superconducting fluctuations above the critical temperature leads to precursor effects of the superconducting phase occurring while the system is still in the normal phase, sometimes far from the critical temperature. The conductivity, the heat capacity, the diamagnetic susceptibility, the sound attenuation, etc. may increase considerably in the vicinity of the transition temperature.

The first numerical estimation of the fluctuation contribution to the heat capacity of a superconductor in the vicinity of T_{c0} was done by Ginzburg in 1960[16]. In that paper he showed that superconducting fluctuations increase the heat capacity even above T_{c0}. In this way fluctuations change the temperature dependence of the specific heat in the vicinity of the critical temperature where, according to the phenomenological Landau theory of second-order phase transitions, a jump should take place. The range of temperatures where the fluctuation correction to the heat capacity of a bulk, clean, conventional superconductor is relevant was estimated by Ginzburg to be $\frac{\delta T}{T_{c0}} \sim 10^{-18}$. In the modern theory of phase transitions the relative temperature width of the fluctuation region is called the Ginzburg Number, Gi.

5.1.1 The Ginzburg number

This quantity is defined as

$$Gi \equiv 1 - \frac{T^*}{T_{c0}}, \tag{5.1}$$

where T^* is the Ginzburg-Levanyuk temperature. At this particular temperature fluctuations start to be important. The piece of physical information that will allow us to understand a little more about superconductors is that at this exact temperature the **fluctuation** contribution to the heat capacity is equal to the **mean field** contribution to the heat capacity. On this chapter we are going to calculate both mean-field and fluctuation contribution to the heat capacity. We will find T^* in terms of the Ginzburg-Landau coefficients(a, b and $\mathcal{K}$) and mean-field critical temperature(T_{c0}) and use it to calculate the Ginzburg number. With this number we will be able to know how much the temperature will shift from its mean-field result in consequence of thermal fluctuations.

5.2 Partition function and free energy

To calculate system properties we need to find the correct expression to the partition function, $\mathcal{Z}$. The partition function is composed of two different contributions: fluctuation and mean field. Because the free energy is of the form $F = F[\Delta(\mathbf{r})]$ we need to integrate all possible configurations of the system. In particular, for the fluctuation contribution we will need to integrate over all possible fluctuation fields. This means that we need perform a functional integration. But, what will be the fluctuation "Hamiltonian" for our system? We will need to reinterpret the free-energy functional as a fluctuation "Hamiltonian" and calculate the partition function. To this end we need first to deal with the free-energy functional.

5.2.1 Mean field and fluctuation contribution to the free energy

For a configuration of D-dimensions we have

$$\mathcal{F} = \int_{L^D} d^D\mathbf{r}\Big\{a|\Delta(\mathbf{r})|^2 + \frac{b}{2}|\Delta(\mathbf{r})|^4 + \mathcal{K}|\boldsymbol{\nabla}\Delta(\mathbf{r})|^2\Big\}. \tag{5.2}$$

If we consider that the order parameter varies from the uniform solution by a fluctuation field $\eta(\mathbf{r})$ we can write

$$\Delta(\mathbf{r}) = \Delta_0 + \eta(\mathbf{r}). \tag{5.3}$$

Where $\Delta_0^2 = -\frac{a}{b}$. Then the free-energy functional can be express as

$$\mathcal{F} = F_0 + H. \tag{5.4}$$

F_0 is the mean-field contribution to the free-energy density. H is called fluctuation "Hamiltonian" which is the fluctuation contribution to the free-energy density and only depends on the fluctuation fields $\eta(\mathbf{r})$ and $\eta^*(\mathbf{r})$. We gave it this name because, as we mention before, when we calculate the properties of the system we reinterpret the free energy as the "Hamiltonian". Therefore, the partition function which has the form

$$\mathcal{Z} = \int D[\Delta(\mathbf{r})] \exp\Big\{-\frac{1}{T}\mathcal{F}\Big\},$$

becomes

$$\mathcal{Z} = \exp\Big\{-\frac{1}{T}F_0\Big\} \int D[\eta(\mathbf{r})] \exp\Big\{-\frac{1}{T}H[\eta(\mathbf{r})\eta^*(\mathbf{r})]\Big\}, \tag{5.5}$$

where the integration is perform over all possible configurations of the Cooper pair wave function. Let us plug $\Delta(\mathbf{r}) = \Delta_0 + \eta(\mathbf{r})$ in the free-energy functional. We are only interested in the quadratic terms. We will see further why odd-power terms do not contribute to Gaussian fluctuations. Let's calculate each of the 3 terms of F individually. We have

$$a|\Delta(\mathbf{r})|^2 \to a(\Delta_0 + \eta(\mathbf{r}))(\Delta_0 + \eta^*(\mathbf{r})) = a\Delta_0^2 + a|\eta(\mathbf{r})|^2 + a\Delta_0\eta^*(\mathbf{r}) + a\Delta_0\eta(\mathbf{r}).$$

Keeping only the quadratic terms we obtain

$$a|\Delta(\mathbf{r})|^2 \to a\Delta_0^2 + a|\eta(\mathbf{r})|^2. \tag{5.6}$$

For the next term

$$\frac{b}{2}|\Delta(\mathbf{r})|^4 \to \frac{b}{2}\Big(\Delta_0 + \eta(\mathbf{r})\Big)^2\Big(\Delta_0 + \eta^*(\mathbf{r})\Big)^2.$$

Keeping only quadratic terms we get

$$\frac{b}{2}|\Delta(\mathbf{r})|^4 \to \frac{b}{2}\Big(\Delta_0^4 + \Delta_0^2\eta^*(\mathbf{r})^2 + 4\Delta_0^2|\eta(\mathbf{r})|^2 + \eta^2(\mathbf{r})\Delta_0^2\Big). \tag{5.7}$$

The last term becomes

$$\mathcal{K}\big|\boldsymbol{\nabla}\Delta(\mathbf{r})\big|^2 \to \mathcal{K}\big|\boldsymbol{\nabla}\left(\Delta_0 + \eta(\mathbf{r})\right)\big|^2 = \mathcal{K}|\boldsymbol{\nabla}\eta(\mathbf{r})|^2. \tag{5.8}$$

Δ_0 is not position dependent. Collecting the terms proportional to Δ_0 we obtain

$$F_0 = \int_{L^D} d^D\mathbf{r}\Big\{a\Delta_0^2 + \frac{b}{2}\Delta_0^4\Big\} = -\frac{a^2}{2b}L^D. \tag{5.9}$$

Now, collecting the remaining terms we obtain the fluctuation "Hamiltonian". It is

$$H = \int_{L^D} d^D\mathbf{r}\Big\{(a + 2b\Delta_0^2)|\eta^2(\mathbf{r})| + \frac{b}{2}\Delta_0^2\eta^2(\mathbf{r}) + \frac{b}{2}\Delta_0^2(\eta^*(\mathbf{r}))^2 + \mathcal{K}|\boldsymbol{\nabla}\eta(\mathbf{r})|^2\Big\}. \tag{5.10}$$

5.2.2 Fourier transform of the Gaussian "Hamiltonian"

We can write the fluctuation contribution to the partition function as

$$\mathcal{Z}_{FLUC} = \int [D\eta(\mathbf{r})] \exp\Big\{-\frac{1}{T} H(\eta(\mathbf{r}), \eta^*(\mathbf{r}))\Big\}. \tag{5.11}$$

As we said before it involves a functional integral. We, however, can deal with this by first transforming the fluctuation fields from configuration space to the momentum space and then separating the real and imaginary parts of this field. We will perform the following Fourier transform into momentum space

$$\eta(\mathbf{r}) = \frac{1}{L^{D/2}} \sum_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{r}} \eta_{\mathbf{q}}, \qquad \eta^*(\mathbf{r}) = \frac{1}{L^{D/2}} \sum_{\mathbf{q}} e^{-i\mathbf{q}\cdot\mathbf{r}} \eta^*_{\mathbf{q}}. \tag{5.12}$$

Now, to make it easier to see each term, let us express the Gaussian "Hamiltonian" as

$$\begin{aligned} H = {}& (a + 2b\Delta_0^2) \int_{L^D} d^D\mathbf{r} |\eta^2(\mathbf{r})| + \frac{b}{2}\Delta_0^2 \int_{L^D} d^D\mathbf{r}\eta^2(\mathbf{r}) \\ & + \frac{b}{2}\Delta_0^2 \int_{L^D} d^D\mathbf{r}(\eta^*(\mathbf{r}))^2 + \mathcal{K} \int_{L^D} d^D\mathbf{r} |\boldsymbol{\nabla}\eta(\mathbf{r})|^2. \end{aligned}$$

Now, we perform the transformation into momentum space. The first integral becomes

$$\int_{L^D} d^D\mathbf{r} |\eta(\mathbf{r})|^2 = \int_{L^D} d^D\mathbf{r} \frac{1}{L^D} \sum_{\mathbf{q},\mathbf{q}'} e^{i(\mathbf{q}-\mathbf{q}')\cdot\mathbf{r}} \eta_{\mathbf{q}}\eta^*_{\mathbf{q}'} = \sum_{\mathbf{q},\mathbf{q}'} \eta_{\mathbf{q}}\eta^*_{\mathbf{q}'}\delta_{\mathbf{q},\mathbf{q}'} = \sum_{\mathbf{q}} |\eta_{\mathbf{q}}|^2.$$

The second integral is

$$\int_{L^D} d^D\mathbf{r}\eta^2(\mathbf{r}) = \int_{L^D} d^D\mathbf{r} \frac{1}{L^D} \sum_{\mathbf{q},\mathbf{q}'} e^{i(\mathbf{q}+\mathbf{q}')\cdot\mathbf{r}} \eta_{\mathbf{q}}\eta_{\mathbf{q}'} = \sum_{\mathbf{q},\mathbf{q}'} \eta_{\mathbf{q}}\eta_{\mathbf{q}'}\delta_{\mathbf{q},-\mathbf{q}'} = \sum_{\mathbf{q}} \eta_{\mathbf{q}}\eta_{-\mathbf{q}}.$$

The third integral becomes

$$\begin{aligned} \int_{L^D} d^D\mathbf{r}(\eta^*(\mathbf{r}))^2 &= \int_{L^D} d^D\mathbf{r} \frac{1}{L^D} \sum_{\mathbf{q},\mathbf{q}'} e^{-i(\mathbf{q}+\mathbf{q}')\cdot\mathbf{r}} \eta^*_{\mathbf{q}}\eta^*_{\mathbf{q}'} \\ &= \sum_{\mathbf{q},\mathbf{q}'} \eta^*_{\mathbf{q}}\eta^*_{\mathbf{q}'}\delta_{\mathbf{q},-\mathbf{q}'} = \sum_{\mathbf{q}} \eta^*_{\mathbf{q}}\eta^*_{-\mathbf{q}}. \end{aligned}$$

The last term is

$$\begin{aligned} \int_{L^D} d^D\mathbf{r} |\boldsymbol{\nabla}\eta(\mathbf{r})|^2 &= \int_{L^D} d^D\mathbf{r} \frac{1}{L^D} \sum_{\mathbf{q},\mathbf{q}'} \boldsymbol{\nabla}\Big(e^{i\mathbf{q}\cdot\mathbf{r}}\eta_{\mathbf{q}}\Big) \cdot \boldsymbol{\nabla}\Big(e^{-i\mathbf{q}\cdot\mathbf{r}}\eta^*_{\mathbf{q}}\Big) \\ &= \sum_{\mathbf{q},\mathbf{q}'} q^2 e^{i(\mathbf{q}-\mathbf{q}')\cdot\mathbf{r}} \eta_{\mathbf{q}}\eta^*_{\mathbf{q}} = \sum_{\mathbf{q}} q^2 |\eta_{\mathbf{q}}|^2. \end{aligned}$$

Collecting all terms we obtain

$$H = \sum_{\mathbf{q}} (a + 2b\Delta_0^2 + \mathcal{K}q^2)|\eta_{\mathbf{q}}|^2 + \frac{b}{2}\Delta_0^2 \Big\{\eta_{\mathbf{q}}\eta_{-\mathbf{q}} + \eta^*_{\mathbf{q}}\eta^*_{-\mathbf{q}}\Big\}. \tag{5.13}$$

Now we separate the real and imaginary parts of the fluctuation field. We can write

$$\eta_{\mathbf{q}} = x_{\mathbf{q}} + i y_{\mathbf{q}}, \tag{5.14}$$

where, $x_{\mathbf{q}} = \mathrm{Re}\{\eta_{\mathbf{q}}\}$ and $y_{\mathbf{q}} = \mathrm{Im}\{\eta_{\mathbf{q}}\}$. Then, the Gaussian "Hamiltonian" becomes

$$H = \sum_{\mathbf{q}} \Big\{ (a + 2b\Delta_0 + \mathcal{K}q^2)(x_{\mathbf{q}}^2 + y_{\mathbf{q}}^2) + \frac{b}{2}\Delta_0^2 (2x_{\mathbf{q}}x_{-\mathbf{q}} - 2y_{\mathbf{q}}y_{-\mathbf{q}}) \Big\}. \tag{5.15}$$

If we denote: $A_{\mathbf{q}} = a + 2b\Delta_0^2 + \mathcal{K}q^2$ and $B = b\Delta_0^2$ we will have the following

$$H = \sum_{\mathbf{q}} \Big\{ A_{\mathbf{q}}\big(x_{\mathbf{q}}^2 + y_{\mathbf{q}}^2\big) + B\big(x_{\mathbf{q}}x_{-\mathbf{q}} - y_{\mathbf{q}}y_{-\mathbf{q}}\big) \Big\}. \tag{5.16}$$

Let us now express it in a more convenient form. Because of the summation over all momenta q we have the following relations

$$\sum_{\mathbf{q}} A_{\mathbf{q}} x_{\mathbf{q}}^2 = \sum_{\mathbf{q}} A_{\mathbf{q}} x_{-\mathbf{q}}^2 \qquad \sum_{\mathbf{q}} B x_{\mathbf{q}} x_{-\mathbf{q}} = \sum_{\mathbf{q}} B x_{-\mathbf{q}} x_{\mathbf{q}},$$
$$\sum_{\mathbf{q}} A_{\mathbf{q}} y_{\mathbf{q}}^2 = \sum_{\mathbf{q}} A_{\mathbf{q}} y_{-\mathbf{q}}^2 \qquad \sum_{\mathbf{q}} B y_{\mathbf{q}} y_{-\mathbf{q}} = \sum_{\mathbf{q}} B y_{-\mathbf{q}} y_{\mathbf{q}}.$$

Using these relations we can write

$$\begin{aligned} H = & \frac{1}{2}\sum_{\mathbf{q}} \Big[A_{\mathbf{q}} x_{\mathbf{q}}^2 + B x_{\mathbf{q}} x_{-\mathbf{q}} + B x_{-\mathbf{q}} x_{\mathbf{q}} + A_{\mathbf{q}} x_{-\mathbf{q}}^2 \Big] \\ & + \frac{1}{2}\sum_{\mathbf{q}} \Big[A_{\mathbf{q}} y_{\mathbf{q}}^2 - B y_{\mathbf{q}} y_{-\mathbf{q}} - B y_{-\mathbf{q}} y_{\mathbf{q}} + A_{\mathbf{q}} y_{-\mathbf{q}}^2 \Big]. \end{aligned}$$

Now we can express this fluctuation "Hamiltonian" in the matrix form

$$H = \frac{1}{2}\sum_{\mathbf{q}} \left[\big(x_{\mathbf{q}}, x_{-\mathbf{q}}\big) \begin{pmatrix} A_{\mathbf{q}} & B \\ B & A_{\mathbf{q}} \end{pmatrix} \begin{pmatrix} x_{\mathbf{q}} \\ x_{-\mathbf{q}} \end{pmatrix} + \big(y_{\mathbf{q}}, y_{-\mathbf{q}}\big) \begin{pmatrix} A_{\mathbf{q}} & -B \\ -B & A_{\mathbf{q}} \end{pmatrix} \begin{pmatrix} y_{\mathbf{q}} \\ y_{-\mathbf{q}} \end{pmatrix} \right]. \tag{5.17}$$

It is convenient to rewrite this expression as

$$H = \sum_{\mathbf{q}, q_x \geq 0} \left[\big(x_{\mathbf{q}}, x_{-\mathbf{q}}\big) \begin{pmatrix} A_{\mathbf{q}} & B \\ B & A_{\mathbf{q}} \end{pmatrix} \begin{pmatrix} x_{\mathbf{q}} \\ x_{-\mathbf{q}} \end{pmatrix} + \big(y_{\mathbf{q}}, y_{-\mathbf{q}}\big) \begin{pmatrix} A_{\mathbf{q}} & -B \\ -B & A_{\mathbf{q}} \end{pmatrix} \begin{pmatrix} y_{\mathbf{q}} \\ y_{-\mathbf{q}} \end{pmatrix} \right] \tag{5.18}$$

and represent the fluctuation contribution to the partition function in the form

$$\mathcal{Z}_{FLUC} = \int \prod_{\mathbf{q}, q_x \geq 0} \Big[\big(dx_{\mathbf{q}} dx_{-\mathbf{q}} dy_{\mathbf{q}} dy_{-\mathbf{q}}\big)\, e^{-\frac{1}{T} H[x_{\mathbf{q}}, x_{-\mathbf{q}}, y_{\mathbf{q}}, y_{-\mathbf{q}}]} \Big]. \tag{5.19}$$

The auxiliary restriction of the summation and product to the domain $q_x \geq 0$ is a matter of our convenience. One can also use, e.g., $q_y \geq 0$ or $q_z \geq 0$. The final results are not sensitive to such an auxiliary procedure.

5.2.3 Diagonalization of the "Hamiltonian"

As we can see our fluctuation "Hamiltonian" is not diagonal. Calculations with Hamiltonians in the diagonal form are easier. Let us diagonalize the relevant Gaussian "Hamiltonian", introducing new variables $\alpha_{\mathbf{q}}$, $\beta_{\mathbf{q}}$, $\eta_{\mathbf{q}}$, and $\zeta_{\mathbf{q}}$ as follows:

$$\begin{pmatrix} x_{\mathbf{q}}, x_{-\mathbf{q}} \end{pmatrix} \begin{pmatrix} A_{\mathbf{q}} & B \\ B & A_{\mathbf{q}} \end{pmatrix} \begin{pmatrix} x_{\mathbf{q}} \\ x_{-\mathbf{q}} \end{pmatrix} = \begin{pmatrix} \alpha_{\mathbf{q}}, \beta_{\mathbf{q}} \end{pmatrix} \begin{pmatrix} E^{(x)}_{\mathbf{q},+} & 0 \\ 0 & E^{(x)}_{\mathbf{q},-} \end{pmatrix} \begin{pmatrix} \alpha_{\mathbf{q}} \\ \beta_{\mathbf{q}} \end{pmatrix}, \tag{5.20}$$

and

$$\begin{pmatrix} y_{\mathbf{q}}, y_{-\mathbf{q}} \end{pmatrix} \begin{pmatrix} A_{\mathbf{q}} & -B \\ -B & A_{\mathbf{q}} \end{pmatrix} \begin{pmatrix} y_{\mathbf{q}} \\ y_{-\mathbf{q}} \end{pmatrix} = \begin{pmatrix} \xi_{\mathbf{q}}, \zeta_{\mathbf{q}} \end{pmatrix} \begin{pmatrix} E^{(y)}_{\mathbf{q},+} & 0 \\ 0 & E^{(y)}_{\mathbf{q},-} \end{pmatrix} \begin{pmatrix} \xi_{\mathbf{q}} \\ \zeta_{\mathbf{q}} \end{pmatrix}. \tag{5.21}$$

Here, $E^{(x)}_{\mathbf{q},+}$ and $E^{(x)}_{\mathbf{q},-}$ are the eigenvalues of diagonal fluctuation modes associated with the real component of the fluctuation field and $E^{(y)}_{\mathbf{q},+}$ and $E^{(y)}_{\mathbf{q},-}$ are associated with its imaginary component. If the unitary matrix $\mathcal{U}_x$ is made of eigenvectors of $\begin{pmatrix} A_{\mathbf{q}} & B \\ B & A_{\mathbf{q}} \end{pmatrix}$, then

$$\mathcal{U}_x^{\dagger} \begin{pmatrix} A_{\mathbf{q}} & B \\ B & A_{\mathbf{q}} \end{pmatrix} \mathcal{U}_x = \begin{pmatrix} E^{(x)}_{\mathbf{q},+} & 0 \\ 0 & E^{(x)}_{\mathbf{q},-} \end{pmatrix},$$

and we can write

$$\begin{pmatrix} x_{\mathbf{q}}, x_{-\mathbf{q}} \end{pmatrix} \mathcal{U}_x \mathcal{U}_x^{\dagger} \begin{pmatrix} A_{\mathbf{q}} & B \\ B & A_{\mathbf{q}} \end{pmatrix} \mathcal{U}_x \mathcal{U}_x^{\dagger} \begin{pmatrix} x_{\mathbf{q}} \\ x_{-\mathbf{q}} \end{pmatrix} = \begin{pmatrix} \alpha_{\mathbf{q}}, \beta_{\mathbf{q}} \end{pmatrix} \begin{pmatrix} E^{(x)}_{\mathbf{q},+} & 0 \\ 0 & E^{(x)}_{\mathbf{q},-} \end{pmatrix} \begin{pmatrix} \alpha_{\mathbf{q}} \\ \beta_{\mathbf{q}} \end{pmatrix},$$

where

$$\mathcal{U}_x^{\dagger} \begin{pmatrix} x_{\mathbf{q}} \\ x_{-\mathbf{q}} \end{pmatrix} = \begin{pmatrix} \alpha_{\mathbf{q}} \\ \beta_{\mathbf{q}} \end{pmatrix} \quad \text{or} \quad \begin{pmatrix} x_{\mathbf{q}}, x_{-\mathbf{q}} \end{pmatrix} \mathcal{U}_x = \begin{pmatrix} \alpha_{\mathbf{q}}, \beta_{\mathbf{q}} \end{pmatrix}. \tag{5.22}$$

Similarly, if the unitary matrix $\mathcal{U}_y$ is made of eigenvectors of $\begin{pmatrix} A_{\mathbf{q}} & -B \\ -B & A_{\mathbf{q}} \end{pmatrix}$, then

$$\mathcal{U}_y^{\dagger} \begin{pmatrix} A_{\mathbf{q}} & -B \\ -B & A_{\mathbf{q}} \end{pmatrix} \mathcal{U}_y = \begin{pmatrix} E^{(y)}_{\mathbf{q},+} & 0 \\ 0 & E^{(y)}_{\mathbf{q},-} \end{pmatrix},$$

and we have

$$\begin{pmatrix} y_{\mathbf{q}}, y_{-\mathbf{q}} \end{pmatrix} \mathcal{U}_y \mathcal{U}_y^{\dagger} \begin{pmatrix} A_{\mathbf{q}} & -B \\ -B & A_{\mathbf{q}} \end{pmatrix} \mathcal{U}_y \mathcal{U}_y^{\dagger} \begin{pmatrix} y_{\mathbf{q}} \\ y_{-\mathbf{q}} \end{pmatrix} = \begin{pmatrix} \xi_{\mathbf{q}}, \zeta_{\mathbf{q}} \end{pmatrix} \begin{pmatrix} E^{(y)}_{\mathbf{q},+} & 0 \\ 0 & E^{(y)}_{\mathbf{q},-} \end{pmatrix} \begin{pmatrix} \xi_{\mathbf{q}} \\ \zeta_{\mathbf{q}} \end{pmatrix},$$

where

$$\mathcal{U}_y^{\dagger} \begin{pmatrix} y_{\mathbf{q}} \\ y_{-\mathbf{q}} \end{pmatrix} = \begin{pmatrix} \xi_{\mathbf{q}} \\ \zeta_{\mathbf{q}} \end{pmatrix} \quad \text{or} \quad \begin{pmatrix} y_{\mathbf{q}}, y_{-\mathbf{q}} \end{pmatrix} \mathcal{U}_y = \begin{pmatrix} \xi_{\mathbf{q}}, \zeta_{\mathbf{q}} \end{pmatrix}. \tag{5.23}$$

Our next step is to explicitly find the unitary transformations $\mathcal{U}_x$ and $\mathcal{U}_y$. The eigenvalue equation associated with $\mathcal{U}_x$ is

$$\begin{pmatrix} A_{\mathbf{q}} & B \\ B & A_{\mathbf{q}} \end{pmatrix} \begin{pmatrix} u_{\pm}^{(x)} \\ v_{\pm}^{(x)} \end{pmatrix} = E_{\mathbf{q},\pm}^{(x)} \begin{pmatrix} u_{\pm}^{(x)} \\ v_{\pm}^{(x)} \end{pmatrix}. \tag{5.24}$$

A solution for this equation exists when

$$\det \begin{pmatrix} A_{\mathbf{q}} - E_{\mathbf{q},\pm}^{(x)} & B \\ B & A_{\mathbf{q}} - E_{\mathbf{q},\pm}^{(x)} \end{pmatrix} = 0.$$

This, of course, means that

$$E_{\mathbf{q},+}^{(x)} = A_{\mathbf{q}} + B, \qquad E_{\mathbf{q},-}^{(x)} = A_{\mathbf{q}} - B.$$

The eigenvector for $E_{\mathbf{q},+}^{(x)}$ is given by

$$\begin{pmatrix} A_{\mathbf{q}} & B \\ B & A_{\mathbf{q}} \end{pmatrix} \begin{pmatrix} u_{+}^{(x)} \\ v_{+}^{(x)} \end{pmatrix} = (A_{\mathbf{q}} + B) \begin{pmatrix} u_{+}^{(x)} \\ v_{+}^{(x)} \end{pmatrix},$$

where the normalization condition $u_{+}^{(x)2} + v_{+}^{(x)2} = 1$ is assumed. So, we get

$$u_{+}^{(x)} = \frac{1}{\sqrt{2}} \text{ and } v_{+}^{(x)} = \frac{1}{\sqrt{2}}.$$

Proceeding in the same fashion, we get that the components of the eigenvector for $E_{\mathbf{q},-}^{(x)}$ are

$$u_{-}^{(x)} = \frac{1}{\sqrt{2}} \text{ and } v_{-}^{(x)} = -\frac{1}{\sqrt{2}}.$$

So, the unitary transformation associated with the real part of the fluctuation field is given by

$$\mathcal{U}_x = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}. \tag{5.25}$$

This means that

$$\begin{pmatrix} x_{\mathbf{q}} \\ x_{-\mathbf{q}} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} \alpha_{\mathbf{q}} \\ b_{\mathbf{q}} \end{pmatrix}. \tag{5.26}$$

The eigenvalue equation associated with $\mathcal{U}_y$ reads

$$\begin{pmatrix} A_{\mathbf{q}} & -B \\ -B & A_{\mathbf{q}} \end{pmatrix} \begin{pmatrix} u_{\pm}^{(y)} \\ v_{\pm}^{(y)} \end{pmatrix} = E_{\mathbf{q},\pm}^{(y)} \begin{pmatrix} u_{\pm}^{(y)} \\ v_{\pm}^{(y)} \end{pmatrix}.$$

From the condition of a non-trivial solution we get

$$E_{\mathbf{q},+}^{(y)} = A_{\mathbf{q}} + B, \qquad E_{\mathbf{q},-}^{(y)} = A_{\mathbf{q}} - B. \tag{5.27}$$

Then, the eigenvector corresponding to $E^{(y)}_{\mathbf{q},+}$ is given by

$$u^{(y)}_{+} = \frac{1}{\sqrt{2}} \text{ and } v^{(y)}_{+} = -\frac{1}{\sqrt{2}}.$$

For $E^{(x)}_{\mathbf{q},-}$ one obtains

$$u^{(x)}_{-} = \frac{1}{\sqrt{2}} \text{ and } v^{(x)}_{-} = \frac{1}{\sqrt{2}}.$$

Thus, the corresponding unitary transformation is

$$\mathcal{U}_y = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}, \tag{5.28}$$

and

$$\begin{pmatrix} y_{\mathbf{q}} \\ y_{-\mathbf{q}} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} \begin{pmatrix} \xi_{\mathbf{q}} \\ \zeta_{\mathbf{q}} \end{pmatrix}. \tag{5.29}$$

Thus, the diagonalized Gaussian fluctuation “Hamiltonian" writes

$$\begin{aligned} H = & \sum_{\mathbf{q},q_x \geq 0} \begin{pmatrix} \alpha_{\mathbf{q}}, \beta_{\mathbf{q}} \end{pmatrix} \begin{pmatrix} A_{\mathbf{q}} + B & 0 \\ 0 & A_{\mathbf{q}} - B \end{pmatrix} \begin{pmatrix} \alpha_{\mathbf{q}} \\ \beta_{\mathbf{q}} \end{pmatrix} \\ & + \sum_{\mathbf{q},q_x \geq 0} \begin{pmatrix} \xi_{\mathbf{q}}, \zeta_{\mathbf{q}} \end{pmatrix} \begin{pmatrix} A_{\mathbf{q}} + B & 0 \\ 0 & A_{\mathbf{q}} - B \end{pmatrix} \begin{pmatrix} \xi_{\mathbf{q}} \\ \zeta_{\mathbf{q}} \end{pmatrix}. \end{aligned} \tag{5.30}$$

Then, the fluctuation contribution to the partition function becomes

$$\mathcal{Z}_{FLUC} = \int \prod_{\mathbf{q},q_x \geq 0} \left[\left(d\alpha_{\mathbf{q}} d\beta_{\mathbf{q}} d\eta_{\mathbf{q}} d\zeta_{\mathbf{q}} \right) \, \exp\left\{ -\frac{1}{T} H[\alpha_{\mathbf{q}}, \beta_{\mathbf{q}}, \eta_{\mathbf{q}}, \zeta_{\mathbf{q}}] \right\} \right]. \tag{5.31}$$

5.3 Calculation of the heat capacity

The heat capacity is proportional to the second derivative of the free energy with respect to the temperature. Let us calculate the fluctuation contribution to the free energy.

5.3.1 Fluctuation contribution to the free energy

The fluctuation contribution to the free-energy is given by

$$F_{FLUC} = -T \ln Z_{FLUC}. \tag{5.32}$$

Explicitly writing the partition function, we get

$$\begin{aligned} F_{FLUC} &= -T \ln \int \prod_{\mathbf{q},q_x \geq 0} d\alpha_{\mathbf{q}} d\beta_{\mathbf{q}} \exp\left\{ -\frac{1}{T} \sum_{\mathbf{q},q_x \geq 0} (A_{\mathbf{q}} + B)\alpha^2_{\mathbf{q}} + (A_{\mathbf{q}} - B)\beta^2_{\mathbf{q}} \right\} \\ &= -T \ln \int \prod_{\mathbf{q},q_x \geq 0} d\xi_{\mathbf{q}} d\zeta_{\mathbf{q}} \exp\left\{ -\frac{1}{T} \sum_{\mathbf{q},q_x \geq 0} (A_{\mathbf{q}} + B)\xi^2_{\mathbf{q}} + (A_{\mathbf{q}} - B)\zeta^2_{\mathbf{q}} \right\}. \end{aligned}$$

This is simply a Gaussian integral. We find that

$$F_{FLUC} = -T \ln \left(\prod_{\mathbf{q},q_x \geq 0} \sqrt{\frac{\pi T}{A_\mathbf{q} + B}} \sqrt{\frac{\pi T}{A_\mathbf{q} - B}} \sqrt{\frac{\pi T}{A_\mathbf{q} + B}} \sqrt{\frac{\pi T}{A_\mathbf{q} - B}} \right),$$

And finally

$$F_{FLUC} = -T \sum_{\mathbf{q},q_x \geq 0} \left(\ln \frac{\pi T}{A_\mathbf{q} + B} + \ln \frac{\pi T}{A_\mathbf{q} - B} \right),$$

which can be rewritten as

$$F_{FLUC} = -\frac{T}{2} \sum_{\mathbf{q}} \left(\ln \frac{\pi T}{A_\mathbf{q} + B} + \ln \frac{\pi T}{A_\mathbf{q} - B} \right). \tag{5.33}$$

Below the critical temperature, the second term of the fluctuation contribution to the heat capacity is

$$-\frac{T}{2} \sum_{\mathbf{q}} \ln \frac{\pi T}{A_\mathbf{q} - B} = -\frac{T}{2} \sum_{\mathbf{q}} \ln \frac{\pi T}{\mathcal{K} \mathbf{q}^2},$$

this term does not include the parameter a and slowly varies with temperature. To get the critical contribution, we can include only the contribution to the free energy related to $A_\mathbf{q} + B = 2|a| + \mathcal{K}\mathbf{q}^2$. So we write

$$F_{FLUC}^{crit} = -\frac{T_{c0}}{2} \sum_{\mathbf{q}} \ln \frac{\pi T_{c0}}{2|a| + \mathcal{K}\mathbf{q}^2}, \tag{5.34}$$

where the temperature dependence is only kept in a.

5.3.2 Fluctuation contribution to the entropy

The entropy is proportional to the first derivative of the free-energy with respect to the temperature. We have

$$S_{FLUC}^{crit} = -\frac{\partial F_{FLUC}^{crit}}{\partial T} = \frac{T_{c0}}{2} \sum_{\mathbf{q}} \frac{\partial}{\partial T} \ln \frac{\pi T_{c0}}{2|a| + \mathcal{K}\mathbf{q}^2},$$

$$S_{FLUC}^{crit} = \alpha T_{c0} \sum_{\mathbf{q}} \frac{1}{2|a| + \mathcal{K}\mathbf{q}^2}, \tag{5.35}$$

where $|a| = \alpha(T - T_{c0})$. Now, we have everything at our disposal to calculate the fluctuation contribution to the heat capacity.

5.3.3 Fluctuation contribution to the heat capacity

From statistical mechanics we know that

$$C_v = T \frac{\partial S}{\partial T} \tag{5.36}$$

so, the critical contribution is

$$C_{v,FLUC}^{crit} = T_{c0}\frac{\partial S_{FLUC}^{crit}}{\partial T} = T_{c0}^2 2\alpha^2 \sum_{\mathbf{q}} \frac{1}{(2|a| + \mathcal{K}\mathbf{q}^2)^2}. \tag{5.37}$$

Now we can see why we kept the temperature dependency on $|a|$. The critical fluctuation contribution to the heat capacity becomes divergent as $T \to T_{c0}$ because $a \to 0$ in this limit. It is convenient to express this result in terms of superconducting quantities. We do the following

$$C_{v,FLUC}^{crit} = \frac{T_{c0}^2}{4\mathcal{K}^2} 2\alpha^2 \sum_{\mathbf{q}} \frac{1}{(\frac{|a|}{\mathcal{K}} + \frac{q^2}{2})^2},$$

$$C_{v,FLUC}^{crit} = \frac{1}{2\xi_0^4} \sum_{\mathbf{q}} \frac{1}{(\xi^{-2} + \frac{q^2}{2})^2}.$$

where $\xi = \sqrt{\frac{\mathcal{K}}{|a|}}$ is the Ginzburg-Landau coherence length, which makes $\xi_0 = \sqrt{\frac{\mathcal{K}}{\alpha T_{c0}}}$ the zero temperature coherence length. We can see that the asymptotic behavior of ξ is

$$\xi \to \infty \text{ when } T \to T_{c0}.$$

Which means that $C_{v,FLUC}^{crit} \to \infty$ when $T \to T_{c0}$. We can conclude that the critical behavior is due to the divergence of ξ which follows from the fact that $|a| \to 0$ near the critical temperature. This is why the temperature dependence of $|a|$ is decisive in the fluctuation free-energy.

We proceed with the calculations of the fluctuation contribution to the heat capacity for D-dimensions. We go from discreet variables to continuous by using the standard procedure

$$\sum_{\mathbf{q}} \to L^D \int \frac{d^D\mathbf{q}}{(2\pi)^D},$$

for D dimensions. Then, we obtain

$$C_{v,FLUC}^{crit} = 2T_{c0}^2\alpha^2 L^D \int \frac{d^D\mathbf{q}}{(2\pi)^D} \frac{1}{(2|a| + \mathcal{K}\mathbf{q}^2)^2}.$$

Let us solve this integral. First we do a change of variables

$$\mathbf{q}\sqrt{\mathcal{K}} \to \mathbf{p} \text{ which means that } d^D\mathbf{q} = \frac{d^D\mathbf{p}}{(\sqrt{\mathcal{K}})^D}.$$

And so

$$C_{v,FLUC}^{crit} = \frac{2T_{c0}^2\alpha^2 L^D}{\mathcal{K}^{D/2}} \int \frac{d^D\mathbf{p}}{(2\pi)^D} \frac{1}{(2|a| + \mathbf{p}^2)^2}. \tag{5.38}$$

Again, we do a change of variables

$$\frac{\mathbf{p}}{\sqrt{a}} \to \mathbf{m} \text{ which means that } d^D\mathbf{p} = (\sqrt{a})^D d^D\mathbf{m}.$$

And then

$$C_{v,FLUC}^{crit} = \frac{2T_{c0}^2\alpha^2 L^D}{\mathcal{K}^{D/2}|a|^2}|a|^{D/2}\int\frac{d^D\mathbf{m}}{(2\pi)^D}\frac{1}{(2+\mathbf{m}^2)^2}. \tag{5.39}$$

As $|a| = \alpha T_{c0}\tau$ with $\tau = 1 - \frac{T}{T_{c0}}$ we can write

$$C_{v,FLUC}^{crit} = \frac{L^D}{\tau^{2-D/2}}2\frac{\alpha^{D/2}T_{c0}^{D/2}}{\mathcal{K}^{D/2}}\int\frac{d^D\mathbf{m}}{(2\pi)^D}\frac{1}{(2+\mathbf{m}^2)^2}, \tag{5.40}$$

and as

$$\frac{\alpha^{D/2}T_{c0}^{D/2}}{\mathcal{K}^{D/2}} = \frac{1}{\xi_0^D},$$

we finally have that

$$C_{v,FLUC}^{crit} = \frac{L^D}{\tau^{2-D/2}}2\frac{1}{\xi_0^D}\int\frac{d^D\mathbf{m}}{(2\pi)^D}\frac{1}{(2+\mathbf{m}^2)^2}. \tag{5.41}$$

With this result one can see that

$$C_{v,FLUC}^{crit} \propto \begin{cases} \frac{1}{\tau^{1/2}}\frac{1}{\xi_0^3}, & \text{for } D=3; \\ \frac{1}{\tau}\frac{1}{\xi_0^2}, & \text{for } D=2; \\ \frac{1}{\tau^{3/2}}\frac{1}{\xi_0}, & \text{for } D=1. \end{cases} \tag{5.42}$$

We can conclude that the divergence of the heat capacity at the critical temperature is more pronounced in lower dimensions. Now we perform calculations of the integral for D=3, D=2 and D=1.

FOR D=3 equation (5.39) becomes

$$C_{v,FLUC}^{3D,crit} = \frac{2T_{c0}^2\alpha^2 L^3}{\mathcal{K}^{3/2}|a|^{1/2}}\int\frac{d^3\mathbf{m}}{(2\pi)^3}\frac{1}{(2+\mathbf{m}^2)^2} = \frac{2T_{c0}^2\alpha^2 L^3}{\mathcal{K}^{3/2}|a|^{1/2}}\frac{1}{8\pi\sqrt{2}},$$

Finally

$$C_{v,FLUC}^{3D,crit} = \frac{L^3}{4\pi\sqrt{2}}\frac{T_{c0}^2\alpha^2}{\sqrt{\mathcal{K}^3|a|}}. \tag{5.43}$$

For D=2 the Heat Capacity becomes

$$C_{v,FLUC}^{2D,crit} = \frac{2T_{c0}^2\alpha^2 L^2}{\mathcal{K}|a|^2}|a|\int\frac{d^2\mathbf{m}}{(2\pi)^2}\frac{1}{(2+\mathbf{m}^2)^2} = \frac{2T_{c0}^2\alpha^2 L^2}{\mathcal{K}|a|}\frac{1}{8\pi},$$

$$C_{v,FLUC}^{2D,crit} = \frac{L^2}{4\pi}\frac{T_{c0}^2\alpha^2}{\mathcal{K}|a|}. \tag{5.44}$$

For D=1 we have that

$$C_{v,FLUC}^{1D,crit} = \frac{2T_{c0}^2\alpha^2 L}{\mathcal{K}^{1/2}|a|^{3/2}}\int\frac{dm}{(2\pi)^2}\frac{1}{(2+m^2)^2} = \frac{2T_{c0}^2\alpha^2 L}{\mathcal{K}^{1/2}|a|^{3/2}}\frac{1}{16\sqrt{2}}$$

$$C_{v,FLUC}^{1D,crit} = \frac{T_{c0}^2\alpha^2 L}{\mathcal{K}^{1/2}|a|^{3/2}}\frac{1}{8\sqrt{2}}. \tag{5.45}$$

With these calculations we have obtained all the fluctuation contributions we need. Remember, however, that we also need the mean-field contribution to the heat capacity because our goal is to calculate the Ginzburg Number.

5.3.4 Mean-field contribution to the heat capacity

Finally, we need to calculate the mean-field values for the heat capacity which we know that at the Ginzburg-Levanyuk temperature will be the same as the fluctuation contribution. From equation (5.9) we know that

$$F_{m.f.} = -\frac{a^2}{2b} L^D. \tag{5.46}$$

The mean-field contribution to the entropy is

$$S_{m.f.} = -\frac{\partial F_{m.f.}}{\partial T} = -L^D \frac{|a|\alpha}{b}. \tag{5.47}$$

And the mean-field contribution to the heat capacity is

$$C_{v,m.f.} = T_{c0} \frac{\partial S_{m.f.}}{\partial T} = L^D \frac{T_{c0}\alpha^2}{b}. \tag{5.48}$$

5.4 Calculation of Ginzburg number

Before performing calculations for the different dimensions with the proper numerical coefficients let us derive a useful approximation for Gi. When the fluctuation and mean field contributions are equal ($T = T^*$ or $\tau = Gi$) we have that

$$L^D \frac{T_{c0}\alpha^2}{b} \sim \frac{L^D}{\tau^{2-D/2}} \frac{1}{\xi_0^D}\bigg|_{\tau=Gi}. \tag{5.49}$$

We will give this expression in terms of the jump of the mean-field heat capacity at the critical temperature per unity volume, i.e.

$$\Delta c = \frac{T_{c0}\alpha^2}{b}.$$

And so

$$\Delta c \sim \frac{1}{\xi_0^D \tau^{(4-D)/2}}\bigg|_{\tau=Gi},$$

which means that

$$Gi \sim \frac{1}{(\Delta c \xi_0^D)^{\frac{2}{4-D}}}. \tag{5.50}$$

The zero-temperature coherence length ξ_0 plays an important role in the estimation of the fluctuation impact. When ξ_0 decreases Gi increases and so the impact of fluctuation is more pronounced. This increase of the Ginzburg number is dependent on the dimension of the system. We can write

$$Gi \propto \begin{cases} \frac{1}{\xi_0^6} (D = 3); \\ \frac{1}{\xi_0^2} (D = 2); \\ \frac{1}{\xi_0} (D = 1). \end{cases} \tag{5.51}$$

Now, let us calculate Gi, including numerical coefficients. For this calculation we use the following criterion $C^{crit}_{v,FLUC}(T^*) = C_{v,m.f.}(T^*)$, to calculate Gi. **D=3**

$$\frac{L^3}{4\pi\sqrt{2}}\frac{T_{c0}^2\alpha^2}{\mathcal{K}^{3/2}|a(T^*)|^{1/2}} = L^3 T_{c0}\frac{\alpha^2}{b}. \tag{5.52}$$

But

$$\sqrt{|a(T^*)|} = \sqrt{\alpha(T_{c0} - T^*)} = \sqrt{\frac{\alpha}{T_{c0}}Gi}.$$

Substituting this result we obtain

$$\frac{L^3}{4\pi\sqrt{2}}\frac{T_{c0}^2 a^2}{\mathcal{K}^{3/2}\sqrt{\frac{\alpha}{T_{c0}}Gi}} = L^3 T_{c0}\frac{a^2}{b},$$

Solving for Gi we get

$$Gi^{3D} = \frac{T_{c0}b^2}{32\pi^2\alpha\mathcal{K}^3} \tag{5.53}$$

for the 3D case.

D=2

$$\frac{L^2}{4\pi}\frac{T_{c0}^2\alpha^2}{\mathcal{K}|a(T^*)|^2} = \frac{L^2 T_{c0}\alpha^2}{b}. \tag{5.54}$$

Because $a(T^*) = \alpha Gi T_{c0}$ we have

$$Gi^{2D} = \frac{b}{4\pi\alpha\mathcal{K}}. \tag{5.55}$$

D=1

$$\frac{T_{c0}^2\alpha^2 L}{\mathcal{K}^{1/2}|a|^{3/2}}\frac{1}{8\sqrt{2}} = \frac{L T_{c0}\alpha^2}{b}, \tag{5.56}$$

$$Gi^{1D} = \left(\frac{1}{128}\frac{b^2}{\mathcal{K}T_{c0}\alpha^3}\right)^{1/3}. \tag{5.57}$$

5.4.1 Calculation of Gi for deep band

As an example, consider a single-band superconductor with a deep band in the clean limit(see sec. 3.3.6). The values of the coefficients for $D = 3$ are

$$b_{3D} = N(0)\frac{7\zeta(3)}{8\pi^2 T_{c0}^2}, \qquad \mathcal{K}_{3D} = N(0)\frac{7\zeta(3)v_F^2}{8\pi^2 6 T_{c0}^2}, \qquad \alpha_{3D} = \frac{N(0)}{T_{co}}.$$

Substituting this values in the Ginzburg number expression for $3D$ we get

$$Gi^{3D} = T_{c0}^4\frac{32}{36\pi^2}\frac{8\pi^2}{7\zeta(3)}\frac{1}{N^2(0)v_F^6}. \tag{5.58}$$

Where, v_F is the fermi velocity and $N(0)$ is the 3 dimensional density of states (DOS). But, $v_F^6 N^2(0) = \frac{E_F^4}{2\pi^4}$, where E_F is the fermi energy. Therefore

$$Gi^{3D} = \frac{27\pi^4}{14\zeta(3)}\left(\frac{T_{c0}}{E_F}\right)^4. \tag{5.59}$$

For a typical deep band clean single band superconductor like aluminum we have that[17]

$$T_{c0} = 1.2K \approx 0.1MeV; \qquad E_F = 10^4.MeV \tag{5.60}$$

So, the usual value of the Ginzburg number for this kind of superconductor is

$$Gi^{3D} \approx 10^{-18}. \tag{5.61}$$

The Ginzburg-Landau coefficients for $2D$ are

$$b_{2D} = N_{2D}\frac{7\zeta(3)}{8\pi^2 T_{c0}^2}, \qquad \mathcal{K}_{2D} = N_{2D}\frac{7\zeta(3)v_F^2}{8\pi^2 6T_{c0}^2}, \qquad \alpha_{2D} = \frac{N_{2D}}{T_{co}}.$$

Where $N_{2D} = \frac{m}{2\pi}$ which is the 2 dimensional DOS. Then

$$Gi^{2D} = \frac{8\pi}{4\pi}\frac{T_{c0}}{mv_F^2} = \frac{T_{c0}}{\frac{k_F^2}{m}} = \frac{T_{c0}}{E_F}. \tag{5.62}$$

So

$$Gi^{2D} \approx 10^{-5}. \tag{5.63}$$

Clearly, as we have found earlier, the dimensionality player an important role. Finally for $D = 1$ we have that

$$b_{1D} = N_{1D}\frac{7\zeta(3)}{16\pi^2 T_{c0}^2}; \quad \mathcal{K}_{1D} = N_{1D}\frac{7\zeta(3)v_F^2}{16\pi^2 6T_{c0}^2}; \quad \alpha_{1D} = \frac{N_{1D}}{2T_{co}}. \tag{5.64}$$

Where $N_{1D} = \frac{m}{\pi k_F}$ and is the 1 dimensional DOS. The one dimension Ginzburg number is:

$$Gi^{1D} = \left(\frac{1}{128}\frac{b}{a^3}\frac{6}{v_F^2 T_{c0}}\right) \propto \left(\frac{T_{c0}}{E_F}\right)^0 \approx 1. \tag{5.65}$$

For $1D$ case Gi is so large that the mean-field approach does not make sense in the whole temperature range below T_{c0}. This cases are beyond the scope of the Gaussian fluctuation formalism.

5.5 General form of the "Hamiltonian"

As we move forward with our formalism, we need to generalize the fluctuation "Hamiltonian" to make our calculations easier. Suppose that our Hamiltonian with ϵ_+ and ϵ_- as eigenvalues can be expressed as

$$H = \sum_{\mathbf{q}} \left[\epsilon_+ (x_{\mathbf{q}}^2 + y_{\mathbf{q}}^2) + \epsilon_- (x_{\mathbf{q}} x_{-\mathbf{q}} - y_{\mathbf{q}} y_{-\mathbf{q}}) \right], \tag{5.66}$$

where, of course, we already have performed the Fourier transform of the fluctuation field and expressed the “Hamiltonian" in terms of the real and imaginary parts of the field $\eta_{\mathbf{q}}$[18]. After the diagonalization procedure we obtain

$$H = \sum_{\mathbf{q}, q_x \geq 0} \left[\epsilon_{1,\mathbf{q}} (\alpha_{\mathbf{q}}^2 + \xi_{\mathbf{q}}^2) + \epsilon_{2,\mathbf{q}} (\beta_{\mathbf{q}}^2 + \zeta_{\mathbf{q}}^2) \right], \tag{5.67}$$

where one finds

$$\alpha_{\mathbf{q}} = \frac{1}{\sqrt{2}} (x_{\mathbf{q}} + x_{-\mathbf{q}}), \qquad \beta_{\mathbf{q}} = \frac{1}{\sqrt{2}} (x_{\mathbf{q}} - x_{-\mathbf{q}}), \tag{5.68}$$

$$\xi_{\mathbf{q}} = \frac{1}{\sqrt{2}} (y_{\mathbf{q}} - y_{-\mathbf{q}}), \qquad \zeta_{\mathbf{q}} = \frac{1}{\sqrt{2}} (y_{\mathbf{q}} + y_{-\mathbf{q}}).$$

The relations between $\epsilon_\pm$ and $\epsilon_{1(2),\mathbf{q}}$ are

$$\epsilon_+ = \frac{\epsilon_{1,\mathbf{q}} + \epsilon_{2,\mathbf{q}}}{2}, \qquad \epsilon_- = \frac{\epsilon_{1,\mathbf{q}} - \epsilon_{2,\mathbf{q}}}{2}.$$

By comparing with equation (5.33) we can express the fluctuation contribution to the free energy as

$$F_{FLUC} = -\frac{T}{2} \sum_{\mathbf{q}} \left(\ln \frac{\pi T}{\epsilon_{1,\mathbf{q}}} + \ln \frac{\pi T}{\epsilon_{2,\mathbf{q}}} \right), \tag{5.69}$$

where

$$A_{\mathbf{q}} + B = \epsilon_{1,\mathbf{q}}, \qquad A_{\mathbf{q}} - B = \epsilon_{2,\mathbf{q}}.$$

We will use this convenient framework to calculate various averaged products of fluctuation fields.

5.6 Average of the fluctuation fields

Now we are going to calculate some averages of fluctuation fields.

5.6.1 Odd powers of fluctuation field

The average that we are dealing is done over fluctuation fields as we mentioned before. It is given by the following expression

$$\langle \psi(\mathbf{r}) \rangle = \frac{\int D[\eta(\mathbf{r})]\psi(\mathbf{r})e^{-\frac{H}{T}}}{\int D[\eta(\mathbf{r})]e^{-\frac{H}{T}}}. \tag{5.70}$$

Where H is the fluctuation “Hamiltonian" and $\psi(\mathbf{r})$ is an arbitrary function. Therefore, we have that

$$\langle \eta(\mathbf{r}) \rangle = \frac{\int D[\eta(\mathbf{r})]\eta(\mathbf{r})e^{-\frac{H}{T}}}{\int D[\eta(\mathbf{r})]e^{-\frac{H}{T}}}.$$

Performing a Fourier transform we get

$$\langle \eta_{\mathbf{q}} \rangle = \frac{\int D[\eta_{\mathbf{q}}]\eta_{\mathbf{q}}e^{-\frac{H}{T}}}{\int D[\eta_{\mathbf{q}}]e^{-\frac{H}{T}}}.$$

Separating the real and imaginary parts

$$\langle x_{\mathbf{q}} \rangle = \frac{\int D[\eta(\mathbf{r})]x_{\mathbf{q}}e^{-\frac{H}{T}}}{\int D[\eta(\mathbf{r})]e^{-\frac{H}{T}}}, \qquad \langle y_{\mathbf{q}} \rangle = \frac{\int D[\eta(\mathbf{r})]y_{\mathbf{q}}e^{-\frac{H}{T}}}{\int D[\eta(\mathbf{r})]e^{-\frac{H}{T}}}$$

To perform this calculation we are going to use the general diagonal fluctuation “Hamiltonian" that we have obtained last section. We will get the following expression for the average of the real part of the fluctuation field

$$\langle x_{\mathbf{q}} \rangle = \frac{\displaystyle\int \prod_{\mathbf{k},k_x\geq 0} x_{\mathbf{q}} e^{-\frac{1}{T}[\epsilon_{1,\mathbf{k}}(\alpha_{\mathbf{k}}^2+\xi_{\mathbf{k}}^2)+\epsilon_{2,\mathbf{k}}(\beta_{\mathbf{k}}^2+\zeta_{\mathbf{k}}^2)]} \; d\alpha_{\mathbf{k}} d\beta_{\mathbf{k}} d\xi_{\mathbf{k}} d\zeta_{\mathbf{k}}}{\displaystyle\int \prod_{\mathbf{k},k_x\geq 0} e^{-\frac{1}{T}[\epsilon_{1,\mathbf{k}}(\alpha_{\mathbf{k}}^2+\xi_{\mathbf{k}}^2)+\epsilon_{2,\mathbf{k}}(\beta_{\mathbf{k}}^2+\zeta_{\mathbf{k}}^2)]} \; d\alpha_{\mathbf{k}} d\beta_{\mathbf{k}} d\xi_{\mathbf{k}} d\zeta_{\mathbf{k}}} \tag{5.71}$$

Separating the terms for which $\mathbf{k} \neq \mathbf{q}$ we have the following expression

$$\begin{aligned}\langle x_{\mathbf{q}} \rangle =& \frac{\displaystyle\int x_{\mathbf{q}} e^{-\frac{1}{T}[\epsilon_{1,\mathbf{q}}(\alpha_{\mathbf{q}}^2+\xi_{\mathbf{q}}^2)+\epsilon_{2,\mathbf{q}}(\beta_{\mathbf{q}}^2+\zeta_{\mathbf{q}}^2)]} d\alpha_{\mathbf{q}} d\beta_{\mathbf{q}} d\xi_{\mathbf{q}} d\zeta_{\mathbf{q}}}{\displaystyle\int e^{-\frac{1}{T}[\epsilon_{1,\mathbf{q}}(\alpha_{\mathbf{q}}^2+\xi_{\mathbf{q}}^2)+\epsilon_{2,\mathbf{q}}(\beta_{\mathbf{q}}^2+\zeta_{\mathbf{q}}^2)]} d\alpha_{\mathbf{q}} d\beta_{\mathbf{q}} d\xi_{\mathbf{q}} d\zeta_{\mathbf{q}}} \times \\ &\times \frac{\displaystyle\int \prod_{\mathbf{k}\neq\mathbf{q},k_x\geq 0} e^{-\frac{1}{T}[\epsilon_{1,\mathbf{k}}(\alpha_{\mathbf{k}}^2+\xi_{\mathbf{k}}^2)+\epsilon_{2,\mathbf{k}}(\beta_{\mathbf{k}}^2+\zeta_{\mathbf{k}}^2)]} d\alpha_{\mathbf{k}} d\beta_{\mathbf{k}} d\xi_{\mathbf{k}} d\zeta_{\mathbf{k}}}{\displaystyle\int \prod_{\mathbf{k}\neq\mathbf{q},k_x\geq 0} e^{-\frac{1}{T}[\epsilon_{1,\mathbf{k}}(\alpha_{\mathbf{k}}^2+\xi_{\mathbf{k}}^2)+\epsilon_{2,\mathbf{k}}(b_{\mathbf{k}}^2+\zeta_{\mathbf{k}}^2)]} d\alpha_{\mathbf{k}} d\beta_{\mathbf{k}} d\xi_{\mathbf{k}} d\zeta_{\mathbf{k}}}.\end{aligned}$$

The first term in this expression is for $\mathbf{k} = \mathbf{q}$. The product is done over all values of $\mathbf{k}$.

There's no summation over $\mathbf{q}$. Because $x_{\mathbf{q}} = \frac{1}{\sqrt{2}}(\alpha_{\mathbf{q}} + \beta_{\mathbf{q}})$ we have that

$$\langle x_{\mathbf{q}} \rangle = \frac{\displaystyle\int \frac{1}{\sqrt{2}}(\alpha_{\mathbf{q}} + \beta_{\mathbf{q}}) e^{-\frac{1}{T}(\epsilon_{1,\mathbf{q}}\alpha_{\mathbf{q}}^2 + \epsilon_{2,\mathbf{q}}\beta_{\mathbf{q}}^2)} d\alpha_{\mathbf{q}} d\beta_{\mathbf{q}} \int d\xi_{\mathbf{q}} d\zeta_{\mathbf{q}} e^{-\frac{1}{T}\epsilon_{1,\mathbf{q}}\xi_{\mathbf{q}}^2 + \epsilon_{2,\mathbf{q}}\zeta_{\mathbf{q}}^2}}{\displaystyle\int e^{-\frac{1}{T}(\epsilon_{1,\mathbf{q}}\alpha_{\mathbf{q}}^2 + \epsilon_{2,\mathbf{q}}b_{\mathbf{q}}^2)} d\alpha_{\mathbf{q}} d\beta_{\mathbf{q}} \int d\xi_{\mathbf{q}} d\zeta_{\mathbf{q}} e^{-\frac{1}{T}\epsilon_{1,\mathbf{q}}\xi_{\mathbf{q}}^2 + \epsilon_{2,\mathbf{q}}\zeta_{\mathbf{q}}^2}},$$

$$\langle x_{\mathbf{q}} \rangle = \frac{1}{\sqrt{2}} \frac{\displaystyle\int (\alpha_{\mathbf{q}} + b_{\mathbf{q}}) e^{-\frac{1}{T}(\epsilon_{1,\mathbf{q}}\alpha_{\mathbf{q}}^2 + \epsilon_{2,\mathbf{q}}b_{\mathbf{q}}^2)} d\alpha_{\mathbf{q}} d\beta_{\mathbf{q}}}{\displaystyle\int e^{-\frac{1}{T}(\epsilon_{1,\mathbf{q}}a_{\mathbf{q}}^2 + \epsilon_{2,\mathbf{q}}b_{\mathbf{q}}^2)} d\alpha_{\mathbf{q}} d\beta_{\mathbf{q}}}.$$

And because the integral is a odd Gaussian integral its result is obviously zero. For the imaginary part we will follow the same calculation and get

$$\langle y_{\mathbf{q}} \rangle = \frac{1}{\sqrt{2}} \frac{\displaystyle\int (\xi_{\mathbf{q}} + \zeta_{\mathbf{q}}) e^{-\frac{1}{T}(\epsilon_{1,\mathbf{q}}\xi_{\mathbf{q}}^2 + \epsilon_{2,\mathbf{q}}\zeta_{\mathbf{q}}^2)} d\xi_{\mathbf{q}} d\zeta_{\mathbf{q}}}{\displaystyle\int e^{-\frac{1}{T}(\epsilon_{1,\mathbf{q}}\xi_{\mathbf{q}}^2 + \epsilon_{2,\mathbf{q}}\zeta_{\mathbf{q}}^2)} d\xi_{\mathbf{q}} d\zeta_{\mathbf{q}}} = 0.$$

Therefore, the average of odd powers of fluctuation fields don't contribute.

5.6.2 Even powers of fluctuation field

In this subsection our goal is to calculate $\langle |\eta(\mathbf{r})|^2 \rangle$. The first step is to express this field in term of the quasi-particles. We have that

$$\eta(\mathbf{r}) = \frac{1}{L^{D/2}} \sum_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{r}} \eta_{\mathbf{q}} = \frac{1}{L^{D/2}} \sum_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{r}} (x_{\mathbf{q}} + iy_{\mathbf{q}}).$$

If we do $\mathbf{q} \to -\mathbf{q}$ we obtain

$$\eta(\mathbf{r}) = \frac{1}{L^{D/2}} \sum_{\mathbf{q}} e^{-i\mathbf{q}\cdot\mathbf{r}} \eta_{-\mathbf{q}} = \frac{1}{L^{D/2}} \sum_{\mathbf{q}} e^{-i\mathbf{q}\cdot\mathbf{r}} (x_{-\mathbf{q}} + iy_{-\mathbf{q}}).$$

Adding these two expressions we get

$$\eta(\mathbf{r}) = \frac{1}{2L^{D/2}} \sum_{\mathbf{q}} \Big(e^{i\mathbf{q}\cdot\mathbf{r}} (x_{\mathbf{q}} + iy_{\mathbf{q}}) + e^{-i\mathbf{q}\cdot\mathbf{r}} (x_{-\mathbf{q}} + iy_{-\mathbf{q}}) \Big).$$

Restricting the sum to only momenta who has positive components

$$\eta(\mathbf{r}) = \frac{1}{L^{D/2}} \sum_{\mathbf{q}, q_x \geq 0} \Big(e^{i\mathbf{q}\cdot\mathbf{r}} (x_{\mathbf{q}} + iy_{\mathbf{q}}) + e^{-i\mathbf{q}\cdot\mathbf{r}} (x_{-\mathbf{q}} + iy_{-\mathbf{q}}) \Big).$$

Using equation (5.68) we get

$$\begin{aligned} \eta(\mathbf{r}) = & \frac{1}{L^{D/2}} \sum_{\mathbf{q}, q_x \geq 0} e^{i\mathbf{q}\cdot\mathbf{r}} \Big(\frac{\alpha_{\mathbf{q}} + \beta_{\mathbf{q}}}{\sqrt{2}} + i \frac{\xi_{\mathbf{q}} + \zeta_{\mathbf{q}}}{\sqrt{2}} \Big) \\ & + \frac{1}{L^{D/2}} \sum_{\mathbf{q}, q_x \geq 0} e^{-i\mathbf{q}\cdot\mathbf{r}} \Big(\frac{\alpha_{\mathbf{q}} - \beta_{\mathbf{q}}}{\sqrt{2}} - i \frac{\xi_{\mathbf{q}} - \zeta_{\mathbf{q}}}{\sqrt{2}} \Big). \end{aligned} \tag{5.72}$$

For the complex conjugate field we have that

$$\eta^*(\mathbf{r}) = \frac{1}{L^{D/2}} \sum_{\mathbf{q}', q'_x \geq 0} e^{-i\mathbf{q}'\cdot\mathbf{r}} \Big(\frac{\alpha_{\mathbf{q}'} + \beta_{\mathbf{q}'}}{\sqrt{2}} - i \frac{\xi_{\mathbf{q}'} + \zeta_{\mathbf{q}'}}{\sqrt{2}} \Big)$$
$$+ \frac{1}{L^{D/2}} \sum_{\mathbf{q}', q'_x \geq 0} e^{i\mathbf{q}'\cdot\mathbf{r}} \Big(\frac{\alpha_{\mathbf{q}'} - \beta_{\mathbf{q}'}}{\sqrt{2}} + i \frac{\xi_{\mathbf{q}'} - \zeta_{\mathbf{q}'}}{\sqrt{2}} \Big). \tag{5.73}$$

Now we calculate $\eta(\mathbf{r})\eta^*(\mathbf{r})$. Only terms that $\mathbf{q} = \mathbf{q}'$ will contribute for the final calculation of the average. We write

$$|\eta(\mathbf{r})|^2 = \frac{1}{L^D} \sum_{\mathbf{q}, q_x \geq 0} \Big(\alpha_{\mathbf{q}}^2 + \alpha_{\mathbf{q}}^2 e^{2i\mathbf{q}\cdot\mathbf{r}} \alpha_{\mathbf{q}}^2 e^{-2i\mathbf{q}\cdot\mathbf{r}} + \alpha_{\mathbf{q}}^2 + \beta_{\mathbf{q}}^2 - \beta_{\mathbf{q}}^2 e^{2i\mathbf{q}\cdot\mathbf{r}} - \beta_{\mathbf{q}}^2 e^{-2i\mathbf{q}\cdot\mathbf{r}}$$

$$+ \beta_{\mathbf{q}}^2 + \xi_{\mathbf{q}}^2 - \xi_{\mathbf{q}}^2 e^{2i\mathbf{q}\cdot\mathbf{r}} - \xi_{\mathbf{q}}^2 e^{-2i\mathbf{q}\cdot\mathbf{r}} + \xi_{\mathbf{q}}^2 + \zeta_{\mathbf{q}}^2 + \zeta_{\mathbf{q}}^2 e^{2i\mathbf{q}\cdot\mathbf{r}} + \zeta_{\mathbf{q}}^2 e^{-2i\mathbf{q}\cdot\mathbf{r}} + \zeta_{\mathbf{q}}^2 \Big). \tag{5.74}$$

Now we are going to take the average of this expression, but first let's calculate the average of the squared quasiparticles.

$$\langle \alpha_{\mathbf{q}}^2 \rangle = \frac{\displaystyle\int D[\eta_{\mathbf{q}}] \alpha_{\mathbf{q}}^2 e^{-\frac{H}{T}}}{\displaystyle\int D[\eta_{\mathbf{q}}] e^{-\frac{H}{T}}} = \frac{\displaystyle\int \alpha_{\mathbf{q}}^2 e^{-\frac{1}{T}\epsilon_{1,\mathbf{q}}\alpha_{\mathbf{q}}^2} d\alpha_{\mathbf{q}}}{\displaystyle\int e^{-\frac{\epsilon_{1,\mathbf{q}}}{T}} d\alpha_{\mathbf{q}}} = \frac{T}{2\epsilon_{1,\mathbf{q}}}. \tag{5.75}$$

$$\langle \beta_{\mathbf{q}}^2 \rangle = \frac{\displaystyle\int D[\eta_{\mathbf{q}}] \beta_{\mathbf{q}}^2 e^{-\frac{H}{T}}}{\displaystyle\int D[\eta_{\mathbf{q}}] e^{-\frac{H}{T}}} = \frac{\displaystyle\int \beta_{\mathbf{q}}^2 e^{-\frac{1}{T}\epsilon_{2,\mathbf{q}}\beta_{\mathbf{q}}^2} d\beta_{\mathbf{q}}}{\displaystyle\int e^{-\frac{\epsilon_{2,\mathbf{q}}}{T}} d\beta_{\mathbf{q}}} = \frac{T}{2\epsilon_{2,\mathbf{q}}}. \tag{5.76}$$

Because $\xi_{\mathbf{q}}$ has the same eigenvalue as $\alpha_{\mathbf{q}}$ and $\zeta_{\mathbf{q}}$ has the same value as $\beta_{\mathbf{q}}$ the averages of their squared values are simply

$$\langle \xi_{\mathbf{q}}^2 \rangle = \frac{T}{2\epsilon_{1,\mathbf{q}}}, \qquad \langle \zeta_{\mathbf{q}}^2 \rangle = \frac{T}{2\epsilon_{2,\mathbf{q}}}.$$

With these results we can write

$$\langle |\eta(\mathbf{r})|^2 \rangle = \frac{1}{L^D} \sum_{\mathbf{q}, q_x \geq 0} \Big(\langle \alpha_{\mathbf{q}}^2 \rangle + \langle \beta_{\mathbf{q}}^2 \rangle + \langle \xi_{\mathbf{q}}^2 \rangle + \langle \zeta_{\mathbf{q}}^2 \rangle \Big)$$
$$= \frac{2}{L^D} \sum_{\mathbf{q}, q_x \geq 0} \Big(\langle \alpha_{\mathbf{q}}^2 \rangle + \langle \beta_{\mathbf{q}}^2 \rangle \Big).$$

Removing the restriction in the summation we obtain

$$\langle |\eta(\mathbf{r})|^2 \rangle = \frac{1}{L^D} \sum_{\mathbf{q}} \Big(\langle \alpha_{\mathbf{q}}^2 \rangle + \langle \beta_{\mathbf{q}}^2 \rangle \Big).$$

Finally we get

$$\langle |\eta(\mathbf{r})|^2 \rangle = \frac{1}{2L^D} \sum_{\mathbf{q}} \Big[\frac{T}{\epsilon_{1,\mathbf{q}}} + \frac{T}{\epsilon_{2,\mathbf{q}}} \Big]. \tag{5.77}$$

By the same procedures we can find that

$$\langle \eta^2(\mathbf{r}) \rangle = \frac{1}{2L^D} \sum_{\mathbf{q}} \left[\frac{T}{\epsilon_{1,\mathbf{q}}} - \frac{T}{\epsilon_{2,\mathbf{q}}} \right]. \tag{5.78}$$

This average is usually zero. It becomes nonzero only when $\epsilon_{1,\mathbf{q}} \neq \epsilon_{2,\mathbf{q}}$. As we are always working near the critical temperature $\epsilon_{1,\mathbf{q}} \approx \epsilon_{2,\mathbf{q}}$ [18] and so we can consider $\langle \eta^2(\mathbf{r}) \rangle = 0$.

5.7 Fluctuation Shifted Critical Temperature

This section is the culmination of this chapter. We are going to apply the formalism of Gaussian fluctuations to calculate how much the critical temperature is going to shift from its mean field value. As is usual, the critical temperature equation is part of the Ginzburg-Landau equation by the temperature dependence on a. The Ginzburg-Landau equation of course is given by

$$a\Delta(\mathbf{r}) + b\Delta(\mathbf{r})|\Delta(\mathbf{r})|^2 - \mathcal{K}\boldsymbol{\nabla}^2\Delta(\mathbf{r}) = 0.$$

Suppose that the order parameter is given by its average value over fluctuations plus a fluctuation field as $\Delta(\mathbf{r}) = \Delta_0 + \eta(\mathbf{r})$ where $\Delta_0 = \langle \Delta(\mathbf{r}) \rangle$. The Ginzburg-Landau equation becomes

$$a(\Delta_0 + \eta(\mathbf{r})) + b|\Delta_0 + \eta(\mathbf{r})|^2(\Delta_0 + \eta(\mathbf{r})) - \mathcal{K}\boldsymbol{\nabla}^2(\Delta_0 + \eta(\mathbf{r})) = 0. \tag{5.79}$$

Now we collect similar terms

$$\begin{aligned} &\underbrace{a\Delta_0 + b\Delta_0|\Delta_0|^2 - \mathcal{K}\boldsymbol{\nabla}^2\Delta_0}_{\text{(no fluctuation terms)}} \\ &+ \underbrace{a\eta(\mathbf{r}) + 2b\eta(\mathbf{r})|\Delta_0|^2 + b\Delta_0^2\eta^*(\mathbf{r}) - \mathcal{K}\boldsymbol{\nabla}^2\eta(\mathbf{r})}_{\text{(linear in } \eta)} \\ &+ \underbrace{b\eta^2(\mathbf{r})\Delta_0^* + 2b\Delta_0|\eta(\mathbf{r})|^2 + b\eta(\mathbf{r})|\eta(\mathbf{r})|^2}_{\text{(non linear in } \eta)} = 0. \end{aligned} \tag{5.80}$$

Now, we average this equation over fluctuations. However, as we already calculated, the terms linear in η don't contribute and the nonlinear terms give a contribution provided that they are not anomalous, i.e. $\langle \eta^2 \rangle = 0$ and $\langle \eta|\eta|^2 \rangle = 0$. We will obtain the following

$$a\Delta_0 + b|\Delta_0|^2\Delta_0 + 2b\langle|\eta(\mathbf{r})|^2\rangle\Delta_0 - \mathcal{K}\boldsymbol{\nabla}^2\Delta_0 = 0,$$

and we rewrite this equation as

$$\Big(a + 2b\langle|\eta(\mathbf{r})|^2\rangle\Big)\Delta_0 + b|\Delta_0|^2\Delta_0 - \mathcal{K}\boldsymbol{\nabla}^2\Delta_0 = 0. \tag{5.81}$$

We can see that this is a Ginzburg-Landau equation for Δ_0 but with a new coefficient proportional to the local term. From the format of this equation, when we go to the critical temperature the coefficient proportional to the local term has to go to zero. So we have that when $T \to T_{c0}$

$$a + 2b\langle|\eta(\mathbf{r})|^2\rangle_{T_{c0}} = 0. \tag{5.82}$$

Making explicitly the temperature dependence of the coefficient a we obtain

$$\alpha(T_c - T_{c0}) + 2b\langle|\eta(\mathbf{r})|^2\rangle_{T_{c0}} = 0.$$

Finally, the shifted critical temperature is given by

$$T_c = T_{c0} - \frac{2b}{\alpha}\langle|\eta(\mathbf{r})|^2\rangle_{T_{c0}}. \tag{5.83}$$

This is the shifted critical temperature because of fluctuations. To quantify this shift, however, we need to calculate $\langle|\eta_{\mathbf{q}}|^2\rangle$.

5.8 Calculation of $\langle|\eta_{\mathbf{q}}|^2\rangle$

To obtain the expression for $\langle|\eta_{\mathbf{q}}|^2\rangle$ we will go back to equation (5.79) and linearize it. Our goal is to find the equation for the fluctuation fields. We will follow the classical way of the linearization of the Ginzburg-Landau equation but with one important additional ingredient that is related to the mean-field theory of fluctuations. Nonlinear terms in $\eta(\mathbf{r})$ are approximated according to the mean-field recipe. If the product of two operators obeys the relation

$$\langle AB\rangle \simeq \langle A\rangle\langle B\rangle \text{ then, } AB = \langle A\rangle B + A\langle B\rangle - \langle A\rangle\langle B\rangle.$$

The three operator product can be approximated by taking only into account the two operator correlation as

$$\begin{aligned} ABC \simeq\ & \langle A\rangle BC + A\langle BC\rangle - \langle A\rangle\langle BC\rangle \\ &+ \langle B\rangle AC + B\langle AC\rangle - \langle B\rangle\langle AC\rangle \\ &+ \langle C\rangle AB + C\langle AB\rangle - \langle C\rangle\langle AB\rangle. \end{aligned}$$

Following the recipe we obtain

$$\begin{aligned} \eta(\mathbf{r})|\eta(\mathbf{r})|^2 = \eta(\mathbf{r})\eta(\mathbf{r})\eta^*(\mathbf{r}) \simeq & \langle\eta(\mathbf{r})\rangle\eta(\mathbf{r})\eta^*(\mathbf{r}) + \eta(\mathbf{r})\langle\eta(\mathbf{r})\eta^*(\mathbf{r})\rangle - \langle\eta(\mathbf{r})\rangle\langle\eta(\mathbf{r})\eta^*(\mathbf{r})\rangle \\ &+ \langle\eta(\mathbf{r})\rangle\eta(\mathbf{r})\eta^*(\mathbf{r}) + \eta(\mathbf{r})\langle\eta(\mathbf{r})\eta^*(\mathbf{r})\rangle - \langle\eta(\mathbf{r})\rangle\langle\eta(\mathbf{r})\eta^*(\mathbf{r})\rangle \\ &+ \langle\eta^*(\mathbf{r})\rangle\eta^2(\mathbf{r}) + \eta^*(\mathbf{r})\langle\eta^2(\mathbf{r})\rangle - \langle\eta^*(\mathbf{r})\rangle\langle\eta(\mathbf{r})^2\rangle, \end{aligned}$$

which is reduced to (since $\langle\eta^*(\mathbf{r})\rangle = \langle\eta(\mathbf{r})\rangle = \langle\eta^2(\mathbf{r})\rangle = 0$)

$$\eta(\mathbf{r})|\eta(\mathbf{r})|^2 \simeq 2\eta(\mathbf{r})\langle|\eta(\mathbf{r})|^2\rangle. \tag{5.84}$$

Then, the equation (5.80) becomes at $T \geq T_c$ (i.e., for $\Delta_0 = 0$)

$$\underbrace{(a + 2b\langle|\eta(\mathbf{r})|^2\rangle)}_{\text{new coefficient}}\eta(\mathbf{r}) - \mathcal{K}\boldsymbol{\nabla}^2\eta(\mathbf{r}) = 0. \tag{5.85}$$

The functional that generates this equation through the variational principle is

$$F_{sG} = \int_{L^D} d^D\mathbf{r}\Big\{\big[a + 2b\langle|\eta(\mathbf{r})|^2\rangle\big]|\eta(\mathbf{r})|^2 + \mathcal{K}|\boldsymbol{\nabla}\eta(\mathbf{r})|^2\Big\}. \tag{5.86}$$

Based on this functional and in the result written as equation (5.6.2) , we find

$$\langle|\eta_{\mathbf{q}}|^2\rangle = \frac{1}{2L^D}\sum_{\mathbf{q}}\left[\frac{T}{\epsilon_{1,\mathbf{q}}} + \frac{T}{\epsilon_{2,\mathbf{q}}}\right],$$

where comparing to previous results

$$A_{\mathbf{q}} + B = \epsilon_{1,\mathbf{q}}, \qquad A_{\mathbf{q}} - B = \epsilon_{2,\mathbf{q}}$$

and

$$A_{\mathbf{q}} = a + 2b\langle|\eta_{\mathbf{q}}|^2\rangle + \mathcal{K}\mathbf{q}^2, \qquad B = 0.$$

So,

$$\langle|\eta_{\mathbf{q}}|^2\rangle = \frac{1}{L^D}\sum_{\mathbf{q}}\left[\frac{T}{a + 2b\langle|\eta_{\mathbf{q}}|^2\rangle + \mathcal{K}\mathbf{q}^2}\right]. \tag{5.87}$$

Here we can see another example of the usefulness of the general fluctuation hamiltonian that we have derived earlier. In just a few lines of calculations we were able to find the expression that we wanted. Going from discrete to continous variables we have

$$\langle|\eta_{\mathbf{q}}|^2\rangle = \int\frac{d^D\mathbf{q}}{(2\pi)^D}\left[\frac{T}{a + 2b\langle|\eta_{\mathbf{q}}|^2\rangle + \mathcal{K}\mathbf{q}^2}\right]. \tag{5.88}$$

The last step is just to find this average at the critical temperature. The coefficient proportional to the local term in a Ginzburg-Landau equation goes to zero at the critical temperature, which means that $a + 2b\langle|\eta_{\mathbf{q}}|^2_{T_c}\rangle = 0$. Finally we obtain

$$\langle|\eta_{\mathbf{q}}|^2\rangle_{T_c} = \int\frac{d^D\mathbf{q}}{(2\pi)^D}\left[\frac{T_c}{\mathcal{K}\mathbf{q}^2}\right]. \tag{5.89}$$

This integral is of course divergent. To deal with this we have to introduce the infrared and ultraviolet cut-offs as

$$\langle|\eta(\mathbf{r})|^2\rangle_{T_c} = \int_{\Lambda_0}^{\Lambda_\infty}\frac{d^D\mathbf{q}}{(2\pi)^D}\left[\frac{T_c}{\mathcal{K}\mathbf{q}^2}\right]. \tag{5.90}$$

Here Λ_0 is the infrared cut-off that is proportional to the inverse of the Ginzburg-Landau coherence length at the Ginzburg-Levanyuk temperature (justified from the renormalization group analysis)[18]

$$\Lambda_0 \sim \frac{1}{\xi(Gi)}. \tag{5.91}$$

Momenta which is smaller than $\frac{1}{\xi(Gi)}$ should not contribute because $\xi(Gi)$ is an upper limit to the coherence radius in the system. Beyond that we don't yet have means to understand the behavior of the system. The ultra-violet cut-off Λ_∞ is proportional to the inverse of the zero temperature coherence length. Momenta which are larger than $\frac{1}{\xi_0}$ are excluded as ξ_0 is the minimal length in the Ginzburg-Landau theory and so

$$\Lambda_\infty \sim \frac{1}{\xi_0}. \tag{5.92}$$

Now we will calculate $\langle|\eta(\mathbf{r})|^2\rangle_{T_c}$ for $D = 3$, $D = 2$ and $D = 1$ and use this result to calculate the shift of the critical temperature.

5.9 Equation for T_c

5.9.1 T_c shifted by fluctuations for $D = 3$

$$\langle|\eta(\mathbf{r})|^2\rangle_{T_c} = \int_{\Lambda_0}^{\Lambda_\infty} \frac{d^3\mathbf{q}}{(2\pi)^3}\frac{T_c}{\mathcal{K}\mathbf{q}^2} = \frac{T_c}{2\pi^2\mathcal{K}}\left[\frac{c_\infty}{\xi_0} - \frac{c_0}{\xi(Gi)}\right], \tag{5.93}$$

where, c_0 and c_∞ are proportionality coefficients of the cut-offs. Because $\xi(Gi) = \xi_0\sqrt{Gi}$ we can write

$$\langle|\eta(\mathbf{r})|^2\rangle_{T_{c0}} = \frac{T_c}{2\pi^2\mathcal{K}}\frac{c_\infty}{\xi_0}\Big(1 - \frac{c_0}{c_\infty}\sqrt{Gi}\Big). \tag{5.94}$$

The equation for the shifted critical temperature give us

$$\frac{T_{c0} - T_c}{T_c} = \frac{2b}{a}\frac{1}{2\pi^2\mathcal{K}}\frac{c_\infty}{\xi_0}\Big(1 - \frac{c_0}{c_\infty}\sqrt{Gi}\Big). \tag{5.95}$$

From previous calculations we have that

$$Gi^{3D} = \frac{T_{c0}b^2}{32\pi^2 a\mathcal{K}^3}.$$

Then

$$\frac{T_{c0} - T_c}{T_c} = \frac{c_\infty}{\pi^2}\sqrt{32\pi^2 G_i}\Big(1 - \frac{c_0}{c_\infty}\sqrt{G_i}\Big). \tag{5.96}$$

Because the Ginzburg number is very small for $D = 3$ we only need to keep the leading-order contribution in $\sqrt{G_i}$, i.e.,

$$\frac{T_{c0} - T_c}{T_c} = \frac{c_\infty}{\pi^2}\sqrt{32\pi^2 G_i}, \tag{5.97}$$

$$T_c = T_{c0}\left(\frac{1}{1+\frac{8}{\pi}\sqrt{G_i}}\right), \tag{5.98}$$

here we set $c_\infty = \sqrt{2}$ to get the result known form the renormalization group theory.

5.9.2 Shifted T_c for $D = 2$

$$\langle|\eta(\mathbf{r})|^2\rangle_{T_c} = \int_{\Lambda_0}^{\Lambda_\infty} \frac{d^2\mathbf{q}}{(2\pi)^2}\frac{T_c}{\mathcal{K}\mathbf{q}^2} = \frac{1}{2\pi}\int_{\Lambda_0}^{\Lambda_\infty} dq\frac{T_c}{Kq} = \frac{T_c}{2\pi\mathcal{K}}\ln\frac{\Lambda_\infty}{\Lambda_0}, \tag{5.99}$$

$$\langle|\eta(\mathbf{r})|^2\rangle_{T_c} = \frac{T_c}{2\pi\mathcal{K}}\ln\frac{c_\infty}{c_0}\frac{1}{\sqrt{G_i}}. \tag{5.100}$$

Inserting this result in the equation for the shifted critical temperature

$$\frac{T_{c0}-T_c}{T_c} = \frac{2b}{a}\frac{1}{2\pi^2\mathcal{K}}\ln\frac{c_\infty}{c_0}\frac{1}{\sqrt{G_i}} \tag{5.101}$$

The Ginzburg number for 2D is

$$Gi^{2D}\frac{b}{4\pi a\mathcal{K}}.$$

So, we have

$$\frac{T_{c0}-T_c}{T_c} = 4Gi\ln\frac{c_\infty}{c_0}\frac{1}{\sqrt{Gi}}.$$

To get the result that agrees with the renormalization group result we set $\frac{c_\infty}{c_0} = \frac{1}{2}$ and so

$$\frac{T_{c0}-T_c}{T_c} = 2Gi\ln\frac{1}{4Gi},$$

$$T_c = T_{c0}\left(\frac{1}{1+2Gi\ln\frac{1}{4Gi}}\right). \tag{5.102}$$

5.9.3 Calculations of T_c for one spatial dimension

Our previous calculation of Gi for one spatial dimension produced the result $Gi \sim 1$, meaning the failure of the perturbation scheme based on the Gaussian fluctuations. Here, for a further illustration we calculate the shift of the critical temperature due to fluctuations for $D = 1$

$$\begin{aligned}\langle|\eta(\mathbf{r})|^2\rangle_{T_c} &= \int_{\Lambda_0}^{\Lambda_\infty}\frac{dq}{2\pi}\frac{T_c}{\mathcal{K}q^2}\\ &= \frac{T_c}{2\pi\mathcal{K}}\left(\frac{1}{\Lambda_0}-\frac{1}{\Lambda_\infty}\right)\\ &= \frac{T_c}{2\pi\mathcal{K}}\left(\frac{\xi(Gi)}{c_0}-\frac{\xi_0}{c_\infty}\right)\\ &= \frac{T_c}{2\pi\mathcal{K}}\frac{\xi_0}{c_\infty}\left(\frac{c_\infty}{c_0}\frac{1}{\sqrt{Gi}}-1\right).\end{aligned}$$

Inserting this result in the equation for the shifted critical temperature we have

$$\frac{T_{c0}-T_c}{T_c} = \frac{b}{a\pi\mathcal{K}}\sqrt{\frac{\mathcal{K}}{aT_{c0}}}\Big(\frac{c_\infty}{c_0}\frac{1}{\sqrt{Gi}} - 1\Big).$$

The expression for the Ginzburg number for one spatial dimension is

$$Gi = Gi^{1D} = \left(\frac{1}{128}\frac{b^2}{\mathcal{K}T_{c0}a^3}\right)^{1/3}.$$

Then

$$\frac{b}{a\pi\mathcal{K}}\sqrt{\frac{\mathcal{K}}{aT_{c0}}} = \frac{1}{\pi}\sqrt{128Gi^3}.$$

Finally

$$\begin{aligned}\frac{T_{c0}-T_c}{T_c} &= \frac{1}{c_\infty\pi}\sqrt{128Gi^3}\Big(\frac{c_\infty}{c_0}\frac{1}{\sqrt{Gi}} - 1\Big)\\ &= \underbrace{\frac{1}{\pi c_0}\sqrt{128}Gi}_{\sim 1} - \underbrace{\frac{1}{\pi c_\infty}\sqrt{128}G_i^{3/2}}_{\sim 1},\end{aligned}$$

which are beyond the scope of perturbation theory. For $D = 1$ fluctuations are huge and we cannot invoke any framework based on the Gaussian picture of fluctuations.

5.10 Fluctuation driven shift of critical temperature for a two-band system

To end this work we will take the formalism we did for a two-band system and calculate the shift of the critical temperature. We will see that bellow a certain threshold the thermal fluctuation kills the superconducting state. We consider the standard microscopic model of a two-band superconductor introduced in the last chapter, where one band is deep ($\nu = 1$) and the other one is shallow ($\nu = 2$). We model this situation by assuming that the Fermi velocity in band 2 is much smaller than that in band 1, we set their ratio equal to zero. The condensate is formed due to the conventional s-wave pairing in both bands with the intraband interaction strength $g_{\nu,\nu}$ ($\nu = 1, 2$) and the inter band coupling $g_{12} = g_{21}$ of the Josephson type [19]. So we plot in figure 14

$$\frac{T_{c0}-T_c}{T_c} = 2G_i^{2D}\ln\frac{1}{4Gi^{2D}}, \tag{5.103}$$

where,

$$Gi^{2D} = \frac{b}{4\pi a\mathcal{K}} = G^{2D}i_{\text{deep}}\frac{1+S^4}{1+S^2}, \tag{5.104}$$

with S introduced in the previous chapter eq. (4.50) and $Gi_{\rm deep}$ the Ginzburg number of the deep band. As it has been found previously, the mean-field critical temperature in units of $T_{c0,1}$ is given by

$$\frac{T_{c0}}{T_{c0,1}} = \exp\left\{(1+\chi)\left(\frac{1}{\lambda_{11}} - \frac{\lambda_{22} - \lambda_{11}S}{\lambda_{11}\lambda_{22} - \lambda_{12}^2}\right)\right\}, \tag{5.105}$$

where $T_{c0,1}$ is the mean-field critical temperature of an uncoupled band 1. Considering $Gi_{\rm deep} = 10^{-5}$ and using $\lambda_{11} = 0.25$ and $\lambda_{22} = 0.3$, and $N_1 = N_2$, we find the dependence of the critical temperature shift on λ_{12} illustrated in Fig. 14. The qualitative behavior is not sensitive to a particular choice of λ_{11}, λ_{22}, $\chi = N_2/N_1$ and $Gi_{\rm deep}$. In real materials we usually have $\lambda_{11}, \lambda_{22} \simeq$ 0.1-0.4, $\lambda_{12} \ll \lambda_{11}, \lambda_{22}$, and $N_1 \approx N_2$. In addition, 10^{-5} is a conservative estimation of the Ginzburg number for real materials with quasi-2D bands.

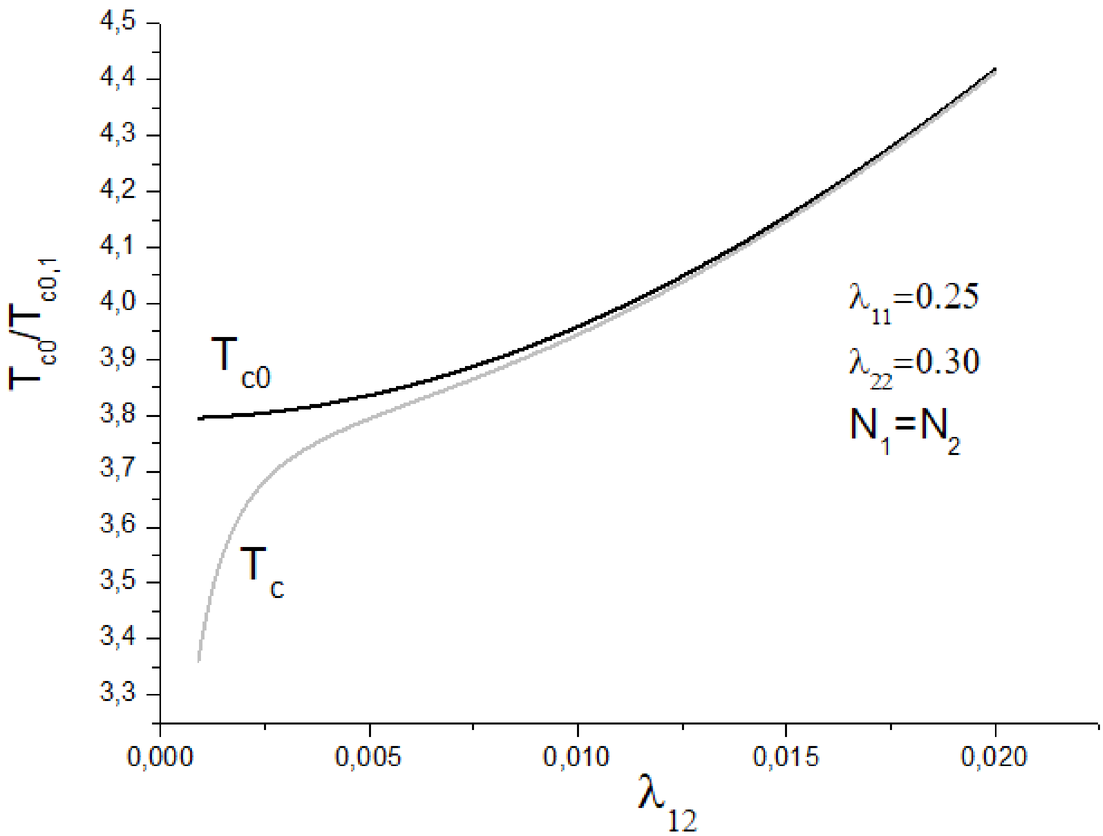


Figure 14: The mean-field T_{c0},and fluctuation-renormalized T_c critical temperatures, plotted versus the inter-band coupling λ_{12}.

We can see from this figure that the fluctuations are reduced and eventually suppressed in the presence of the inter-band coupling between shallow-band (unstable) and deep-band (stable) condensates. Thus, the interplay of different condensates in one material can significantly change the physical picture: for ia single shallow band the condensate is suppressed by fluctuations while in the combination of deep and shallow band one observes the mean-field regime already at relatively small inter-band couplings.

6 SUMMARY AND FUTURE WORK

6.1 Summary

In the introductory **Chapter 2** of this thesis we were able to see how the Meissner effect was explained by the idea of the electrons forming a macroscopic condensate in the same single-particle quantum state, a superfluid which flows through the metal without resistance explaining how the cables in figure 1 in the general introduction chapter can have the same current. Next we have proved that the formation of this condensate of fermions is possible because below a certain temperature, two free electrons above the Fermi sea are less favorable thermodynamically than an in-medium bound state of these two electrons. Therefore, the composite boson (the Cooper pair) is formed even for weak interaction between fermions as long as it is attractive.

Even with the London equations and Cooper instability superconductivity was not yet fully understood. So, we continued our study by investigating the phenomenological theory of Ginzburg and Landau, see **Chapter 3**. We obtained the Ginzburg-Landau equations by using the concept of the order parameter which is nonzero below the critical temperature. Because the order parameter is small near T_c, it is possible to expand the free-energy functional and use the variational principle to obtain the first and second Ginzburg Landau equations which describes the order parameter and the supercurrent. Finally, we have introduced two characteristics lengths, the Ginzburg-Landau coherence length and the London penetration depth, and discussed the Ginzburg-Landau parameter which quantifies the difference between two conventional types of superconductivity.

Though the Ginzburg-Landau theory can describe many important features of the superconducting state, it was, in its original formulation, a phenomenological theory. To go deeper into microscopic details of superconductivity, the BCS approach is discussed in **Chapter 3**. We have employed the BCS-Bogoliubov Hamiltonian and found that the excitation spectrum has a energy gap in the uniform superconductor. Both the BCS and Ginzburg-Landau theories explain experimental data(fig. 10) and therefore they are both consistent with the data. To connect these two theories, we have used the formalism of Green functions developed by Gor'kov. By expressing the order parameter in terms of the anomalous Green function and by using the perturbative expansion of the microscopic gap equation in small deviation from the critical temperature, we have got the Ginzburg-Landau equation for the order parameter with coefficients expressed in terms of the normal state Green functions. Thus, we have demonstrated (following Gor'kov) how the Ginzburg-Landau formalism is linked to the microscopic parameters of the superconducting system.

In **Chapter 4** we have considered how the Gor'kov equations can be generalized to other physically interesting cases. We have constructed these equation in the paramagnetic limit where the external magnetic field only acts on the spin of the electrons promoting the tendency to Cooper pairing with non-zero momentum, the FFLO state. We have derived the corresponding Ginzburg Landau formalism with the coefficients depending on the applied field. By calculating when the coefficients for the squared gradient and nonlinear terms in the Ginzburg-Landau equation become zero, we have found the point where the superconducting, normal and FFLO state meets. For another illustration, we have considered the Gor'kov equations generalized to the case of a two-band system. We have found the equation for the mean-field critical temperature and have shown that the implementation of the two-band Ginzburg Landau theory produces the effective single-component GL formalism but with the coefficients averaged over both contributing bands.

Despite the great success of the mean field theory in the form of the BCS-Bogoliubov Hamiltonian, there are plenty of superconductors where the mean-field approach should be corrected by including fluctuations. To deal with them we have considered the Gaussian theory of thermal fluctuations in **Chapter 5**. We have assumed that the order parameter deviates from the uniform stationary solution due to the contribution of fluctuation fields and constructed the Gaussian fluctuation "Hamiltonian". Using this"Hamiltonian" we have investigated various aspects of fluctuation effects. In particular, we have calculated the Ginzburg number Gi that measure the temperature range with strong fluctuations near the mean-field critical temperature. We have also calculated the shift of the critical temperature due to fluctuations within the generalized Gaussian scheme taking into account the interaction between fluctuation modes. Finally, we have applied the generalized Gaussian scheme to calculate the fluctuation shift of the critical temperature in a two band system with one shallow and one deep bands. We have shown that fluctuations are reduced in the presence of the inter-band coupling between unstable shallow-band condensate and stable deep-band condensate.

6.2 Future Work

Further applications of the generalized Gaussian model of thermal fluctuations will be considered for multiband superconductors in the paramagnetic limit during my PhD program.

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