Master Thesis

Anisotropic Three-Component Superconductors

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Abstract

Since first discovery in 1911 by Heike Kamerlingh Onnes, superconductivity has always been an extremely active research field. A conventional superconductor (SC) is described by a single complex order parameter, and its behavior can be easily classified by studying the ratio of two characteristic length scales: the magnetic penetration depth $\lambda$ and the coherence length $\xi$. However, a single component model is not sufficient to describe all kinds of superconductors: iron pnictides, require a multiband models with two or more order parameters. Moreover, many superconducting materials present spatial anisotropies, which should be included in the theoretical framework to fully describe their behavior. As an example, the three band anisotropic superconductor Sr$_2$RuO$_4$ is a material of central interest today. The intention of this work is to describe how anisotropies change the behavior of a three-band SCs using a phenomenological Ginzburg-Landau model with Josephson potential. This potential leads to a variety of situations exhibiting phase frustration, which we study for specific sets of Ginzburg-Landau coefficients. Then we introduce anisotropies in the system and study how topological excitations change compared to the isotropic case. Our goal is to show that the additional couplings introduced by the anisotropy tensor structurally change the vortex structure, yielding non-Abrikosov vortices. Using a non-linear conjugate gradient method, we start with specific sets of parameters and initial guesses and study the convergence to equilibrium states.

Key words: Superconductivity, multi-band superconductor, three components superconductor, anisotropies, BTRS, topological excitations, vortex matter
**Sammanfattning**


**Nyckelord:** Supraledning, flerkomponentssupraledare, tre-komponentssupraledare, anisotropi, BTRS, topologiska excitationer, virveltillstånd
Preface

This thesis is the result of my Master degree project carried out at KTH’s Theoretical Physics Department, under the supervision of Prof. Egor Babaev. The work started by getting acquainted with finite element simulations, and in particular with FreeFem++ environment. Once that was applied successfully to simple Ginzburg Landau models, I started studying the behaviour of topological excitations in three band anisotropic superconductors. This part of the work took a great amount of time, since in three band systems the number of degrees of freedom is high, and to reach a good level of convergence in the simulations a lot of core-hours are required.

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Chapter 1

Introduction

Conventional superconductors are described by a single complex order parameter which plays the role of a macroscopic wave function. In this physical system there are two main fundamental lengthscales, namely the magnetic penetration depth $\lambda$ and the matter field coherence length $\xi$. Their ratio offers the possibility of easily classifying the superconductor behavior in presence of magnetic field. When $\lambda < \xi$, we have a positive surface energy between superconducting and normal domains. In this case, we have no magnetic field penetrating inside the superconductor bulk. This effect is called Meissner-Ochsenfeld. However, once the external field reaches a critical value, proper of the specific superconductor, we assist to a phase transition yielding back to the normal state. In this case we talk of Type - I superconductors. If instead we have $\lambda > \xi$, the situation can be radically different. For external magnetic fields that are smaller than the first critical field, i.e. $H < H_{c1}$, the system remains in the Meissner state. At $H = H_c$ the situation changes, in fact the surface energy between superconducting and normal states becomes negative, therefore the formation of interfaces is suddenly favorable. These interfaces are in the form of vortices. Since the superconducting field is charged, vortex excitations are coupled with the magnetic field. One of the most surprising feature of vortices is related to the magnetic field flux that they carry: in one component superconductors each vortex brings a quantum of magnetic flux, namely $\Phi_0 = \frac{2\pi h}{e}$. If one keeps increasing the magnetic field, we assist to an increase of the vortex density in the material. For $H > H_{c2}$, superconductivity is not thermodynamically convenient anymore and the system undergoes a transition back to the normal state. This is classified as Type- II superconductivity. The situation becomes even more interesting when we start dealing with multi-band superconductors. These models describe materials where we have simultaneous formation of different bands leading to different superconducting components. These components can also interact, for example via cooper pairs tunneling. While the magnetic penetration depth $\lambda$ remains unique, each band will be characterized by a proper coherence length $\xi$. This has an interesting consequence: if $\xi_1 < \lambda$ and $\xi_2 > \lambda$ we are in neither of the case discussed above.
This new regime is called Type-1.5 superconductivity. The existence of superconductors with two gaps was theoretically predicted in 1959 [39], and experimentally measured almost fifty years later with the discovery of MgB$_2$ [33]. After that, multi-band superconductivity was found also in the high temperature iron based superconductors [43]. These materials are thought to be described by models ranging from one to four bands. Moreover, many materials are not isotropic, therefore being able to adapt the models to describe superconductivity to anisotropic system can lead to the discovery of new phenomena. Anisotropies were first taken into account by Gork’ov [28], while obtaining the Ginzburg Landau coefficients for a two bands superconductor starting from BCS theory [5]. One of the interesting features of anisotropic superconductors regards the lengthscales: in fact we start having different lengthscales in different direction. Also the magnetic field happens to have direction dependent penetration depth. This yields to a wider range of possible phenomena. For two bands anisotropic superconductors, an extensive work concerning length scale hierarchies is reported in [38][40][42].

1.1 Ginzburg-Landau theory

Ginzburg Landau theory provides an extremely useful tool to phenomenologically describe superconductors close to the critical temperature. The phase transition at $T_c$ signals the appearance of an ordered state in which the electrons are at least partially condensed into frictionless superfluid. The state of the superconductor is represented by a complex field order parameter $\psi$ and its free energy functional is given by:

$$F = F_N + \int_{\mathbb{R}^d} d^d x \left[ \frac{\hbar^2}{2m^*} \left| \left( \nabla + i \frac{e^*}{\hbar c} A \right) \psi \right|^2 + \alpha |\psi|^2 + \beta |\psi|^4 + \frac{\left( \nabla \times A \right)^2}{8\pi} \right]$$

(1.1)

Where $m^*$ and $e^*$ are effective mass and charge, and are directly linked to the mass and charge of the particle responsible for superconductivity. $F_N$ represents the free energy of the material when it is in a normal state, which can be easily considered as energy offset. $A$ is the vector potential. Experiments indicate $m^* = 2m_e$ and $e^* = 2e$, where $m_e$ is the electron mass. This suggests that the particle leading to superconductivity are bound state of electrons. Thus, it is convenient to choose a normalization for the order parameter such that $|\psi(\mathbf{r})| = n_s^*(\mathbf{r})$, where $n_s^*(\mathbf{r})$ represents the superconducting particle density. We are allowed to make this choice thanks to the freedom in $\alpha$ and $\beta$. However, Ginzburg Landau theory does not explain why electron condensate in pairs and give rise to a frictionless fluid. These answers were given by Bardeen Cooper Schrieffer in 1957 [5], when BCS theory was first published, even though its connection with GL theory was still unknown. Two years later, Gor’kov [20], using Green Functions formalism derived Ginzburg Landau equations as a consequence of the free energy functional reported in Eq.(1). Its particular structure is due to the vicinity to the critical temperature. In this way, Gor’kov managed to ascribe a physical meaning to the order parameter $\psi$. 
1.1. Ginzburg-Landau theory

Let us now focus on the coefficients $\alpha$ and $\beta$. Following Gor’kov derivation and Matsubara formalism it is possible to express them in in terms of inter/intra-band coupling coefficients and impurity level. However, as the Ginzburg Landau theory for second order phase transitions states, we know that, the coefficients of the second order term must be $\alpha \propto 1 - \frac{T}{T_c}$. This means that if $T < T_c$ then $\alpha < 0$ an order parameter $|\psi| \neq 0$ will lower the energy, leading to a minimum. By contrast if $T > T_c$ then $\alpha > 0$ and the most favorable situation occurs for $|\psi| = 0$.

Moreover GL theory completely covers and justifies all the previously existing London theory of superconductivity, and explains the magnetic flux quantization. As an example let us consider the simplest solution, i.e. $|\psi| = \text{const}$ and $A = 0$. From Eq.(1) it is clear that a uniform field leads to a smaller energy then a non uniform one. Hence we have:

\[
F = F_N + \alpha|\psi|^2 + \frac{\beta}{2}|\psi|^4
\] (1.2)

To obtain the equation of motion let us minimize the free energy functional, i.e. $\frac{\delta F}{\delta|\psi|} = 0$ which leads to the equation of motion for $|\psi|:

\[
\left( \alpha + \beta |\psi|^2 \right) |\psi| = 0
\] (1.3)

Whose possible solutions are $|\psi| = 0$ and $|\psi| = \sqrt{-\frac{\alpha}{\beta}}$. The fist one leads to $F = F_N$, i.e. the normal state in which we have no cooper pairs formation. The second one leads to:

\[
F = F_N - \frac{\alpha^2}{2\beta}
\] (1.4)

In this case we obtain a state leading to an even smaller energy, but for this solution to be possible, we need the coefficient $\alpha$ to be negative. It is also important to check that these states actually represent minima of the free energy. We can easily do that by studying the concavity of the free energy in that point, i.e.:

\[
\frac{\partial^2 F}{\partial|\psi|^2} = 2\alpha + 6\beta|\psi|
\] (1.5)

Therefore in the two possible minima we have:

\[
\frac{\partial^2 F}{\partial|\psi|^2} \bigg|_{|\psi|=\psi_0} = -4\alpha > 0 \quad \text{if} \quad T < T_c
\] (1.6)

\[
\frac{\partial^2 F}{\partial|\psi|^2} \bigg|_{|\psi|=\psi_0} = 2\alpha > 0 \quad \text{if} \quad T > T_c
\] (1.7)

This confirms the fact that below the critical temperature the superconducting state is preferred, while above $T_c$ the ground state corresponds to the normal state. Moreover, Eq.(1.4) directly explains the presence of the critical field in Type 1
superconductors. In fact, the energy $\Delta F = \frac{\alpha^2}{2\beta}$ is what we need to provide to bring
the superconductor back into a normal state, therefore we can define the critical
field as follows:

$$\frac{H_c^2}{4\pi} = \frac{\alpha^2}{\beta}$$ (1.8)

This requires $\beta$ to be positive, which is coherent with GL theory assumptions.
To conclude this brief introduction about Ginzburg Landau theory, it is worth
underlying how it offers an extremely interesting and deep picture of particle-drive
phenomena from a field theory perspective.
1.2 Ground state excitations

Now that the conditions to have a stable superconducting ground state are clear, let us study what happens when we apply a perturbation to it. This is the first step necessary to understand the fundamental topological excitations, i.e. the vortices. We will start by studying the simplest case of a single component isotropic superconductor, whose free energy, written in dimensionless units, is:

$$F = \int d^3x \left\{ \left| (\nabla + iqA)\psi \right|^2 + d|\psi|^2 + \frac{1}{2} \theta|\psi|^4 + \frac{(\nabla \times A)^2}{2} \right\}$$ (1.9)

Let us suppose now that the order parameter and the vector potential are respectively:

$$\psi = \left[ \bar{u}_i + \varepsilon(r) \right] e^{i[\bar{\theta}_i + \phi_i]}$$ (1.10)
$$A = a(r)$$ (1.11)

Where $\bar{u}_i$ and $\bar{\theta}_i$ are the ground state values, obtained as in the previous section. $\varepsilon(r), \phi(r), a(r)$, are instead small perturbations. Moreover we assume cylindrical symmetry in the system. Substituting in the free energy, we can write the functional as:

$$\mathcal{F} = a\bar{u}^2 + \frac{b}{2} \bar{u}^4 + 2\varepsilon(a + b\bar{u}^2)\bar{u} + \left( \nabla \varepsilon \right)^2 + \bar{u}^2 \left( \nabla \phi \right)^2 + \varepsilon^2 \left( 2a + 6b\bar{u}^2 \right) +$$
$$+ \frac{(\nabla \times a)^2}{2} + \frac{1}{2} q^2 a^2 \bar{u}^2$$ (1.12)

Since in a superconducting ground state the order parameter is $\bar{u} = \sqrt{\frac{a}{b}}$, we notice that $\mathcal{F}^{(1)} = 0$. Moreover we can introduce the following notation:

$$\Gamma = (\varepsilon) \quad \nabla(\Gamma) = (\nabla \varepsilon) \quad \mathcal{M}^2 = (2a + 6b\bar{u}^2000)$$ (1.13)

Where $\hat{\phi} = \bar{u}\phi$. Then Eq.(1.12) becomes$^1$:

$$\mathcal{F} = (\nabla \Gamma)^2 + \Gamma^T \mathcal{M}^2 \Gamma + \frac{(\nabla \times a)^2}{2} + \frac{1}{2} q^2 a^2 \bar{u}^2$$ (1.14)

We can notice that this linearized free energy is the sum of two remarkable free energies. We have a Klein-Gordon free energy for what concerns the field modulus and phase, and Proca free energy for the vector potential. Moreover, it is worth

---

$^1$We will neglect the constant term $\mathcal{F}^{(0)}$ since it is irrelevant to the equation of motion.
underlining how in the linearized free energy, the vector potential and superconducting field perturbation are decoupled. The vector potential couples instead to the ground state of the superconductor trough the charge $q$. We can now derive the equation of motion for the modulus and phase of the macroscopic wave function and for the vector potential. In the functional differentiation we will assume that the fields perturbations vanish at the boundaries of the system. We have then:

$$\frac{\delta F}{\delta \Gamma} = 0 \Rightarrow \nabla^2 \Gamma + \mathcal{M}^2 \Gamma = 0 \quad (1.15)$$

$$\frac{\delta F}{\delta \mathbf{a}} = 0 \Rightarrow \nabla \times \nabla \times \mathbf{a} - q^2 \bar{u}^2 \mathbf{a} = 0 \quad (1.16)$$

By introducing $\nabla \times \mathbf{a} = \mathbf{b}$ we obtain the equation of motion for the magnetic field as follows:

$$\nabla \times \nabla \times \mathbf{b} = q^2 \bar{u}^2 \mathbf{b} \quad (1.17)$$

Using the relation $\nabla \times \nabla \times \mathbf{b} = \nabla (\nabla \cdot \mathbf{b}) - \nabla^2 \mathbf{b}$, and the solenoidality of the magnetic field, i.e. $\nabla \cdot \mathbf{b} = 0$, we obtain:

$$\nabla^2 \mathbf{b} - m_b^2 \mathbf{b} = 0 \quad m_b = q^2 \bar{u}^2 \quad (1.18)$$

Let us now analyze more in detail the physical consequences of these equations. Starting by Eq.(1.18), we can notice that the magnetic field has acquired a mass $m_b = q^2 \bar{u}^2$. This equation is the London equation for perturbations to the gauge field. In fact, the order parameter is assumed to be constant everywhere, except for a local perturbation. Hence the magnetic field has to vanish everywhere except for the perturbed area. By solving its equation of motion, keeping in mind that we assumed cylindrically symmetric perturbations, we obtain:

$$\mathbf{b}(r) = \mathbf{b}(0)e^{-m_b r} \quad (1.19)$$

We define penetration depth the inverse of the field mass, i.e. $\lambda = m_b^{-1} = \frac{1}{q\bar{u}}$. It is $\lambda$ to describe how far the magnetic field can penetrate in the superconductor. This is an evidence of the Anderson-Higgs mechanism. If we had no superconductivity in the ground state, then we would have $m_a^2 = 0$ and the magnetic field would be massless again. Let us now focus on what happens to the perturbations of the magnetic field. The equation of motion for the perturbation of the modulus is:

$$\nabla^2 \varepsilon + \left(2a + 6b\bar{u}^2\right)\varepsilon^2 = 0 \quad \rightarrow \quad \bar{u} = \sqrt{-\frac{a}{b}} \quad \rightarrow \quad \nabla^2 \varepsilon - 4a = 0 \quad (1.20)$$

Since $\alpha > 0$ by hypothesis, the requirement of a perturbation vanishing at infinity is fulfilled, yielding:

$$\varepsilon(r) = \varepsilon(0)e^{-\frac{r}{\xi}} \quad \text{with} \quad \xi = \frac{1}{2\sqrt{\alpha}} \quad (1.21)$$

Let us finally focus on what happens to the phase. From Eq.(1.15), we have:

$$\nabla^2 \phi = 0 \quad (1.22)$$
This means that we have a massless mode, since the mass associated to the phase recovery is zero. This equation reflects the local $U(1)$ symmetry of the Ginzburg Landau free energy. By adding more superconducting components and potential terms we would obtain a more complicated and non diagonal mass matrix $M^2$. This means that to obtain the coherence lengths as done above, we would need to diagonalize the matrix. Therefore, the eigenvectors would also be linear combination of the modes associated to the single superconducting components. The physical consequence of this is the presence of collective modes at which more than one condensate takes part. We could also obtain phase collective modes, the so called Leggett modes [26][27].
1.3 Flux quantization and vortex solutions

One of the most successful results of Ginzburg Landau theory is the possibility to describe the presence and interaction of vortices in superconductors. To introduce this topic, let us start by considering a single component 2D isotropic superconductor with a hole in the bulk, as shown in Figure 1.1

Let us now calculate the magnetic flux within the contour \( \sigma \). In the Meissner state, supercurrents occurring around the hole rapidly screen the magnetic field. Hence, along the contour we can assume \( J(\sigma) = 0 \). Hence the magnetic flux results:

\[
\Phi = \int_{S(\sigma)} d^2x \, \mathbf{B} \cdot \mathbf{n} = \{\mathbf{B} = \nabla \times \mathbf{A}\} = \oint_{\sigma} dl \cdot \mathbf{A} \tag{1.23}
\]

In a one component isotropic superconductor the vector potential is coupled to the gradient of the order parameter phase, resulting in the supercurrent:

\[
J = -\lambda^2 \left( \frac{\nabla \theta}{q} + \mathbf{A} \right) \tag{1.24}
\]

Re-arranging with respect to the vector potential and substituting into Eq.(1.23), we obtain:

\[
\Phi = -\oint_{\sigma} dl \cdot \left( \lambda^2 J + \frac{\nabla \theta}{q} \right) \tag{1.25}
\]

Since we assumed the superconductor to be in Meissner state, and the hole to be in the bulk, we have a lot of freedom in the choice of the contour \( \sigma \). Hence, we can choose it such that:

\[
\lambda^2 \oint_{\sigma} dl \cdot J = 0 \tag{1.26}
\]

That leads to:

\[
\Phi = -\frac{1}{q} \oint_{\sigma} dl \cdot \nabla \theta = -\frac{\Delta \theta}{q} \tag{1.27}
\]

Since the macroscopic wave function must be a single valued function, we have that \( \Delta \theta = 2\pi N \), where \( N \) is an integer number, to which we will refer as winding
number. Hence we obtain that the flux trough the superconductor is quantized, because it can only be a multiple of $\Phi_0$:

$$\Phi = -N\Phi_0 \quad \Phi_0 = \frac{2\pi}{q} \quad (1.28)$$

We can therefore define the vortex charge as:

$$N = \frac{1}{2\pi} \oint \mathbf{l} \cdot \nabla \theta \quad (1.29)$$

Let us now study more in details the structure and properties of vortices. Physically, a vortices are points in 2D or lines in 3D around which the order parameter phase winds $N$ times and the modulus decays to zero. These topological defects are strongly related to the $U(1)$ symmetry of the model. The presence of the gauge field plays a fundamental role in this scenario, in fact the phase winding produces a phase gradient, that with no magnetic field would be present also at infinite distance from the singularity. This would cost an enormous amount of energy, since the free energy is directly dependent on these gradients. Hence the vector potential couples with the phase gradient, and effectively winds around the vortex as well. In this way the vector potential compensates the phase winding leading to energetically stable states. This means that, if we have a stable state with a vortex and no external magnetic field, we have to expect a magnetic field produced by the presence of the vortex.

The first thing we need to study to understand the behavior of these excitations are their equation of motion$^2$

$$\frac{\delta F}{\delta \psi^*} = 0 \quad (1.30)$$

$$= \frac{\delta}{\delta \psi^*} \int_\Omega d^3x \left\{ \frac{1}{2} \left[ (\partial_j - iqA_j)\psi^* \right] \left[ (\partial_j + iqA_j)\psi \right] + a\psi\psi^* + \frac{b}{2} \psi^2\psi^2* \right\} \quad (1.31)$$

$$= \frac{1}{2} \frac{\delta}{\delta \psi^*} \left\{ \int_{\partial\Omega} d^2x \psi^* (\nabla + iq\mathbf{A}) \cdot \mathbf{n} - \int_\Omega d^3x \psi^* (\nabla + iq\mathbf{A})^2 \psi \right\} \quad (1.32)$$

$$+ (a + b|\psi|^2)\psi \quad (1.33)$$

$$\Rightarrow (\nabla + iq\mathbf{A})^2\psi = 2a\psi + 2b|\psi|\psi \quad (1.34)$$

$^2$We spend some time deriving them since this single component case is handy. In multicomponent cases the equation of motion are more complex, but the underlying structure such as the assumptions for the boundary conditions remain the same.
Chapter 1. Introduction

With the boundary condition of no normal current, i.e. \((\nabla + iq\psi) \cdot \mathbf{n} = 0\). For the vector potential we have:

\[
\frac{\delta F}{\delta A_k} = 0
\]

\[
= \frac{1}{2} \frac{\delta}{\delta A_k} \int d^3x \left[ (\nabla - iqA_j)\psi^*(\nabla + iqA_j)\psi + (\nabla \times \mathbf{A})^2 \right]
\]

\[
= q \text{Im}\{\psi^*(\nabla + iqA_k)\psi\} + \frac{\delta}{\delta A_k} \int d^3x \partial_i \delta A_j (\partial_i A_j - \partial_j A_i)
\]

\[
= q \text{Im}\{\psi^*(\nabla + iqA_k)\psi\} + \frac{\delta}{\delta A_k} \oint_{\partial\Omega} d^2x n_i [(\partial_i A_j - \partial_j A_i)\delta A_j + \partial_i (\delta A_j n_i)]
\]

\[
= q \text{Im}\{\psi^*(\nabla + iqA_k)\psi\} + \frac{\delta}{\delta A_k} \oint_{\partial\Omega} d^2x (B \times n)_j
\]

\[
\Rightarrow (\nabla \times \nabla \times \mathbf{A})_k + q^2 |\psi|^2 A_k = -q \text{Im}\{\psi^* \nabla \psi\}
\]

Where we assumed the boundary condition \(B \times \mathbf{n} = 0\). Recapping we have:

\[
(\nabla + iq\mathbf{A})^2 = 2\left(a + b|\psi|^2\right)\psi
\]

\[
\nabla \times \nabla \times \mathbf{A} + q^2 |\psi|^2 \mathbf{A} = q \text{Im}\{\psi^* \nabla \psi\}
\]

With the boundary conditions:

\[
\begin{cases}
(\nabla \psi + iq\psi \mathbf{A}) \cdot \mathbf{n} = 0 \\
\mathbf{B} \times \mathbf{n} = 0
\end{cases}
\]

Since we assumed cylindrical symmetry we can perform the following ansatz. Using \(N\) for the winding number we have:

\[
\psi = f(r)e^{i\theta} \quad A = \frac{a(r)}{r} \mathbf{u}_\phi
\]

Substituting into Eq.(1.30) yields to the coupled equations:\(^3\)

\[
- \frac{1}{r} \frac{\partial}{\partial r} \left[ \frac{1}{r} \frac{\partial f(r)}{\partial r} \right] + \left[ \frac{1}{r^2} (N + qa(r)) - 2(a + bf^2(r)) \right] f(r) = 0
\]

\[
\frac{\partial}{\partial r} \left[ \frac{1}{r} \frac{\partial a(r)}{\partial r} \right] + \frac{1}{r} (q^2 a(r) + qN) f(r)^2 = 0
\]

\(^3\)In the following equations we are using the differential form of the identity \(\oint \nabla \theta \cdot d\mathbf{l} = 2\pi N \Rightarrow \nabla \theta = \frac{N}{r}\)
It is worth noticing that thanks to cylindrical symmetry terms like $\nabla \theta \cdot \nabla f$ and $A \cdot \nabla |\psi|$ vanish. Moreover, to have vortex-like solutions we need the field to recover its ground state value for $r \to \infty$ and to be in its normal state for $r = 0$, hence:

$$f(r = 0) = 0 \quad f(r \to \infty) \to \sqrt{-\frac{a}{b}}$$ (1.49)

We can also obtain the asymptotic value of the vector potential by considering Eq.(1.48) in the limit $r \to \infty$. Considering only the leading order:

$$q^2 a(r) - qN = 0 \quad \Rightarrow \quad A(r \to \infty) = -\frac{N}{qr} u_\theta$$ (1.50)

By solving Eq.(1.47) and Eq.(1.48) we are able to fully describe interactions between vortices, taking into account their kinetic energy, magnetic interactions and core core interaction. However, given the highly non-linearity of those equations have no analytical solution.

A very useful approximation is the London limit, in which we have $|\psi| \sim const$. In this case we would neglect the core-core interaction, but at the same time we would be able to have analytical expressions for kinetic energy and magnetic interaction. In this regime we also have $\xi \ll \lambda$, which means that the order parameter recovers way faster compared to the magnetic field attenuation, as displayed in Fig.1.2

![Figure 1.2: Comparison between $|\psi_1|$ and $|B_z|$](image)
In this approximation we can obtain a very nice equation for the magnetic field by taking the curl of Eq. (1.44) yielding:

\[
\nabla \times \nabla \times \mathbf{B} + \lambda^{-2} \mathbf{B} = \frac{1}{q} \nabla \times \nabla \theta
\]

(1.51)

\[
\nabla \times \nabla \times \mathbf{B} = \nabla (\nabla \cdot \mathbf{B}) - \nabla^2 \mathbf{B}
\]

(1.52)

\[
\Rightarrow \lambda^2 \nabla^2 \mathbf{B} - \mathbf{B} = -\frac{1}{q} \nabla \times \nabla \theta
\]

(1.53)

Since \( \mathbf{A} = A(r) \mathbf{u}_\theta \Rightarrow \mathbf{B} = B(r) \mathbf{u}_\theta \). Moreover we have \( \nabla \theta = \frac{N}{r} \mathbf{u}_\theta \Rightarrow \nabla \times \nabla \theta = 2\pi N \delta(r - r_0) \). We can then solve Eq. 1.53 with the boundary condition \( B(r \to \infty) \to 0 \); calling \( \Phi = N \Phi_0 \) we have:

\[
\lambda^2 \nabla^2 B_z - B_z = \Phi \delta(r - r_0) \quad \Rightarrow \quad B_z(r) = \frac{\Phi}{2\pi \lambda^2} K_0 \left( \frac{|r - r_0|}{\lambda} \right)
\]

(1.54)

Where \( K_0(r) \) is the zeroth order modified Bessel function of the second kind. Since it is diverging for \( r \to 0 \), we can estimate the magnetic field in the vortex core introducing a cutoff for \( r \sim \xi \). This is reasonable since in the center of the vortex we have a normal conductor. Hence we have:

\[
B_z(0) \approx \frac{\Phi}{2\pi \lambda^2} \ln \left( \frac{\lambda}{\xi} \right)
\]

(1.55)

With energy per unit of length in \( z \) direction:

\[
E_v = \frac{\Phi}{2} B_z(0) \approx \frac{1}{4\pi} \left( \frac{\Phi}{\lambda} \right)^2 \ln \left( \frac{\lambda}{\xi} \right)
\]

(1.56)

Eq. (1.53) is linear, therefore in this limit we can easily obtain the magnetic field and interaction energy of multiple vortices, even though core-core interaction remains neglected. For example, in case of two vortices with \( (N_1, N_2) \) in position \( r_1 \) and \( r_2 \) we have:

\[
B_z(r) + \lambda^2 B(z) = \Phi_0 [N_1 \delta(r - r_1) + N_2 \delta(r - r_2)]
\]

(1.57)

With energy per unit of length:

\[
E = \frac{\Phi}{2} B_z(0) \approx \frac{1}{4\pi} \left( \frac{\Phi}{\lambda} \right)^2 \ln \left( \frac{\lambda}{\xi} \right) + \frac{\Phi_0^2 N_1 N_2}{2\pi \lambda^2} K_0 \left( \frac{|r_1 - r_2|}{\lambda} \right)
\]

(1.58)

Where the interaction energy is:

\[
E_{int} = \frac{\Phi_0^2 N_1 N_2}{2\pi \lambda^2} K_0 \left( \frac{|r_1 - r_2|}{\lambda} \right)
\]

(1.59)

We can notice that the interaction energy is quadratic in the winding numbers. We can notice that in the London limit, two vortices with same windings will always
repel each other, while having opposite winding numbers yield attraction. In this case the total topological charge must be conserved. For the interested reader, a much more complete treatment of multi-band superconductivity can be found in [2] [25] [1].
1.4 First and second critical fields

Before proceeding to the multicomponent case it is worth studying how the critical fields change in presence of vortex excitations in the superconducting field. In fact, the critical field obtained at the beginning in fact was for a type-1 superconductor, i.e. for a superconductor in which the transition is between normal and Meissner state. In a type-2 instead we can have the formation of a vortex state, therefore we will have more critical fields to take into account. The critical field we obtain before, i.e. :

\[ H_c = \frac{|\alpha|}{\sqrt{\beta}} = \frac{\Phi_0}{4\pi \lambda \xi} \]  
\hspace{1cm} (1.60)

Determines the field for which it is not energetically convenient to have superconductivity anymore. However, vortices will enter the system for fields that are smaller than this one, but sufficiently big to destroy the uniform ground state. To estimate this energy we need to introduce in the free energy a term for the external magnetic field. Let us then perform a Legendre transformation to start working with the Gibbs free energy:

\[ G = F - \int d^3x \mathbf{B} \cdot \mathbf{H} \]  
\hspace{1cm} (1.61)

The superconductor will enter in a stable vortex state when the condition \( G(1\text{ vortex}) - G(0\text{ vortex}) < 0 \). Hence we can find the lower critical field by requiring \( G(1) - G(0) = 0 \), that leads to:

\[ H_{c1} = \frac{1}{4\pi} \frac{\Phi_0}{\lambda^2} \ln \left( \frac{\lambda}{\xi} \right) \]  
\hspace{1cm} (1.62)

If we compare Eq.(1.62) with Eq.(1.60), it is clear that \( H_{c1} < H_c \) in a type-2 superconductor where \( \lambda > \xi \), while \( H_{c1} > H_c \) for a type 1 superconductor. Hence in type 1 superconductors, vortex states are energetically unfavorable, since superconductivity is destroyed for lower fields. Focusing on a type two superconductor, for \( H > H_{c1} \) we will start assisting to vortex formation. The more we increase the external magnetic field the more vortices we will create. At a certain field value, \( H_{c2} \), we are going to reach a state in which vortex cores overlap, creating a macroscopic area in which superconductivity is destroyed in favor of the normal state. This field is called second or upper critical field and it is given by:

\[ H_{c2} = \frac{\Phi_0}{4\pi \xi^2} \]  
\hspace{1cm} (1.63)

Comparing it with \( H_c \) we notice that \( H_{c2} > H_c \), meaning that a type-2 superconductor can maintain superconductivity at much higher field than a type 1.
1.5 Multicomponent Ginzburg Landau

It is possible to use Ginzburg Landau theory to describe multicomponent superconductors. In this case we need to use more order parameters, specifically, one complex order parameter per phase. In this case the free energy functional becomes (once rescaled to be dimensionless):

$$F = \sum_{\alpha}^{N} \int_{\mathbb{R}^d} d^d x \left[ \frac{1}{2} |D\psi_\alpha|^2 + a_\alpha |\psi|^2 + \frac{b_\alpha}{2} |\psi|^4 + \frac{(\nabla \times A)^2}{2} \right]$$

(1.64)

Where \(N\) is the number of components, \(D_j = \partial_j + i q A_j\) is the covariant derivative, \(a_\alpha < 0\ \forall \alpha\) and \(b_\alpha > 0\ \forall \alpha\). Since there are not inter-band terms, all the component will have independent equation of motion, therefore we can now focus on the free energy functional per component, i.e.:

$$F_\alpha = \frac{1}{2} |D\psi_\alpha|^2 + a_\alpha |\psi|^2 + \frac{b_\alpha}{2} |\psi|^4$$

(1.65)

Here we can identify the the covariant derivative \(\frac{1}{2} |D\psi_\alpha|^2\) as the kinetic energy of the field, and the quadratic and quartic term as the potential. We have then:

$$\mathcal{K}_\alpha = |(\nabla + i q A)\psi_\alpha|^2$$

(1.66)

$$\mathcal{V}_\alpha = a_\alpha |\psi|^2 + \frac{b_\alpha}{2} |\psi|^4.$$  

(1.67)

This underlines that the model that we are using to describe superconductivity is well known in classical field theory: it is the non-relativistic limit of the \(U(1)\) gauge theory for the scalar complex massive field \(\psi = |\psi|e^{i\theta}\), with the self interaction term \(|\psi|^4\).

The potential is plotted in Fig.1.3. We can obtain the equation of the different matter fields by imposing \(\frac{\delta F}{\delta \psi_\alpha^*} = 0\) and using boundary conditions (1.45), obtaining:

$$D_j D_j \psi_\alpha - 2 \left( a_\alpha + b_\alpha |\psi|^2 \right) \psi = 0$$

(1.68)

The first symmetry which is worth studying is the \(U(1)\) symmetry. As first thing, we notice that, under the assumption of no magnetic field and uniform matter field, we have:

$$|\psi_{0\alpha}|^2 = \frac{-a_\alpha}{b_\alpha} \Rightarrow |\psi_{0\alpha}| = \sqrt{-\frac{a_\alpha}{b_\alpha}}$$

(1.69)

This solution leaves the phase completely free. Hence any field of the form

$$\psi_\alpha = \psi_{0\alpha} e^{i\theta}$$

(1.70)

is solution in the uniform case. This result is well displayed in Fig.1.3. The equation of motion fixes the modulus of the order parameter, that is represented as a vector.
in the Gauss plane. Since the potential only depends on the modulus, any rotation, generated by the term \( e^{i\theta} \), will lead to an equivalent physical situation. Since the field is uniform, also the phase must be constant, hence we speak of global \( U(1) \) symmetry. As the system goes in the ground state, one value of the phase is chosen, and therefore we say that the system has broken the \( U(1) \) global symmetry. Since the considered free energy describes a \( N \) component superconductor without inter-band couplings, each component has \( U(1) \) symmetry, and the whole system therefore has \( U(1)^N \) symmetry. Let us now consider a spatially varying fields with minimal coupling with the vector potential \( \mathbf{A} \). For the sake of simplicity we will study a single component. In fact, until we introduce inter-band couplings all components behave qualitatively in the same way. Considering the free energy functional is Eq.1.65, let us study what happens under a \( U(1) \) rotation of the field, i.e.:

\[
\psi'_\alpha = \psi_\alpha e^{i\phi(r)}
\]

We have:

\[
F_\alpha = \frac{1}{2} \left( \nabla + iq \mathbf{A} \right) \psi_\alpha e^{-i\phi} \right|^2 + a_\alpha |\psi'_\alpha|^2 + \frac{b_\alpha}{2} |\psi'_\alpha|^4 \tag{1.72}
\]

\[
= \frac{1}{2} e^{-i\phi(r)} \left[ \nabla + iq \left( \frac{-\nabla \phi}{q} + \mathbf{A} \right) \right] |\psi'_\alpha|^2 + a_\alpha |\psi'_\alpha|^2 + \frac{b_\alpha}{2} |\psi'_\alpha|^4 \tag{1.73}
\]

\[
= \left\{ \mathbf{A}' = \mathbf{A} - \frac{\nabla \phi}{q} \right\} \tag{1.74}
\]

\[
= \frac{1}{2} \left( \nabla + iq \mathbf{A}' \right) |\psi'_\alpha|^2 + a_\alpha |\psi'_\alpha|^2 + \frac{b_\alpha}{2} |\psi'_\alpha|^4 \tag{1.75}
\]
We can notice that the field $\psi'_\alpha$ has the same free energy functional $F_\alpha$ up to a gauge term. This means that these two fields are describing the same physical situation. Moreover, it is interesting to see how it is the phase of the field to couple with the vector potential gauge. However, in this case the $U(1)$ symmetry is not global anymore. In fact, since the field is non-uniform, we have a position dependent phase, which implies a local $U(1)$ symmetry, i.e.:

$$\theta' = \theta + \phi(r)$$  \hspace{1cm} (1.76)

$$A' = A - \frac{\nabla \phi}{q}$$ \hspace{1cm} (1.77)

This free energy functional presents also a discrete symmetry, namely $\mathbb{Z}_2$ symmetry. In fact we can perform a complex conjugate transformation on the order parameter $\psi_\alpha \to \psi^*_\alpha$, and still have the same functional. This symmetry is commonly referred to as time reversal symmetry. Let us now derive a crucial quantity in a superconductor, the current density $J = \sum_{\alpha} j_\alpha$. To find $j_\alpha$ we can perform a functional derivative of the free energy wrt $A$, neglecting the magnetic field free energy. Calling $F' = F - \int \frac{(\nabla \times A)^2}{2}$, and $\rho^2 = \sum_{\alpha} |\psi_\alpha|$ we have:

$$J = -\frac{\delta F'}{\delta A}$$ \hspace{1cm} (1.78)

$$= \sum_{\alpha} \frac{i q}{2} (\psi^* \nabla \psi_\alpha - \psi_\alpha \nabla \psi^*) - q^2 \rho^2 \mathbf{A}$$

$$= \{\psi_\alpha = |\psi_\alpha| e^{i \theta}\}$$

$$= -\sum_{\alpha} \frac{i q}{2} \left\{ |\psi_\alpha| \nabla |\psi_\alpha| + i |\psi_\alpha|^2 \nabla \theta_\alpha - |\psi_\alpha|^2 \nabla \theta_\alpha + i |\psi_\alpha|^2 \nabla \theta_\alpha - q^2 |\psi_\alpha|^2 \mathbf{A} \right\}$$

$$\Rightarrow J = -\sum_{\alpha} q |\psi_\alpha|^2 \{ \nabla \theta_\alpha + q \mathbf{A} \}$$ \hspace{1cm} (1.79)

This result highlights how it is the phase of the superconducting field to couple with the vector potential and generate supercurrents. Moreover, the bigger the modulus of a certain component is, the higher will be its influence on the current density. It is also worth introducing the definition $\lambda^{-2}_\alpha = q^2 |\psi_\alpha|^2$. These coefficients define the contribution of each component to the Meissner screening of the magnetic field. We could now proceed as for the one component case to study the linearized equation of motion for ground state excitations. Without potential terms we would get still a diagonal mass matrix, i.e. independent gapped modes for the matter field and gapless mode for the phase difference. In this case we just report the results

\footnote{If we include it, then by putting this functional derivative to 0 we obtain the equation of motion of the vector potential}
for the two component case. A more detailed analysis of it is presented in [22] [15].

The mass matrix in the basis \( f = (\varepsilon_1, \varepsilon_2, \phi_{12})^T \) is given by:

\[
\mathcal{M}^2 = \begin{pmatrix}
  a_1 + 3b_1 & 0 & 0 \\
  0 & a_2 + 3b_2 & 0 \\
  0 & 0 & 0
\end{pmatrix}
\]

(1.80)

While the equation for the vector potential is:

\[
\nabla \times \nabla \times A = q^2 (\bar{u}_1^2 + \bar{u}_2^2) a
\]

(1.81)

In this case the lengthscale of the system is the magnetic field penetration depth and it is given by the recovery length of the gauge field, which in this case is:

\[
\lambda^{-2} = \frac{q^2}{\bar{u}_1^2 + \bar{u}_2^2} = \sum_{\alpha} \lambda_{\alpha}^{-2}
\]

(1.82)

### 1.6 Fractional Vortices

It is now worth studying how the flux quantization changes in a multicomponent superconductor. Proceeding in the same was as did in the single component case, we integrate the current density along a contour sufficiently big to have \(|J(r \to \infty)| \to 0\). Using Eq.(1.79) for the current density we obtain:

\[
\oint_{\sigma(r \to \infty)} J \cdot dl = -\oint_{\sigma} \sum_{\alpha} q |\psi_{\alpha}|^2 \{\nabla \theta_{\alpha} + q A\}
\]

(1.83)

\[
0 = \sum_{\alpha} \lambda_{\alpha}^{-2} \oint_{\sigma} \nabla \theta_{\alpha} \cdot dl + \left( \sum_{\alpha} \lambda_{\alpha}^{-2} \right) \oint_{\sigma} A \cdot dl
\]

(1.84)

\[
\Rightarrow \oint_{S(\sigma)} B \cdot n \, dS = -\sum_{\alpha} \lambda_{\alpha}^{-2} \oint_{\sigma} \nabla \theta_{\alpha} \cdot dl
\]

(1.85)

Using the definitions of \( \lambda^{-2}, \lambda_{\alpha}^{-2}, \rho^2 = \sum_{\alpha} |\psi_{\alpha}|^2 \) and that \( \oint_{\sigma} \nabla \theta_{\alpha} \cdot = 2\pi N_{\alpha} \) we get\(^6\)

\[
\Phi = -\Phi_0 \sum_{\alpha} \frac{|\psi_{\alpha}|^2}{\rho^2} N_{\alpha}
\]

(1.86)

Therefore we can notice that in a multicomponent superconductor each vortex carries a fraction \( \frac{|\psi_{\alpha}|^2}{\rho^2} \) of the flux quantum. That is why we talk of fractional vortices. Fractional vortices exhibit very interesting features that are analytically obtainable in the London limit. However, in the present work the London limit will not be used due to highly frustrated situations. We invite the interested reader to check [14] [2] [3] [11] [13] [4] [6] [19].

\(^6\)In this case \( N_{\alpha} \) is the total winding per component.
1.7 Anisotropic superconductors

Normally, most of superconducting materials are anisotropic, therefore it is crucial to know how the Ginzburg-Landau theory changes consequently. Adding anisotropies physically means that we are imposing different energy weights for “moving” in different directions. This means that the potential terms of the free energy will remain unchanged, whether the kinetic part becomes, using summation connection on the roman indices:

$$K = \sum_\alpha \left(D_j^* \psi_\alpha^* Q_{jk}^\alpha (D_k \psi_\alpha)\right)$$  \hspace{1cm} (1.87)

The \(\{i, j\}\) indeces define the spatial directions, while the greek index \(\alpha\) denotes the superconducting component. The terms \(Q_{ij}^\alpha\) define the weight of the field covariant derivatives in the different spatial directions. For example if \(Q_{xx}^\alpha \ll Q_{yy}^\alpha\), it means that in the \(\alpha\)-th component it is much more expensive to have a sharp varying field in the \(y\) direction than along \(x\). If we were in a single component system, we could simply rescale the system’s coordinate and vector potential, to make it isotropic. In a multi-band superconductor however, this procedure can “isotropise” only a single band, while the others will remain anisotropic. We will now study how the current density changes in these conditions. Let us consider the following free energy, for an anisotropic multicomponent superconductor:

$$F = \sum_\alpha N \int_{\mathbb{R}^d} d^d x \left[\frac{1}{2} (D_j^* \psi_\alpha^*) Q_{jk}^\alpha (D_k \psi_\alpha) + F_{pot} + \frac{(\nabla \times A)^2}{2}\right]$$  \hspace{1cm} (1.88)

Proceeding as in Eq.(1.78):

$$J_k = -\frac{\delta F'}{\delta A_k}$$  \hspace{1cm} (1.89)

$$= \sum_\alpha \frac{i q}{2} Q_{kj}^\alpha (\psi_\alpha^* \partial_j \psi_\alpha - \psi_\alpha \partial_j \psi_\alpha^*) - q^2 |\psi_\alpha|^2 Q_{kj}^\alpha A_j$$

$$= \left\{ \psi_\alpha = |\psi_\alpha| e^{i \theta} \right\}$$

$$= \sum_\alpha -q |\psi_\alpha|^2 Q_{kj}^\alpha (\partial_j \theta_\alpha + q A_j)$$  \hspace{1cm} (1.90)

As first thing we notice that the coefficients defining the influence of each band to the Meissner screening are not scalar anymore but rank 2 tensors. Naming:

$$\left(\lambda_{\alpha}^{-2}\right)_{kj} = q^2 |\psi_\alpha|^2 Q_{kj}^\alpha$$  \hspace{1cm} (1.91)

We obtain:

$$J_k = -\sum_\alpha \left(\lambda_{\alpha}^{-2}\right)_{kj} \left(\frac{1}{q} \partial_j \theta_\alpha + A_j\right)$$  \hspace{1cm} (1.92)
The contribution of each component to the total current is then:

\[ j_k = -\left( \lambda^{-2}_\alpha \right)_{kj} \left( \frac{1}{q} \partial_j \theta_\alpha + A_j \right) \]  

(1.93)

This result explicitly underlines how different directions can lead to different currents and magnetic field screening. We can check that this result is consistent with Eq.(1.78) by asking \( Q^\alpha_{jk} = (1)_{jk} \). The magnetic field is given by the Maxwell equation\(^7\) \( \epsilon_{ijk} \partial_j B_k = J_i \). We can now consider an explicit example for a two band superconductor with small anisotropies, i.e.:

\[
Q^1_{jk} = \begin{pmatrix} Q^1_{xx} & 0 \\ 0 & Q^1_{yy} \end{pmatrix} \quad Q^\alpha_{jk} = \begin{pmatrix} Q^1_{xx} (1 + \varepsilon) & 0 \\ 0 & Q^1_{yy} (1 + \varepsilon) \end{pmatrix}
\]  

(1.94)

Then we can rearrange Eq.(1.92) with respect to \( A \). Introducing the notation \( \hat{\lambda}^2_L = \left[ \Sigma_\alpha \lambda^{-2}_\alpha \right]^{-1} \), where \( (\hat{\lambda}^{-2}_\alpha)_{jk} = (\lambda^{-2}_\alpha)_{kj} = q^2 |\psi_\alpha|^2 Q^\alpha_{kj} \), we have:

\[
A = \hat{\lambda}^2_L J - \frac{1}{q} \sum_{\alpha=1,2} \hat{\lambda}^2_L \lambda^{-2}_\alpha \nabla \theta_\alpha
\]  

(1.95)

Taking the curl of the vector potential yields:

\[
B = \nabla \times \hat{\lambda}^2_L J - \frac{1}{q} \nabla \times \sum_{\alpha=1,2} \hat{\lambda}^2_L \lambda^{-2}_\alpha \nabla \theta_\alpha
\]  

(1.96)

Supposing to be dealing with a 2D superconductor in the London model, we will have \( J = J(x, y) \) and the same for \( \nabla \theta_\alpha \), that implies \( B = B_z u_z \). Hence, the expanded expression turns out to be:

\[
B_z = \frac{1}{q \rho^2} \left( \frac{\partial_x J_y}{Q^1_{yy}} - \frac{\partial_y J_x}{Q^1_{xx}} \right) - \frac{1}{q \rho^2} \left[ |\psi_1|^2 (\nabla \times \nabla \theta_1)_z + |\psi_2|^2 (\nabla \times \nabla \theta_2)_z \right] - \frac{|\psi_2|^2}{q \rho^4} \left( \varepsilon_{yy} \partial_x J_y - \varepsilon_{xx} \partial_y J_x \right) - \frac{|\psi_2|^2 |\psi_1|^2}{q \rho^4} \left[ \varepsilon_{yy} \partial_x \partial_y (\theta_2 - \theta_1) - \varepsilon_{xx} \partial_y \partial_x (\theta_2 - \theta_1) \right]
\]  

(1.97)

\[\text{nonumber}\]

\[
\]  

(1.98)

\[
\]  

(1.99)

With \( \rho^2 = \sum_\alpha |\psi_\alpha|^2 \). Supposing not to have vortices, i.e. \( (\nabla \times \nabla \theta_1)_z = 0 \) and \( (\nabla \times \nabla \theta_2)_z = 0 \), expression (1.97) becomes:

\[
B_z = \frac{1}{q \rho^2} \left( \frac{\partial_x J_y}{Q^1_{yy}} - \frac{\partial_y J_x}{Q^1_{xx}} \right) - \frac{|\psi_2|^2}{q \rho^4} \left( \varepsilon_{yy} \partial_x J_y - \varepsilon_{xx} \partial_y J_x \right) - \frac{|\psi_2|^2 |\psi_1|^2}{q \rho^4} \left[ \varepsilon_{yy} \partial_x \partial_y (\theta_2 - \theta_1) - \varepsilon_{xx} \partial_y \partial_x (\theta_2 - \theta_1) \right]
\]  

(1.100)

\[\text{nonumber}\]

\[
\]  

(1.101)

\[\text{This equation can also be obtained by setting } \delta F/\delta A = 0\]
1.7. Anisotropic superconductors

We can notice that Eq. 1.101 highlights the fact that anisotropies couple phase differences to the magnetic field. In this case, even simple fluctuations of \(\theta_{21} = \theta_2 - \theta_1\) can lead to magnetic field. If we now take the isotropic limit, i.e. \(Q_{xx}^1 = Q_{yy}^1 = 1\) and \(\varepsilon_{xx}, \varepsilon_{yy} \to 0\), expression (1.101) becomes:

\[
B_z = \frac{1}{q\rho^2} (\partial_x J_y - \partial_y J_x)
\]

(1.102)

Which corresponds to the magnetic field of a isotropic superconductor with no vortices.

However, the result we just obtained for the current density can be further generalized by adding mixed kinetic terms. Let us see what is their effect on the current density. The most general form for the free energy functional in an anisotropic superconductor is:

\[
F = \frac{N}{\sum_{\alpha,\beta} d^d x} \left[ \frac{1}{2} (D^*_j \psi^*_\alpha) Q_{jk}^\alpha \psi_\alpha + F_{pot} + \frac{(\nabla \times A)^2}{2} \right]
\]

(1.103)

That can be rewritten as:

\[
F = \frac{N}{\sum_{\alpha} d^d x} \left[ \frac{1}{2} (D^*_j \psi^*_\alpha) Q_{jk}^\alpha \psi_\alpha + F_{pot} + \frac{(\nabla \times A)^2}{2} \right] + \frac{1}{2} \sum_{\alpha \neq \beta} \int_{\mathbb{R}^d} d^d x (D^*_j \psi^*_\alpha) Q_{jk}^{\alpha \beta} (D^*_k \psi^*_\beta)
\]

(1.104)

Hence the current density is:

\[
J_k = -\frac{\delta F'}{\delta A_k} \quad \Rightarrow \quad J_k = \sum_{\alpha} -q|\psi_\alpha|^2 Q_{jk}^\alpha (\partial_j \theta_\alpha + qA_j) - \frac{\delta F_{mix}}{\delta A_k}
\]

(1.105)

Let us then focus on \(\frac{\delta F_{mix}}{\delta A_k}\); We have:

\[
\frac{\delta F_{mix}}{\delta A_m} = \frac{1}{2} \sum_{\alpha \neq \beta} \frac{\delta}{\delta A_m} \int_{\mathbb{R}^d} d^d x (D^*_j \psi^*_\alpha) Q_{jk}^{\alpha \beta} (D^*_k \psi^*_\beta)
\]

(1.106)

Since the free energy must be real we have that the tensor \(Q_{jk}^{\alpha \beta}\) needs to be symmetric under spacial index interchange, hence \(Q_{jk}^{\alpha \beta} = Q_{kj}^{\alpha \beta}\) and have symmetric real part and antisymmetric imaginary part for what concerns the component index.
However, we will start by considering it just as a real symmetric tensor. Hence we have:

\[ Q_{jk}^{\alpha \beta} = Q_{kj}^{\alpha \beta} = Q_{k}^{\beta \alpha} = Q_{j}^{\beta \alpha} \]  

(1.107)

The current density is given by:

\[ J_{k}^{\text{mix}} = -\frac{\delta F_{\text{mix}}}{\delta A_k} \]

(1.108)

\[ = -q^2 \sum_{\alpha \neq \beta} Q_{k}^{\alpha \beta} \left\{ \frac{1}{q} \text{Im} \left\{ (\psi_{\alpha}^* \partial_j \psi_{\alpha}) \right\} + A_j \text{Re} \left\{ (\psi_{\alpha} \psi_{\beta}^*) \right\} \right\} \]

(1.109)

\[ = -q^2 \sum_{\alpha \neq \beta} Q_{k}^{\alpha \beta} \left\{ \frac{1}{q} \left[ (|\psi_{\beta}| \partial_j |\psi_{\alpha}|) \sin (\theta_{\alpha} - \theta_{\beta}) + |\psi_{\alpha}| |\psi_{\beta}| \cos (\theta_{\alpha} - \theta_{\beta}) \partial_j \theta_{\alpha} \right] \right. \]

\[ + \left. |\psi_{\alpha}| |\psi_{\beta}| A_j \cos (\theta_{\alpha} - \theta_{\beta}) \right\} \]

(1.110)

We can now order expression (1.112) with respect to the vector potential \( A \) and take its curl to obtain the magnetic field \( B \). Introducing the following notation:

\[ (\lambda^2_{k})_{k} = q^2 |\psi_{\alpha}|^2 Q_{k}^{\alpha \beta} \delta^{ab} \]

We can notice how in this case, also the gradients of the modulus of the order parameter can have an influence in the overall current. We can now order expression (1.112) with respect to the vector potential \( A \) and take its curl to obtain the magnetic field \( B \). Introducing the following notation:

\[ (\lambda^2_{k})_{k} = q^2 \sum_{\alpha \neq \beta} Q_{k}^{\alpha \beta} |\psi_{\alpha}| |\psi_{\beta}| \cos \theta_{\alpha \beta} \]  

(1.113)

and

\[ (\lambda^{-2}_{k})_{k} = q^2 \sum_{\beta} Q_{k}^{\alpha \beta} |\psi_{\alpha}| |\psi_{\beta}| \cos \theta_{\alpha \beta} \]  

(1.114)

With \( \theta_{\alpha \beta} = \theta_{\alpha} - \theta_{\beta} \). Using summation convention we have:

\[ B_i = \epsilon_{iml} \left[ \partial_m (\lambda^2_{k})_{lk} \right] \left\{ -J_k - q \sum_{\alpha \neq \beta} Q_{k}^{\alpha \beta} |\psi_{\beta}| \partial_j |\psi_{\alpha}| \sin \theta_{\alpha \beta} - \sum_{\alpha} (\lambda^{-2}_{k})_{k} \frac{\partial_j \theta_{\alpha}}{q} \right\} \]

(1.115)

\[ - \epsilon_{iml} \left[ \lambda^2_{lk} \partial_m J_k - \sum_{\alpha} \left[ (\lambda^2_{k})_{lk} \partial_m \left( (\lambda^{-2}_{k})_{k} \right) \frac{\partial_j \theta_{\alpha}}{q} - (\lambda^{-2}_{k})_{lk} \frac{\partial m \partial_j \theta_{\alpha}}{q} \right] \right] \]

(1.116)

\[ - q \epsilon_{iml} (\lambda^2_{k})_{lk} \sum_{\alpha \neq \beta} Q_{k}^{\alpha \beta} \left\{ \partial_m |\psi_{\beta}| \partial_j |\psi_{\alpha}| \sin \theta_{\alpha \beta} + |\psi_{\beta}| \partial_m \partial_j |\psi_{\alpha}| \sin \theta_{\alpha \beta} \right\} \]

+ |\psi_{\beta}| \partial_j |\psi_{\alpha}| \cos \theta_{\alpha \beta} \partial_m \theta_{\alpha \beta} \]
We can notice that in the most general case the number of terms generating the magnetic fields increases. In fact, we find first and second order derivatives not only in the phase but also in the modulus of the superconducting fields.

1.8 Anisotropic Vortices

When anisotropies are present in the system the vortex structures change and one of the first evidence is the loss of cylindrical symmetry. While in the isotropic model each solution has $S0(2)$ symmetry, in the anisotropic case the symmetry is reduced to a four-fold one, therefore the ansatz proposed in Eq. (1.46) is no longer valid and the situation becomes analytically much more complicated. The interested reader can find an extensive treatment of two components anisotropic superconductors in [38][40][42].
Chapter 2

Three component superconductors

Let us now enter the core topic of the present work: three components superconductors. Multiband superconductivity was theoretical pioneered in [39]; the experimental results reported in [21] with in the theoretical followup [32] represent a strong motivation to investigate further the theory of three component superconductors. Moreover, as shown in [4], it is possible to microscopically derive a multi-component Ginzburg Landau theory for $s + is$ superconducting states, which provides an extremely powerful tool to discover new phenomena. Since most of the superconducting materials are also anisotropic, we will use an anisotropic GL theory. In the present work we will not derive the Ginzburg-Landau coefficient microscopically, therefore each band will be described by our choice of $(a_\alpha, b_\alpha)$. Moreover the three different components can interact via Josephson coupling, which is included in the free energy functional as:

$$F_P = \frac{1}{2} \sum_{\beta > \alpha}^{3} \eta_{\alpha \beta} (\psi_\alpha \psi_\beta^* + \psi_\beta \psi_\alpha^*)$$

(2.1)

This kind of coupling is the simplest we could think of, but while in a two band system it does not lead to any peculiar phenomena, in the three band case it leads to highly frustrated situations. The new physics arises from the presence of three inter-band Josephson coupling instead of just one. This leads to situations in which the Josephson terms cannot be minimized all simultaneously, and compete to find the most favorable phase locking. The result of this frustration is the so called time reversal symmetry breaking. Moreover, in the present work we will be analyzing
anisotropic superconductors, therefore the free energy functional reads:

\[
F = \sum_{\alpha, \beta}^3 \left( D_j^* \psi^*_\alpha \right) Q_{jk}^{\alpha \beta} \left( D_k \psi_\beta \right) + \sum_{\alpha}^3 \left( a_\alpha |\psi_\alpha|^2 + \frac{b_\alpha}{2} |\psi_\alpha|^4 \right) + \frac{1}{2} \sum_{\beta > \alpha}^3 \eta_{\alpha \beta} \left( |\psi_\alpha| \psi^*_\beta + |\psi_\beta| \psi^*_\alpha \right) + \left( \nabla \times A \right)^2
\]

Let us now study the terms of Eq.(2.2). The tensor \(Q_{ij}^{\alpha \beta}\) contains all the information about the anisotropies, and we will assume it to be diagonal, both in the component and spatial indices. This physically means that we do not have inter-component scattering, and that the spatial anisotropies allow a diagonal representation for all the three components. Another important aspect to analyze concerns the coefficients \((a_\alpha, b_\alpha)\). In fact, since we have additional potential terms, we can face the situation in which \(a_\alpha > 0\) but the band still has nonzero superfluid density: in this case we would talk of passive bands. In the usual case of \(a_\alpha < 0\) we would talk of active band. The reason why \(a_\alpha\) might change sign is due to its temperature dependence. Starting from microscopic theory it is possible to derive a proper relation for it. A work concerning the methods to do it is presented in [24]. Moreover, it is worth rewriting the Josephson term to highlight its dependence on the phase differences among the different components. Writing \(\psi_\alpha = |\psi_\alpha|e^{i\theta_\alpha}\) and using \(\cos x = \frac{1}{2}(e^{ix} + e^{-ix})\), we obtain:

\[
F = \sum_{\alpha}^3 \left( D_j^* \psi^*_\alpha \right) Q_{j}^{\alpha \beta} \left( D_j \psi_\beta \right) + \sum_{\alpha}^3 \left( a_\alpha |\psi_\alpha|^2 + \frac{b_\alpha}{2} |\psi_\alpha|^4 \right) + \frac{1}{2} \sum_{\beta > \alpha}^3 \eta_{\alpha \beta} |\psi_\alpha| |\psi_\beta| \cos(\theta_\alpha - \theta_\beta) + \left( \nabla \times A \right)^2
\]

We will study only situation in which the superconductor is frustrated, in which we cannot assume \(|\psi_\alpha| = \text{const}\), therefore the London limit is not applicable. Fluctuations around the ground state of three band superconductors are also studied in [9], [8] and [12].

### 2.1 Ground state

As seen in the previous section, the ground state depends only on the potential terms, and is not affected by anisotropies. Hence, to determine it we need to minimize with respect to the order parameters the following expression:

\[
F_P = \sum_{\alpha}^3 \left( a_\alpha |\psi_\alpha|^2 + \frac{b_\alpha}{2} |\psi_\alpha|^4 \right) + \sum_{\beta > \alpha}^3 \eta_{\alpha \beta} |\psi_\alpha| |\psi_\beta| \cos(\theta_\alpha - \theta_\beta)
\]

In general it is not possible to obtain an analytical result, since the Josephson terms introduce coupling between the bands. Before obtaining the equation of motion for
2.1. Ground state

the fields ground state, we can have an insight of what is going to happen by studying the sign of the Josephson coefficients $\eta_{\alpha\beta}$. Supposing to have only active bands, we can have:

1. $\eta_{\alpha\beta} < 0 \ \forall \alpha, \beta$, then the free energy is minimized if all the phase differences are zero, that means $\theta_1 = \theta_2 = \theta_3$

2. $\eta_{12}, \eta_{13} < 0$ and $\eta_{23} > 0$. In this case, to achieve the minimum energy value, one would require $\theta_1 = \theta_2$, $\theta_1 = \theta_3 \Rightarrow \theta_2 = \theta_3$ but also $\theta_2 = \theta_3 + \pi$, which clearly contradicts the previous requirement. Hence this scenario leads to a frustrated superconductor.

3. $\eta_{12} < 0$ and $\eta_{13}, \eta_{23} > 0$. Here we need $\theta_1 = \theta_2$, $\theta_1 = \theta_3 + \pi$ and $\theta_2 = \theta_3 + \pi \Rightarrow \theta_1 = \theta_3$ which contradicts the previous requirement. Hence we are again in a frustrated case.

4. $\eta_{\alpha\beta} > 0 \ \forall \alpha\beta$. Here we need $\theta_1 = \theta_2 + \pi$, $\theta_1 = \theta_3 + \pi$ and $\theta_2 = \theta_3 + \pi \Rightarrow \theta_1 = \theta_3$ which contradicts the previous requirement. Hence we are again in a frustrated case.

Differently from the two band case, here we can have phase frustration simply by introducing a bilinear Josephson. In a two components superconductor we have symmetry with respect to the change of sign of the Josephson coupling constant, i.e. $\eta_{12} \rightarrow -\eta_{12}$ implies $\theta_{12} \rightarrow \theta_{12} + \pi$. In the three bands case, as we have seen, this is not happening. Let us now derive the equation of motion. Since the fields are complex and the free energy only depends on phase differences we can take derivative with respect to the modulus and the phase differences. Naming the ground state fields as follows $\psi_{\alpha 0} = \tilde{u}_\alpha e^{i\theta_\alpha}$, and $\theta_{\alpha\beta} = \theta_\alpha - \theta_\beta$, we have:

$$a_1 \bar{u}_1 + b_1 \bar{u}_1^3 + \frac{\eta_{12}}{2} \bar{u}_2 \cos \bar{\theta}_{12} + \frac{\eta_{13}}{2} \bar{u}_3 \cos \bar{\theta}_{13} = 0 \quad (2.5)$$

$$a_2 \bar{u}_2 + b_2 \bar{u}_2^3 + \frac{\eta_{12}}{2} \bar{u}_1 \cos \bar{\theta}_{12} + \frac{\eta_{23}}{2} \bar{u}_3 \cos \bar{\theta}_{23} = 0 \quad (2.6)$$

$$a_3 \bar{u}_3 + b_3 \bar{u}_3^3 + \frac{\eta_{13}}{2} \bar{u}_1 \cos \bar{\theta}_{13} + \frac{\eta_{23}}{2} \bar{u}_2 \cos \bar{\theta}_{23} = 0 \quad (2.7)$$

$$\eta_{12} \bar{u}_1 \bar{u}_2 \sin \bar{\theta}_{12} + \eta_{13} \bar{u}_1 \bar{u}_3 \sin \bar{\theta}_{13} = 0 \quad (2.8)$$

$$\eta_{12} \bar{u}_1 \bar{u}_2 \sin \bar{\theta}_{12} - \eta_{23} \bar{u}_2 \bar{u}_3 \sin \bar{\theta}_{23} = 0 \quad (2.9)$$

$$\eta_{13} \bar{u}_1 \bar{u}_3 \sin \bar{\theta}_{13} + \eta_{23} \bar{u}_2 \bar{u}_3 \sin \bar{\theta}_{23} = 0 \quad (2.10)$$

Unless being in very peculiar cases, it is not possible to find analytical solutions to these equations. In the following work we will always solve them numerically. We will now study some of the frustrated ground state, that we will use in the next chapter to study excited states.

The method used to obtain the minimum energy order parameter starts from an initial guess and then progressively minimizes the energy using a non linear conjugate gradient procedure. We know that the ground state has a global $U(1)$
symmetry, but at the same time, we can notice that we also have a $\mathbb{Z}_2$ symmetry\(^1\). In fact, under the transformation $\psi_\alpha \rightarrow \psi_\alpha^*$, we have $\theta_{\alpha\beta} \rightarrow -\theta_{\alpha\beta}$. Since $|\psi_\alpha|$ is phase independent and $\cos(-\theta_{\alpha\beta}) = \cos(\theta_{\alpha\beta})$, the free energy remains unchanged. Hence our model presents a $U(1) \times \mathbb{Z}_2$ symmetry, that will be naturally broken by the choice of the ground state. Now the ground state phase differences between components start playing a fundamental role. Let us fix the gauge by assuming $\theta_3 = 0$, which means $\theta_{13} = \theta_1$ and $\theta_{23} = \theta_2$. In case $\theta_1 = \pi$ and $\theta_2 = -\pi$, we have $\theta_{12} = 2\pi$, and this particular state is invariant under complex conjugation, because $U(1)$ group is mod $(2\pi)$. However, this is not always the case and for certain sets of parameters we will obtain more ground states with minimal free energy. These situations will lead to interesting excited states.

The method we used to spot the presence of $\mathbb{Z}_2$ symmetry breaking was to repeat many time the ground state minimization using random initial guess.

## 2.2 Examples

Let us start by studying the simplest case, i.e. $a_\alpha = -1$, $b_\alpha = 1$ and $\eta_{\alpha\beta} = 0.5 \forall \alpha, \beta$. The values of the phases are shown in Fig.2.1

![Figure 2.1](image1.png)

*Figure 2.1:* Possible ground state phases obtained by minimizing the potential free energy using random initial states. We can notice the phase frustration happening.

We can notice that the values of the field’s phases are not the same each step. They oscillate between $\frac{2\pi}{3}$ and $-\frac{2\pi}{3}$. Maintaining our gauge convention, we can easily plot them on a gauss plane as complex vectors, as shown in Fig.2.2 Once the gauge is fixed, $\theta_{12}$ can be immediately derived from $\theta_1$ and $\theta_2$

\(^1\)More cases of time reversal symmetry breaking are presented in [7],[16], [30], [31],[37]
2.2. Examples

Figure 2.2: Representation of the ground state phases on a unit circle. We can notice that by complex conjugating all the order parameters, the phase differences remain the same in module, hence do not change the energy value.

If we complex conjugate the state we obtain another ground state having the same energy. This is a very simple example of the frustration phenomena that we can have in three components superconductors. We will see in the next chapter which kind of excitation can be created thanks to this symmetry breaking.

Let us now study what happens when we change some parameters in the potential free energy. In particular, we will study what happens by changing the bilinear Josephson coupling constants. In particular, we will vary $\eta_{12}$, and set $\eta_{13} = \eta_{23} = -1$.

If we consider:

$$F_P = F(a_\alpha, b_\alpha) + \eta_{12}|\psi_1||\psi_2| \cos \theta_{12} + \eta_{13}|\psi_1||\psi_3| \cos \theta_{13} + \eta_{23}|\psi_2||\psi_3| \cos \theta_{23} \quad (2.11)$$

Let us start by supposing $|\eta_{12}| \ll |\eta_{23}|, |\eta_{13}|$, then we have that the value of $|\psi_1||\psi_2| \cos \theta_{12}$, becomes less relevant. Assuming $\eta_{13}, \eta_{23} < 0$, then the ground state will be for $\theta_1 = \theta_3$ and $\theta_2 = \theta_3$. If $\eta_{12} < 0$ we will also have $\theta_{12} = 0$ and a non-frustrated superconductor. As we start to increase $\eta_{12}$, it is reasonable to have moduli variation, still maintaining the same phase locking. We can have an insight of this by expanding about $\theta = 0 \cos \theta = 1 - \frac{\theta^2}{2}$. Therefore, neglecting constant terms we would have:

$$F_P = F(a_\alpha, b_\alpha) + |\eta_{12}|\psi_1||\psi_2|\theta_{12}^2 + |\eta_{13}|\psi_1||\psi_3|\theta_{13}^2 + |\eta_{23}|\psi_2||\psi_3|\theta_{23}^2 \quad (2.12)$$
Where each $|\psi_{\alpha}|$ and $\theta_{\alpha\beta}$ is implicitly function of $\eta_{12}$. Therefore, within a certain range of $\eta_{12}$ values, we can expect to have a linear decrease of $\psi_2$ and $\psi_1$, to compensate the increase of $\eta_{12}$, but still no phase variation. This allows a "slower" increase of the free energy. Then, after a certain critical value, the phases will lose the initial locking and will start variating with $\eta_{12}$. A plot of the phases and moduli variation is shown in Figure 2.3.

![Figure 2.3: Phase and moduli variation with respect $\eta_{12}$; We can notice that the system does not exhibit frustration until the critical value $\eta_{\text{crit}} = 0.282$; here we can also spot a change in the moduli variation](image)

We can notice how $|\psi_1|$ and $|\psi_2|$ change exactly in the same way. It is interesting what happens to $|\psi_3|$ for $\eta > \eta_{\text{crit}}$; its sudden drop indicates a cooper pairs decrease in the third band. Therefore the potential terms $abs\psi_3(\eta_{13}|\psi_3|\cos\theta_{13} + \eta_{23}|\psi_2|\cos\theta_{23})$ decrease their weight in the overall potential.

Hence the remaining term is $\eta_{12}|\psi_1||\psi_2|\cos\theta_{12}$. As we can see from Figure 2.3, $\phi_{12} \rightarrow \pi$, which minimizes the potential. We also present plots of the three different order parameters as complex vectors on the unit circle. Fixing the gauge such that $\theta_3 = 0$, it is really possible to notice that in certain cases the $\mathbb{Z}_2$ symmetry breaking leads to a different ground state, while in others, e.g. $\eta_{12} < \eta_{\text{crit}}$, to the same state.
2.2. Examples

Figure 2.4: Representation of the phase difference as complex vectors on a unit circle as \( \eta_{12} \) changes

For example by complex conjugating the situation in Fig.2.4a, we end up in the same state, while in Fig.2.4b, 2.4c we have frustration, and therefore the possibility to have domain walls.

Before studying the excitations of this kind of superconductors, it is interesting to see what happens when we end up having passive bands, i.e. when some of the \( a_\alpha \) coefficients are positive. In that case the superconductivity in the \( \alpha \)-th band is very fragile, since it only depends by the Josephson terms. Let us consider the following case:

\[
(a_1, b_1) = (1, 1) \quad (a_2, b_2) = (1, 1) \quad (\eta_{12}, \eta_{13}, \eta_{23}) = (2, 3, 3)
\] (2.13)

Since we are dealing with passive bands, it is not immediate to determine whether we are dealing with a frustrated case or not.

Figure 2.5: Phase difference values with random initial guess for passive bands. We can notice that we start in a non frustrated situation
Figure 2.6a shows the result of varying $\eta_{12}$. We can notice that we start in a non frustrated situations, in which all the phases are the same and the state exhibit $U(1)$ symmetry. For $\eta > \eta_{\text{crit}} = 2.536$ we enter in the $U(1) \times \mathbb{Z}_2$ regime. Here we notice that the third band starts to get depleted to compensate the phase differences changes. Then for $\eta \gg \eta_{\text{crit}}$, we end up again in a $U(1)$ regime, where $\theta_{12} \rightarrow 2\pi$ and $|\theta_{13}| = |\theta_{23}| = \pi$. To compensate these phase differences $|\psi_3| \rightarrow 0$.

![Graph](image)

(a) Order parameter phases and moduli variation as $\eta_{12}$ changes in the case of passive bands.

(b) $\eta_{12} < \eta_{\text{crit}}$

(c) $\eta_{12} > \eta_{\text{crit}}$

(d) $\eta \gg \eta_{\text{crit}}$

**Figure 2.6:** Order parameters as $\eta_{12}$ changes. We can notice the phase frustration happening for $\eta_{12} > \eta_{\text{crit}}$

Proceeding as done before we find that the ground state does not exhibit frustration. The phase values oscillate between $\pm \pi$, as shown in Figure 2.5a. A better visual representation of the possible ground states is provided in Figure 2.5b. In this case if we perform a complex conjugation, the state is the same. Maintaining the same values for $(a_\alpha, b_\alpha)$ coefficients, let us study what happens to the phases and moduli when we variate the Josephson coupling constants.
In conclusion of this chapter we can notice that, to have a superconducting ground state, it does not really matter whether we are dealing with active or passive bands. Clearly, this remains true as far as we have Josephson potential terms that can compensate for the positive $a_\alpha$ coefficients. The second interesting feature regards the tight relation between modulus and phase. In fact, in both the analyzed cases, every time we enter in the $U(1) \times \mathbb{Z}_2$ regime, we notice that the moduli start compensating the phase change. In our cases, $|\psi_1|, |\psi_2|$ always increased, while $|\psi_3|$ dropped. This is specific to our choice of the Josephson coefficient to variate.
Chapter 3

Excitated states

Recent experimental works show the need of more than two components models to fully describe the behavior of new superconductors [32][10]. In [32], a four component microscopic model is used to describe the non equilibrium behavior of optimally doped Ba$_{1-x}$K$_x$Fe$_2$As$_2$. However, after some approximation the model is reduced to an effective three band one. The behavior of three band s + is wave superconductors, is deeply analysed in [14],[17],[18], in which a detailed analysis of possible stable topological excitations is presented to the reader. However, a lot of possible superconducting materials are anisotropic, therefore knowing how anisotropies affect the behavior of the superconductors is crucial. The two component case is studied in [38],[40] and [42]. At the moment, no work on anisotropic three component superconductor has been carried out. Given its relevance in the current research, in this chapter we study how anisotropies change the behavior of topological excitations in three band superconductors, described by GL free energy. Our focus is on vortex excitations: we study different sets of coefficients leading to active and passive bands respectively. In both case we analyze how the increasing crystal anisotropies affects the equilibrium states. Then we start studying clusters of vortices, to understand their interaction.

From now on we take into account the full free energy functional, including also the kinetic part, which will play a fundamental role:

$$\mathcal{F} = \sum_{\alpha}^{3} (D_{j}^{*} \psi_{\alpha}^{*}) Q_{j}^{\alpha} (D_{j} \psi_{\alpha}) + \sum_{\alpha}^{3} \left( a_{\alpha} |\psi_{\alpha}|^{2} + \frac{b_{\alpha}}{2} |\psi_{\alpha}|^{4} \right) + \sum_{\beta > \alpha}^{3} \eta_{\alpha \beta} |\psi_{\alpha}| |\psi_{\beta}| \cos (\theta_{\alpha} - \theta_{\beta}) + \frac{(\nabla \times A)^{2}}{2}$$

(3.1)
3.1 Active Bands

Let us start the study of the excitation with a very simple case of anisotropies in a superconductor having all active bands, i.e. $a_{\alpha=1,2,3} < 0$. As previously said, it is possible to derive these coefficients microscopically, as function of interband and intraband couplings and impurities. However, we are mainly interested in a phenomenological study of the excitations behavior in presence of anisotropies. The first set of coefficient we study is reported below:

\[(a_1, b_1) = (-0.1, 0.5) \quad (a_2, b_2) = (-1, 0.5) \quad (a_3, b_3) = (-0.5, 0.5) \quad (3.2)\]

\[(\eta_{12}, \eta_{13}, \eta_{23}) = (0.3, 0.3, 0.3) \quad (3.3)\]

And the anisotropies:

\[(Q_1)_{ij} = \begin{pmatrix} 1 & 0 \\ 0 & 0.1 \end{pmatrix} \quad (Q_2)_{ij} = \begin{pmatrix} 0.1 & 0 \\ 0 & 1 \end{pmatrix} \quad (Q_3)_{ij} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad (3.4)\]

Our initial guess is a single winded vortex per component, i.e. $(N_1, N_2, N_3) = (1, 1, 1)$. The resulting moduli are displayed in Figure 3.1a,3.1b,3.1c.

(a) First order parameter modulus $|\psi_1|$. We can notice the non-cylindrical symmetric core structure due to the presence of anisotropies

(b) Second order parameter modulus $|\psi_2|$. We can notice how the presence of the anisotropies generates a smooth vairating field along y
3.1. Active Bands

(c) Third order parameter $|\psi_3|$. The third band is isotropic, however the shape of the third vortex is affected by the core structure of the excitations in the other two bands.

**Figure 3.1:** Order parameters moduli in active band case

As expected, the first band results squeezed in the $x$ direction while the second band in the $y$ direction. This is because, given the choice of the anisotropies, in the first band it is much more expensive to have sharp derivative along $x$, while in the second component is more expensive to have sharp derivative along $y$. The third component is left isotropic, but the shape of the vortex is slightly influenced by the other two bands. The relative phase are shown in Figures 3.2a, 3.2b, 3.2c:

(a) Phase difference $|\theta_{12}|$. We can notice a non-trivial structure exhibiting four-fold symmetry due to the presence of the anisotropies.

(b) Phase difference $|\theta_{13}|$. We can notice a non-trivial structure exhibiting four-fold symmetry due to the presence of the anisotropies.
Figure 3.2: Phase differences in active band case

The pattern of the phase difference is typical when dealing with multicomponent anisotropic superconductors. The two band case is discussed in [38] and [40]. The reason of this particular results can be found in the linearized theory where the anisotropy matrices create additional couplings between the phase gradient and the gauge field. For an analytical treatment read [41]. The magnetic field is represented in Figure 3.3a. As expected in case of anisotropies, we have magnetic field inversion [40], which is shown in Figure 3.3b.

(a) Magnetic field generated by the vortices. We can notice the lack of cylindrical symmetry due to the anisotropies

(b) Anisotropies add couplings between phase difference and magnetic field. One of the consequences is the presence of magnetic field inversion.

Figure 3.3: Magnetic Field in active band case
3.2 Passive Bands

In this case we will instead study a new set of coefficients, leading to two passive bands and just one active one. Hence we have \( a_1 < 0 \) and \( a_{2,3} > 0 \). Specifically:

\[
(a_1, b_1) = (-1, 1) \quad (a_2, b_2) = (1, 0.5) \quad (a_3, b_3) = (3, 0.5)
\]

(3.5)

\[
(\eta_{12}, \eta_{13}, \eta_{23}) = (-2, 2.7, -4)
\]

(3.6)

![Figure 3.4: Ground state moduli for the considered parameter set. We can notice that the third band is almost depleted if compared with the other two.](image)

The ground state for this set of parameters is shown in Figure 3.4. We can immediately see that the third band results way more depleted than the other two. We will now insert a vortex excitation in each band to study how the excited state changes the phase and moduli distribution. In Figure 3.5c, we can notice that the third band remains depleted compared to the other two, as in the ground state. However, inserting vortex excitations in the system gives rise to unbalances in the phase relations, which are coupled to the moduli amplitude by the Josephson potential. This introduces complex competitions, that lead to non trivial excited states. For example, vortices have different sizes in the different bands and this is one of the reason why one band may undergo a deeper depletion compared to others. Moreover, due to the phase gradients introduced by the kinetic terms in Eq.(3.1), the phase relationship of an excited equilibrium state can be completely different from the ground state. While \( \theta_{12} \) remains zero, \( \theta_{13}, \theta_{23} \), exhibit a phase jump reported in Figure 3.6a and 3.6b.

The reason of the indentation in the phase difference plots lies in the fact that \( \pi \) and \( -\pi \) are the same state. The shape of the vortex in the third band is a consequence of this phase difference structure. Still maintaining the cylindrical symmetry, it exhibits a moat core structure in which, in addition to the central zero, we have a concentric ring where the order parameter is zero. The Josephson
(a) First order parameter modulus $|\psi_1|$, in isotropic system with single winded topological excitation. We can notice how in this case we recover the cylindrical symmetry

(b) Second order parameter modulus $|\psi_2|$ in isotropic system with single winded topological excitation. We have cylindrical symmetry also in this case.

(c) Third order parameter modulus in $|\psi_3|$ isotropic system with single winded topological excitation. In this case we have a moat core vortex, which has nontrivial but cylindrical-symmetric core structure

Figure 3.5: Passive band moduli

coupling $\eta_{12} = -2$ locks the phase difference $\theta_{12} = 0$. At the same time, there is the competing term $\eta_{23}$ which would prefer $\theta_{23} = 0$, while $\eta_{13} = 2.7$ would prefer the phase locking $\theta_{13} = \pi$. In the uniform ground state, the term weighted by $\eta_{23}$ dominates, and therefore we end up having $\theta_1 = \theta_2 = \theta_3$. However, one of the costs of it, is the depletion of the third band. Once we add vortex excitations,
3.2. Passive Bands

(a) Phase difference $\theta_{13}$. The values acquired in the central area by $\theta_{13}$ is $\pi$. It is interesting to notice the jump in the nodal ring of $|\psi_3|$

(b) Phase difference $\theta_{23}$. The values acquired by $\theta_{23}$ in the central area is $\pi$. It is interesting to notice the jump in the nodal ring of $|\psi_3|$

Figure 3.6: Phase differences

the spatial variation of the moduli of the order parameters can be seen as new effective Josephson coupling terms, i.e. $\tilde{\eta}_{ij} = \eta_{ij} f_i(r) f_j(r)$. Hence the variation of the moduli can create areas in which a certain phase coupling is more favorable. This will be particularly evident in anisotropic system, where additional phase gradients will give rise to peculiar patterns. An interesting parameter to display is the modulus of the partial current densities, i.e. the current densities generated by each phase. The mathematical expression is reported in Eq.3.7:

$$j_\alpha = \lambda^{-2} \left( \nabla \theta_\alpha q + A \right)$$

(3.7)

The result is reported in Figures 3.7a,3.7b,3.7c.
Chapter 3. Excited states

(a) Partial current density generated by the first component $|j_1|$. Since we are considering the isotropic limit we can notice cylindrical symmetry

(b) Partial current density generated by the second component $|j_2|$. Since we are considering the isotropic limit we can notice cylindrical symmetry

(c) Partial current density generated by the third component $|j_3|$. Since we are considering the isotropic limit we can notice cylindrical symmetry

Figure 3.7: Partial current densities
3.2. Passive Bands

Let us now introduce some anisotropies in the system, in particular let us consider:

\[
(Q_1)_{ij} = \begin{pmatrix} 1 & 0 \\ 0 & 0.168 \end{pmatrix} \quad (Q_2)_{ij} = \begin{pmatrix} 0.168 & 0 \\ 0 & 1 \end{pmatrix} \quad (Q_3)_{ij} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}
\]

As expected in Figure 3.8a, $|\psi_1|$ is stretched in $x$-direction, since it is more expensive to have derivatives along $y$ and the other way around for $|\psi_2|$ in Figure 3.8b. In Figure 3.8c we can notice a radical change of the situation.

(a) First order parameter module $|\psi_1|$. We can notice the presence of anisotropies by the very smooth field spatial variation along $x$.

(b) Second order parameter module $|\psi_2|$. We can notice the smooth derivatives in the $y$ direction, accordingly to our choice of anisotropy matrices.
(c) Third order parameter module $|\psi_3|$. In this case we completely lose the vortex structure and we assist to strong modulus overshootings. This structure is a clear evidence of the simultaneous presence of anisotropy and phase frustration.

Figure 3.8: Order parameter moduli

An interesting behavior is displayed by $|\psi_3|$ in Figure 3.8c, where we lose the moat core structure of Fig. 3.5c and we assist to strong overshooting. However, the phase winding is maintained in all three the components. Therefore in three component superconductors, we can have more kinds of flux carrying solitons, with different structures than the classical Abrikosov vortex. We can display this result in an alternative fashion, by taking planar sections of these vortices along different axes. The result is shown in Fig. 3.9a-3.9c.

(a) Cross section of the first order parameter module. The direction-dependent core size is here enhanced.

(b) Cross section of the second order parameter module. The direction-dependent core size is here enhanced.
3.2. Passive Bands

> Figure 3.9: Modulus cross sections

The section along \( x \) in Figure 3.9c has the structure of normal stretched vortex. By contrast along \( y \) we assist to two highly peaked overshoots. We can investigate the origin of this phenomenon by studying the relative phases. \( \theta_{12}, \theta_{13} \) and \( \theta_{23} \) are shown in Figures 3.10a-3.10b-3.10c respectively. We can notice that the pattern of the phase differences is qualitatively similar to Fig. 3.2a-3.2c. This is completely reasonable since the additional couplings between the phase gradients and gauge field, introduced by the anisotropies, do not depend on the choice of the potential coefficients. Moreover, we can notice a \( y \)-elongated phase jump from \( \pm \pi \rightarrow \mp \pi \) in Fig 3.10b,3.10c, which is similar to what we saw in Fig.3.6a,3.6b.

(a) Phase difference \( \theta_{12} \). We can notice the untrivial structure with four-fold symmetry.

(b) Phase difference \( \theta_{13} \). We can notice the untrivial structure with four-fold symmetry At \( y = 0 \) we assist to a jump \( \pi \rightarrow -\pi \) and vice versa.
Chapter 3. Excited states

(c) Phase difference $\theta_{23}$. We can notice the untrivial structure with four-fold symmetry. At $y = 0$ we assist to a jump $\pi \rightarrow -\pi$ and vice versa.

Figure 3.10: Phase differences

The value of the phase differences is coupled to the value of the field moduli via the bilinear Josephson potential. Since the Josephson coupling only depends on the cosine of the phase difference, and $\cos(x) = \cos(-x) = \cos(|x|)$, let us plot the moduli of the three phase differences instead.

(a) Modulus of the phase difference $|\theta_{12}|$. We can notice the four-fold symmetric structure.

(b) Modulus of the phase difference $|\theta_{13}|$. We can notice the four fold symmetric structure. The phase jump $\pi \rightarrow -\pi$ is clearly not visible here.

We can notice that the shape of $|\psi_3|$ displayed in Fig. 3.8c, follows the “butterfly wing” four-fold symmetric pattern of the phase differences. This is one of the examples in which the non linearity of the model introduces extremely strong
3.2. Passive Bands

Figure 3.11: Phase difference moduli

couplings between the phase and the moduli that can lead to non trivial equilibrium states.

Figures 3.12a, 3.12b, 3.12c show the partial current densities, which are given by:

\[ j_k = \left( \lambda_{\alpha}^{-2} \right)_{k_j} \left( \frac{1}{q} \partial_j \theta_{\alpha} + A_j \right) \]  

(3.9)

The modulus of the total current density and the modulus of the magnetic field are instead represented in Fig. 3.13a and 3.13b respectively.

(a) First component partial current density \( |j_1| \). We can notice the effect of the presence of anisotropies on the spatial distribution

(b) Second component partial current density \( |j_2| \). The effect of the anisotropies on the spatial distribution is clear here as well
(c) Third component partial current density $|j_3|$. We can notice the unconventional structure. Due to the extremely smaller modulus, its influence on the magnetic field will not be visible.

**Figure 3.12:** Current densities

Finally, the presence of anisotropies leads to a soft magnetic field inversion at the corners of our grid. The result is displayed in Figure 3.13c. In the isotropic case this kind of phenomenon does not occur.

(a) Total current density $|J_{tot}|$. We can notice that the spatial pattern of the third component partial current is not visible

(b) Magnetic field $B_z$. We can notice the anisotropy influence on the spatial distribution
We can now change the anisotropy matrices, introducing coefficients of the same order as the Josephson coupling. Namely:

\[
(Q_1)_{ij} = \begin{pmatrix} 2 & 0 \\ 0 & 1 \end{pmatrix} \quad (Q_2)_{ij} = \begin{pmatrix} 1 & 0 \\ 0 & 2 \end{pmatrix} \quad (Q_3)_{ij} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}
\] (3.10)

As before, it is more expensive to have sharp field derivatives along \( x \) for component one and along \( y \) for the second component. Therefore \( |\psi_1| \) will be stretched along \( x \) and \( |\psi_2| \) will be elongated along \( y \), even though in this case the anisotropy is softer. The three moduli are displayed in Figure 3.14a-3.14c.
Chapter 3. Excited states

We can notice a new unconventional structure due to the substantial reduction of anisotropies

Figure 3.14: Order parameters modulus

While nothing unexpected happens to $|\psi_1|$ and $|\psi_2|$, we can notice that $|\psi_3|$ assumes a shape that is more similar to an elongated vortex, still maintaining overshoots inside. We can also see how the three nodes are already in the same position as in Fig 3.8c. The phase difference are plotted in Figures 3.15a-3.15c.

(a) Phase difference $\theta_{12}$. Unconventional four-fold symmetric structure. Qualitatively the same as the previous case.

(b) Phase difference $\theta_{13}$. Unconventional four-fold symmetric structure. Qualitatively the same as the previous case.
3.2. Passive Bands

Figure 3.15: Phase differences

We can notice that the phase difference remain qualitatively the same as Fig 3.10a-3.10c. This means that the change in the spatial distribution of the third order parameter is mainly related to the different core-shape of the vortices in the first and second band. An interesting feature is the decreased inversion length of the magnetic field, and its increased oscillation as we can notice from Figure 3.16b.

(a) Magnetic field $B_z$

(b) Magnetic field inversion. We can notice that in this case the inversion length is much smaller than in the strongly anisotropic scenario.

Figure 3.16
The situation can radically change if we modify the coefficient of the first component, i.e. the only active one. Maintaining the same value for the anisotropies, let us vary $a_1 = -1 \rightarrow a_1 = -0.1$. We obtain:

(a) First order parameter modulus $|\psi_1|$. We assist to an increased depletion of the first band

(b) Second order parameter modulus $|\psi_2|$. This modulus remains unchanged compared to the previous case

(c) Third order parameter modulus $|\psi_3|$. We can notice that we obtain a new elongated structure without overshooting but with an increased nodal area.

Figure 3.17: Order parameters moduli

We can notice that the third order parameter modulus has completely changed structure. There are no overshoots, but an elongated nodal area directed along the $y$ direction. The phase differences, shown in Figures 3.18a-3.18c are qualitatively similar to Figure 3.10a-3.10c. In this case the responsible of the change is $|\psi_3|$ is the increased depletion of the first band.
3.2. Passive Bands

![Phase difference graphs](a) Phase difference $\theta_{12}$.

(b) Phase difference $\theta_{13}$.

(c) Phase difference $\theta_{23}$.

**Figure 3.18:** We can notice the unconventional four-fold symmetric structure due to the additional coupling introduced by the anisotropies.
3.3 Clustering

Let us study now what happens when, in presence of anisotropies we introduce more vortices in each band. Using the coefficient set:

\[(a_1, b_1) = (-0.1, 0.5) \quad (a_2, b_2) = (-1, 0.5) \quad (a_3, b_3) = (-0.5, 0.5)\]  
\[(\eta_{12}, \eta_{13}, \eta_{23}) = (0.3, 0.3, 0.3)\]  

And

\[(Q_{1})_{ij} = \begin{pmatrix} 1 & 0 \\ 0 & 0.168 \end{pmatrix} \quad (Q_{2})_{ij} = \begin{pmatrix} 0.168 & 0 \\ 0 & 1 \end{pmatrix} \quad (Q_{3})_{ij} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\]  

(3.11) 

(3.12) 

(3.13) 

We can use as initial guess two vortices in each band. The result for the moduli and phases are displayed in Figures 3.19a-3.20c:

(a) $|\psi_1|$. Both vortices maintain the elongated structure along $x$.

(b) $|\psi_2|$. Both vortices present $y$-directed elongation.
(c) $|\psi_3|$. We can notice that the interacting solitons maintain their peculiar spatial structure also while interacting.

**Figure 3.19:** Order parameters moduli

![Figure 3.19](image1)

(a) $\theta_{12}$

(b) $\theta_{13}$

(c) $\theta_{23}$

**Figure 3.20:** We can notice the unconventional phase difference shape for the case of interacting vortices
The magnetic field is shown in Figure 3.21a, and the inverted field in Figure 3.21b. We can notice that the increment in the number of vortices amplifies the field inversion.

(a) Magnetic field $B_z$. Mostly generated by the partial current of component one and two.

(b) Magnetic field inversion. We can notice that the magnetic field inversion pattern is radically different if compared to the single vortex case.

Figure 3.21: Magnetic field

A detailed analysis on the origin of the non-monotonic potential would require a complete mode analysis. However, we have the intuition that the physics behind this effect is similar to what outlined in [38] for a two component anisotropic superconductor. The main difference in this case lies in the presence of a third condensate, which means we will have three modes coupled to the magnetic field. Still, the leading mode is the one giving rise to the inverted field, which mediates the attraction between the two excitations. The short distance repulsive mode instead is to be ascribed to the vortex spatial structure. However the clustering problem in the anisotropic case still requires further investigations.
Chapter 4

Numerical methods

A significant part of this thesis has been learning how to perform the simulations for a three band superconductor. Since we are dealing with a time-independent Ginzburg-Landau theory, the most efficient method is to use finite element simulations. There are more than one available environment to accomplish this task, but among them, FreeFem++ remains the most performing and flexible in terms of parameter control. Another possible language is FeniCS, however, despite a more friendly “grammar” it turns out to have much more overhead time in the computations.

4.1 Finite element method

The finite element method is a numerical method used to solve linear and non-linear partial differential equations with specific boundary conditions. It allows by a discretization of the domain to transform a system of partial differential equations into an algebraic system. The process is structured as follows:

- The continuous domain on which the function is defined gets divided in finite elements through a process named tessellation. Hence the mesh is automatically built using Delaunay-Voronoi algorithm. Each tassel is triangular. If we identify each triangle as $T_k$, then the finite element approximation of the domain $\Omega \rightarrow \text{f.e.m} \rightarrow \Omega_h = \bigcup_{k=1}^{n_t} T_k$, where $n_t$ is the number of triangles.

- The finite element space is defined. It usually consists of a Hilbert space of polynomial functions defined on each element of the mesh and affine in $x, y$. These functions build the canonical basis of the Hilbert space and are continuous, piecewise equal to 1 on one vertex and 0 on all others. Naming
them $\phi_k$, and indicating with $\mathcal{T}_h = \{T_k\}_{k=1}^{n_t}$ the family of triangles in the mesh, we can define the space as:

$$V_h(\mathcal{T}_h, P_2) = \left\{ w(x, y) \mid w(x, y) = \sum_{k=1}^{M} w_k \phi_k(x, y), w_k \in \mathbb{R} \right\}$$

(4.1)

Here $M$ is the dimension of $V_h$, i.e. the number of vertices. $P_2$ indicates that the basis functions are continuous piecewise quadratic. Finally the set of coefficients $w_k$ are called “degrees of freedom of $w$”, and effectively contain all the information about the projection of the analytic function we are interested in, onto the finite dimensional Hilbert space.

• The algebraic system is set depending on the particular differential equation solved. An example for the Poisson equation follows hereby.

Let us consider the following algebraic system:

$$\begin{cases}
\nabla^2 u(x, y) = -f(x, y) & (x, y) \in \Omega \\
\mathbf{n} \cdot \nabla u(x, y) = 0 & (x, y) \in \partial \Omega
\end{cases}$$

(4.2)

Here $u(x, y)$ is our analytical function, $f(x, y)$ the source term function and we impose Neumann boundary conditions. To proceed in discretizing $u$, we need to obtain the weak formulation of the initial problem and perform a Galerkin projection. By performing the weak formulation of 4.2, we allow less regularity in $u$, but at the same time we increase the size of the solution space. In this case, we don’t need anymore $u \in C^2(\Omega)$, but only $u \in L^2(\Omega)$, which mean integrable with respect to its first derivative. To perform this transformation we multiply 4.2 by a test function $v$, and integrate over the space as follows:

$$\int_{\Omega} \mathbf{dr} v(x, y) \nabla^2 u(x, y) = -\int_{\Omega} \mathbf{dr} f v$$

(4.3)

Using the identity:

$$\partial_i (v \partial_i u) = \partial_i u \partial_i v + v \partial_i \partial_i u$$

(4.4)

We can re-write the first integral in Eq. 4.3 as:

$$\int_{\Omega} \mathbf{dr} \nabla \cdot (v \nabla u) - \int_{\Omega} \mathbf{dr} \nabla u \cdot \nabla v = -\int_{\Omega} \mathbf{dr} f v$$

(4.5)

Using Green’s theorem we have:

$$\int_{\partial \Omega} \mathbf{dr} \mathbf{u} \cdot \mathbf{n} \cdot \nabla v - \int_{\Omega} \mathbf{dr} \nabla u \cdot \nabla v = 0$$

(4.6)

Therefore we end up with:

$$\int_{\Omega} \mathbf{dr} \nabla u \cdot \nabla v = \int_{\Omega} \mathbf{dr} f v$$

(4.7)

Naming the bilinear form $\int_{\Omega} \mathbf{dr} \nabla u \cdot \nabla v = a(u, v)$ and the source functional $\int_{\Omega} \mathbf{dr} f v = F(v)$, we are left with the weak formulation $a(u, v) = F(v)$. If $a(u, v)$ and $F(v)$ are
continuos and positively constrained, it is possible to show the weak formulation admits a unique solution. What we need to do now is to discretize $u$; we can use the basis of the previously defined Hilbert space to accomplish this task:

$$u = \sum_{k=1}^{M} u_k \phi_k$$  \hspace{1cm} (4.8)

There is no need to discretize $v$ because, being an arbitrary well behaved function, it can be chosen to be one of the basis functions $\phi_k$. Hence, we end up with:

$$a \left( \sum_{k=1}^{M} u_k \phi_k, \phi_i \right) = F(\phi_i)$$  \hspace{1cm} (4.9)

And since $a(u,v)$ is bilinear it can be described as a stiffness matrix, whose matrix elements are:

$$A_{jk} = a(\phi_j, \phi_k) \quad f_k = F(\phi_k)$$  \hspace{1cm} (4.10)

Here the proble is easily solved.

### 4.2 Ginzburg Landau Functional

Unfortunately in the GL theory the situation is more complicated, because we are dealing with highly non-linear partial differential equations, which cannot be reduced to an easy algebraic formulation. Just to give an insight on how different the problem is, let us consider a simple GL functional without any potential term, i.e. a $U(1)^N$ model. The functional, written using Einstein index convention, is reported in Eq.

$$F = \sum_{\alpha} \int_{\Omega} \mathbf{d}r \left[ (D_j \psi_\alpha)(D_j \psi_\alpha) + a_\alpha|\psi_\alpha|^2 + \frac{b_\alpha}{2}|\psi_\alpha|^4 + \frac{(\nabla \times A)^2}{2} \right]$$  \hspace{1cm} (4.11)

And the equation of motion is obtained by requiring:

$$\delta F[\psi_1, \ldots, \psi_N, A] = 0 \quad \Rightarrow \quad 0 = \int_{\Omega} \mathbf{d}r \left[ \sum_{\alpha} \left( \frac{\delta F}{\delta \psi_\alpha} \delta \psi_\alpha + \frac{\delta F}{\delta A} \cdot \delta A \right) \right]$$  \hspace{1cm} (4.12)

Even tough we cannot obtain a algebraic formulation, we still reduce the problem to its weak formulation as before. Following analogous steps as before we end up with the boundary conditions:

$$\int_{\partial \Omega} d^2x \delta \psi_\alpha n_j (\partial_j + iqA_j) \psi_\alpha = 0$$  \hspace{1cm} (4.13)

$$\int_{\partial \Omega} d^2x A_l \varepsilon_{ijk} B_j n_j = 0$$  \hspace{1cm} (4.14)

The method used to minimise the energy, once we obtain the weak formulation of the problem is the Non Linear Conjugate Gradient (NLCG). This method consists in an unconstrained optimization for nonlinear problems. The interested reader can find exhaustive informations in [34]
4.3 Initial Guess

In this work, we have treated mainly three components superconductors, where each of them is described by a complex scalar field. FreeFem is able to treat complex field, however it turns out much more handy to to treat each field as two scalar fields. Therefore we end up performing minimization with eight degrees of freedom, namely:

\[
\begin{align*}
\text{Re}\{\psi_1\}, \text{Im}\{\psi_1\}, \text{Re}\{\psi_2\}, \text{Im}\{\psi_2\}, \text{Re}\{\psi_3\}, \text{Im}\{\psi_3\}, A_x, A_y
\end{align*}
\]  

(4.15)

To minimize the free energy we perform iterations with the NLCG method until the relative variation of the norm of the functional gradient with respect to the eight degrees of freedom is on average less than \(10^{-7}\). To study the properties of topological excitation we need to provide an initial guess which should have similar properties to the solution we are looking for. Hence the initial guess is defined accordingly:

\[
\psi_\alpha = |\psi_\alpha|(x,y)e^{i\theta_\alpha(x,y)}
\]  

(4.16)

\[
|\psi_\alpha|(x,y) = \bar{u}_\alpha \prod_{k=1}^{N} \sqrt{\frac{1}{2} \left[ 1 + \tanh \left( \frac{4}{\xi_\alpha} r_{\alpha,k}(x,y) - \xi_j \right) \right]}
\]  

(4.17)

\[
\theta_\alpha(x,y) = \bar{\theta}_\alpha + \sum_{k=1}^{N} \arctan \left( \frac{y - y_{\alpha,k}}{x - x_{\alpha,k}} \right)
\]  

(4.18)

Where \(\psi_\alpha^0 = \bar{u}e^{i\bar{\theta}}\) the ground state and \(r_{\alpha,k} = \sqrt{(x - x_{\alpha,k})^2 + (y - y_{\alpha,k})} \). The parameter \(\xi_\alpha\) is instead the guessed core size. Finally to start the minimization we also need a guess for the vector potential \(A\), which can be obtained by solving the Maxwell equation \(\nabla \times B = J\), where the supercurrent \(J\) is obtained by the initial guess.
Chapter 5

Conclusion

Recent discoveries in iron-based superconductors require more than two-component models to describe the experimental results [32],[10]. In [32] an effective microscopic three-band model is used to describe the properties of Ba$_{1-x}$K$_x$Fe$_2$As$_2$. Moreover, it is widely known that the Ginzburg-Landau theory is an extremely useful and powerful model to qualitatively describe superconductors. Eilenberger solutions show that phenomenological GL models can fit microscopic theory in a wide temperature range. The two component case can be found in [36], where the GL coefficients are derived and the applicability conditions discussed. In addition to this, three-component superconductors show unique behaviors, which cannot be found in two- or one-band models. The new physics comes from the the competitions of the three components mediated by the Josephson coupling terms, which can lead to phase frustration. In this scenario, the three potential terms cannot reach their most favourable phase-locking arrangement simultaneously. Then, it is important to consider that many superconducting materials have anisotropic lattices, therefore the models used to describe them need to be adapted accordingly. Motivated by the worked carried out in [14],[17],[18], for three-band isotropic s + is wave superconductors, and in [38],[40],[42] for two-band anisotropic SC, we decided to extend the analysis of the anisotropic Ginzburg-Landau model to three band superconductors.

An example of anisotropic three-band superconductor that exhibits unconventional vortex behavior [35] is Sr$_2$RuO$_4$, the theory of which is discussed in [29], and microscopically in [23]. We started with a brief overview on how anisotropies change the GL model, and the main related physical quantities. Then, we carefully studied the frustration phenomena occurring in the ground state for certain sets of parameters. The presence of the anisotropies only affects the kinetic terms in the Ginzburg-Landau free energy, therefore the ground states remain the same as in the isotropic case. We observed an extremely strong correlation between phase difference and field’s moduli variation, which is related to the lack of an optimal solution for the individual Josephson terms. In the final chapter we analyzed equilibrium topological excitations for certain sets of GL coefficients, yielding both active and
passive bands. We studied single vortex states, and compared the isotropic case to the anisotropic one. We found that the structure of the topological excitations can change completely as a consequence of the spatial anisotropies. The additional couplings between phase gradients and gauge field yield peculiar patterns in the phase differences; these, in a frustrated situation, lead to depletion or overshoots in the order parameter modulus, resulting in flux carrying excitations that are very different from standard Abrikosov vortices. Finally we studied a two-vortex equilibrium state. We noticed how the inter-vortex force is not monotonic, but short range repulsive and long range attractive. The prediction of this work can be experimentally checked using scanning SQUID microscopy, scanning Hall probe microscopy and muon spin rotation measurements.
Bibliography


