Vortex-matter in Multi-component Superconductors

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Abstract

The topic of this thesis is vortex-physics in multi component Ginzburg-Landau models. These models describe a newly discovered class of superconductors with multiple superconducting gaps, and possess many properties that set them apart from single component models. The work presented here relies on large scale computer simulations using various numerical techniques, but also some analytical methods.

In Paper I, *Type-1.5 Superconducting State from an Intrinsic Proximity Effect in Two-Band Superconductors*, we show that in multiband superconductors, even an extremely small interband proximity effect can lead to a qualitative change in the interaction potential between superconducting vortices by producing long-range intervortex attraction. This type of vortex interaction results in an unusual response to low magnetic fields, leading to phase separation into domains of two-component Meissner states and vortex droplets.

In paper II, *Type-1.5 superconductivity in multiband systems: Effects of interband couplings*, we investigate the appearance of Type-1.5 superconductivity in the case with two active bands and substantial inter-band couplings, such as intrinsic Josephson coupling, mixed gradient coupling, and density-density interactions. We show that in the presence of these interactions, the system supports type-1.5 superconductivity with fundamental length scales being associated with the mass of the gauge field and two masses of normal modes represented by mixed combinations of the density fields.

In paper III, *Semi-Meissner state and nonpairwise intervortex interactions in type-1.5 superconductors*, we demonstrate the existence of nonpairwise interaction forces between vortices in multicomponent and layered superconducting systems. Next, we consider the properties of vortex clusters in a semi-Meissner state of type-1.5 two-component superconductors. We show that under certain conditions nonpairwise forces can contribute to the formation of very complex vortex states in type-1.5 regimes.

In paper IV, *Length scales, collective modes, and type-1.5 regimes in three-band superconductors*, we consider systems where frustration in phase differences occur due to competing Josephson inter-band coupling terms. We show that gradients of densities and phase differences can be inextricably intertwined in vortex excitations in three-band models. This can lead to very long-range attractive intervortex interactions and the appearance of type-1.5 regimes even when the intercomponent Josephson coupling is large. We also show that field-induced vortices can lead to a change of broken symmetry from $U(1)$ to $U(1) \times Z_2$ in the system. In the type-1.5 regime, it results in a semi-Meissner state where the system has a macroscopic phase separation in domains with broken $U(1)$ and $U(1) \times Z_2$ symmetries.

In paper V, *Topological Solitons in Three-Band Superconductors with Broken Time Reversal Symmetry*, we show that three-band superconductors with broken time reversal symmetry allow magnetic flux-carrying stable topological solitons. They can be induced by fluctuations or quenching the system through a phase transition. It can provide an experimental signature of the time reversal symmetry breakdown.
Preface

This thesis contains a summary of my scientific work at the Department of Theoretical Physics at KTH since I was admitted in the fall of 2009. The first part contains an introduction to the theoretical framework of my work, the Ginzburg-Landau theory. The second part contains a summary of the results reported in my papers along with some of the main conclusions.

Scientific articles

Paper I

_Type-1.5 Superconducting State from an Intrinsic Proximity Effect in Two-Band Superconductors_, Egor Babaev, Johan Carlström, and Martin Speight.

Paper II

_Type-1.5 superconductivity in multiband systems: Effects of interband couplings_, Johan Carlström, Egor Babaev and Martin Speight.

Paper III

_Semi-Meissner state and nonpairwise intervortex interactions in type-1.5 superconductors_, Johan Carlström, Julien Garaud, and Egor Babaev

Paper IV

_Length scales, collective modes, and type-1.5 regimes in three-band superconductors_, Johan Carlström, Julien Garaud, and Egor Babaev

Paper V

_Topological Solitons in Three-Band Superconductors with Broken Time Reversal Symmetry_, Julien Garaud, Johan Carlström, and Egor Babaev
Comments on my contribution to the papers

Papers I and II
In these papers I developed all the code, conducted all simulations/numerical computations and made a major contribution to writing the article.

Paper III
I made the suggestion that multi-body forces can affect the structure formation in Type-1.5 superconductors, computed the inter-vortex forces and wrote the majority of the article.

Paper IV
My contributions consist of predicting that vortex-matter in frustrated superconductors induce phase-differences and thus give rise to chiral clusters. I also made the majority of the numerics and writing.

Paper V
I made major contributions to identifying new physics and writing article.
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Part I

Background
Superconductivity is a state characterised by two fundamental properties: Absence of electrical resistance, and perfect diamagnetism. It occurs in a wide range of systems, from metals to ceramics, organic compounds and even astronomical objects like neutron stars.

The discovery of superconductivity occurred in 1911, following an intense debate about the conductive properties of metals at low temperature that took place in the beginning of the twentieth century. Among experimental physicists, this debate spurred a pursuit of ever decreasing temperatures, leading to the liquefaction of helium in 1908 and subsequently to the discovery that the resistivity of mercury disappears at approximately 4.2 K in 1911 [11].

The Dutch physicist Heike Kamerlingh Onnes, who was responsible for these two breakthroughs was awarded the Nobel prize in physics 1913 with the motivation: "For his investigations on the properties of matter at low temperatures which led, inter alia, to the production of liquid helium".

It is interesting that the motivation does not even mention superconductivity. Kamerlingh Onnes does however spend part of his Nobel lecture on it:

"As has been said, the experiment left no doubt that, as far as accuracy of measurement went, the resistance disappeared. At the same time, however, something unexpected occurred. The disappearance did not take place gradually but abruptly. From 1/500 the resistance at 4.2 K drops to a millionth part. At the lowest temperature, 1.5 K, it could be established that the resistance had become less than a thousand-millionth part of that at normal temperature. Thus the mercury at 4.2 K has entered a new state, which, owing to its particular electrical properties, can be called the state of superconductivity."

However, Onnes had in fact only uncovered one of the two hallmarks of superconductivity - absence of electrical resistance. The second; that superconductors expel magnetic fields, and are in that respect perfect diamagnets was discovered by Meissner and Ochsenfeld in 1933 [24, 35]. This phenomena is known as the Meissner effect after one of its discoverers.

An early step towards a theoretical understanding of superconductors was taken in 1935 by the London brothers with the formulation of the London equations:

$$E = \frac{\partial}{\partial t}(\Lambda J_s), \quad \Lambda = \frac{4\pi \lambda^2}{c^2} = \frac{m}{n_s c^2}$$  \hspace{1cm} (1)

$$B = -c \nabla \times (\Lambda J_s).$$  \hspace{1cm} (2)

Here, $m$ is the mass, $c$ is the charge, and $n_s$ is the density of superconducting electrons. By Amperes law, the latter of the two may be written

$$\nabla^2 B = \frac{B}{\lambda^2}.$$  \hspace{1cm} (3)

Thus, the current is exponentially screened from the interior of the superconductor with some length scale $\lambda$, which is called the penetration depth.

London theory does however not account for the manner in which superconductivity is destroyed in the presence of strong magnetic fields. This was only
understood with the advent of Ginzburg-Landau (GL) theory, which was introduced in 1950. The idea of Ginzburg and Landau was based on Landau's theory of second order phase transitions, but as order parameter they choose a complex wave function. With a spatially varying wave function as order parameter, GL theory explains the destruction of superconductivity in magnetic fields and predicts the existence of two classes of superconductors: Type-I and Type-II.

Ginzburg and Landau did however not derive their theory from any microscopic model. In fact, such a model did not appear until 1957, when Bardeen, Cooper and Schriefer introduced the BCS theory [8]. The central idea of this theory is that electron phonon interaction causes a small attraction between electrons. This attraction is sufficient to cause the formation of bound pairs of electron with equal but opposite momentum and spin, s.k. Cooper pairs. Shortly after this publication it was shown by Gorkov that GL theory in fact emerges from BCS theory as a limiting case, being accurate near the critical temperature, where the order parameter is small [35].

The work presented in this thesis aims at extending our understanding of superconductivity phenomena, in particular showing that there are new types of superconductors that cannot be classified according to the traditional Type-I/Type-II dichotomy. Before delving any further into the classification of superconductors, or indeed the history of this topic, it is however necessary to introduce the GL theory, which is also the theoretical framework of the work presented here.
Chapter 1

Ginzburg Landau theory

As mentioned in the previous section, Ginzburg and Landau postulated that a superconductor can be modelled by taking Landau theory of phase transitions and introducing a complex wave function as order parameter. According to Landau theory we can approximate the free energy by a Taylor expansion in the order parameter. Keeping only the two first terms in the expansion and introducing a kinetic energy term we get

\[ F - f_n = \alpha |\psi|^2 + \frac{\beta}{2} |\psi|^4 + \frac{\hbar^2}{2m^*} \left| \left( \nabla + \frac{e^*}{\hbar c} A \right) \psi \right|^2 + \frac{B^2}{8\pi}. \]  

(1.1)

This very much resembles the energy of a quantum mechanical system, but unlike in the Schrödinger equation, this expression features a nonlinear term. The wave function is interpreted as the density of superconducting particles so \( n_s = |\psi|^2 \) while \( f_n \) is the free energy in the normal state.

Because we only have two terms in the Landau expansion, we must have \( \beta > 0 \) to ensure that the energy has a lower bound and that the density of superconducting electrons does not diverge. In order to have a nonzero density of superconducting electrons (and thus any superconductivity taking place at all) we require that \( \alpha < 0 \).

Many of the important properties of this model become apparent when rescaling some of these parameters. Consider the case \( \alpha < 0 \): First we introduce

\[ \xi = \sqrt{\frac{\hbar^2}{2m^*|\alpha|}}, \quad \lambda = \sqrt{\frac{m^*c^2}{4\pi e^2|\alpha/\beta|}}, \quad \gamma = \frac{e^*}{\sqrt{|\alpha|m^*c}}. \]  

(1.2)

Next, we choose \( \sqrt{2}\xi \) as our length scale and \( |\alpha/\beta| \) as the unit for the density of cooper pairs. Dropping a few constant terms we obtain

\[ F = \frac{\alpha^2}{2\beta} (|\psi|^2 - 1)^2 + \frac{1}{2} \left| \left( \nabla + i \frac{e^*}{\sqrt{|\alpha|m^*c}} A \right) \psi \right|^2 \frac{\alpha^2}{\beta} + \frac{B^2}{16\pi \xi^2}. \]  

(1.3)
Finally, we rescale $A$ by $\gamma$ and note that $\gamma^{-2}\beta/\alpha^2 = 4\pi\lambda^2$. Introducing the parameter $\kappa = \lambda/\xi$ and choosing $\alpha^2/\beta$ as the unit for our energy density, we obtain

$$F = \frac{1}{2}(|\psi|^2 - 1)^2 + \frac{1}{2}(|\nabla + iA|)^2 + \frac{\kappa^2}{4}B^2. \quad (1.4)$$

Writing the GL free energy in this form clearly shows that there is only one parameter that determines the properties of this model, namely, $\kappa$.

Alternatively, one can write the wave function in complex polar form so that

$$\psi = \chi e^{i\phi}, \quad \frac{1}{2}(|\nabla + iA|^2) = \frac{1}{2}(\nabla\chi)^2 + \frac{1}{2}\chi^2(\nabla\phi + A)^2 \quad (1.5)$$

### 1.1 Quantum vortices and field quantization

One of the most remarkable features of this theory is that it describes macroscopic properties of a thermodynamic system, yet features a complex wave function and so inherits certain fundamental properties of quantum mechanical systems, something that can result in so called quantum vortices: Line-like singularities where the amplitude of the wave function becomes zero, and where the complex phase winds by $2\pi$.

Consider an isolated vortex line along the $z-$axis around which the phase winds by $2\pi$. For our purpose we can regard this as a two dimensional system with a phase winding around the origin. Except in some very exotic systems, such a vortex possess rotational symmetry, and can thus be treated using circular coordinates. The free energy then becomes

$$F = \int rdr \left\{ \frac{1}{2}(\chi^2 - 1)^2 + \frac{1}{2}(\nabla\chi)^2 + \frac{1}{2}\chi^2 \left( \frac{1}{r} + A \right)^2 + \frac{\kappa^2}{4r^2}((\nabla \times A)^2) \right\} \quad (1.6)$$

Working with the gauge $\nabla \cdot A = 0$ we can introduce $A = a(r)\hat{\theta}/r$ to get

$$F = \int rdr \left\{ \frac{1}{2}(\chi^2 - 1)^2 + \frac{1}{2}((\chi')^2 + \frac{1}{2}\chi^2 \frac{1}{r^2}(1 + a)^2 + \frac{\kappa^2}{4r^2}(a')^2) \right\}. \quad (1.7)$$

Due to rotational symmetry we must have $A(0) = 0$ and so we conclude that $a(0) = 0$. For the energy to be finite this implies $\chi(0) = 0$ and so the density of superconducting electrons is zero in the center of the vortex as stated above. Finite energy also implies $a(r \to \infty) = 1$. Likewise we must have $\chi(r \to \infty) = 1$.

So, we have the proper boundary conditions required to formulate the differential equations that determine the shape of a vortex:

$$\chi'' + \frac{1}{r}\chi' - \frac{1}{r^2}(1 + a)^2\chi = \frac{\partial U}{\partial \chi} \quad (1.8)$$

$$a'' - \frac{1}{r}a' = \frac{2}{\kappa^2}\chi^2(1 + a) \quad (1.9)$$
1.1. QUANTUM VORTICES AND FIELD QUANTIZATION

where $U$ is the potential energy. Considering the limit $r \to \infty$ we expect that the deviations from the ground state are small. Introducing $\epsilon = \chi - 1$ and $\alpha = a + 1$ and linearizing the equations we obtain

$$
\epsilon'' + \frac{1}{r} \epsilon' = \frac{\partial^2 U}{\partial \chi^2} \bigg|_{\chi = 1} \epsilon = 4\epsilon
$$
(1.10)

$$
\alpha'' - \frac{1}{r} \alpha' = \frac{2}{\kappa^2} \alpha.
$$
(1.11)

The first line (for $\epsilon$) is a modified Bessel's equation, and the solution is correspondingly a modified Bessel function of second kind. The second equation (for $\alpha$) can be rewritten as a modified Bessel's equation by the substitution ($\alpha = \tilde{\alpha} r$). The results is

$$
\epsilon \sim K_0(2r)
$$
(1.12)

$$
\tilde{\alpha} \sim K_1(\sqrt{2}r/\kappa) \to A \sim \hat{\theta}(q_0 K_1(\sqrt{2}r/\kappa) - 1/r).
$$
(1.13)

Thus, far away from the vortex, $\epsilon$ and $\tilde{\alpha}$ decay exponentially. Recalling that we choose as our length scale $\sqrt{2}\xi$ we find that in a generic representation we have

$$
\epsilon \sim K_0(\sqrt{2}r/\xi)
$$
(1.14)

$$
\tilde{\alpha} \sim K_1(r/\kappa \xi) = K_1(r/\lambda).
$$
(1.15)

The parameters $\xi$ and $\lambda$ thus give the length scale at which the amplitude and gauge field (and thus also magnetic field) changes, and are correspondingly called the coherence length and penetration depth respectively. The coherence length appears with a factor $\sqrt{2}$ for what appears to be historical reasons. If $\kappa = 1/\sqrt{2}$, then the amplitude and magnetic field decay by the same length scale. While the equation 1.9 permits no analytical solution, it is straightforward to obtain the shape of a vortex numerically. Such a solution can be seen in Fig. 1.1.

The asymptotic behaviour derived here reveals a very important property of quantum vortices, namely that of flux quantisation: We have

$$
\lim_{r \to \infty} a(r) = -1 \Rightarrow \lim_{r \to \infty} A(r) = -\hat{\theta} \frac{r}{r}
$$
(1.16)

Conducting a line integration along a circle $C$ with radius $r$ around the vortex we obtain

$$
\lim_{r \to \infty} \oint_C A \cdot dl = \int_{\Omega} d\Omega \cdot B = -2\pi.
$$
(1.17)

Thus, the vortex line carries a unit of magnetic flux which is $2\pi$ in these units. This argument easily extends to multiple vortices. If we require that the energy is finite, then we obtain

$$
\lim_{r \to \infty} (\nabla \varphi + A) = 0
$$
(1.18)
Figure 1.1: Cross section of a vortex showing density and magnetic field deviation from the ground state. In the case $\kappa = 1/\sqrt{2}$ (b) we see that $1 - \chi^2$ and $B$ fall onto the same line. In contrast, $\kappa < 1/\sqrt{2}$ (a) gives a deviation in density that decays slower than the magnetic field, while $\kappa > 1/\sqrt{2}$ (c) gives slower decay of the magnetic field.

and thus

$$\lim_{r \to \infty} \oint_C \vec{A} \cdot d\vec{l} = n2\pi,$$  \hspace{1cm} (1.19)

where $n$ is the number of vortices enclosed by the $C$.

1.2 Analytical approximation of vortex interaction

As mentioned in the previous section, calculating the shapes of vortices generally requires numerical methods, as do in fact most problems that arise in GL theory. Despite this, one can obtain a great deal of insight into vortex interaction from analytical approximation. We start by dividing the energy contributions into two parts:

$$F_I = \frac{1}{2}(\chi^2 - 1)^2 + \frac{1}{2}(\nabla \chi)^2 \hspace{1cm} (1.20)$$

$$F_{II} = \frac{\kappa^2}{4}(\nabla \times \vec{A})^2 + \frac{1}{2} \chi^2(\nabla \varphi + \vec{A})^2 \hspace{1cm} (1.21)$$

To make this calculation tractable, we treat $F_I$ in the limit where $\kappa \ll 1/\sqrt{2}$. In this way, it decouples from $F_{II}$ since the penetration depth is much smaller than the coherence length. Likewise, we treat $F_{II}$ in the limit $\kappa \gg 1/\sqrt{2}$. This implies that the amplitude is depleted in a small region around the singularity, while the magnetic field penetrates much further. Also, we linearize $F_I$. This gives the free
energy density

\[ F_I = 2\epsilon^2 + \frac{1}{2}(\nabla \epsilon)^2, \quad \epsilon = \chi - 1 \]  
(1.22)

\[ F_{II} = \frac{\kappa^2}{4}(\nabla \times A)^2 + \frac{1}{2}(\nabla \varphi + A)^2 \]  
(1.23)

which should give a faithful representation of the behaviour of the vortex far away from the core. Next, we consider the variation of \( F_{II} \) with respect to \( A \):

\[ \delta F_{II} = \frac{\kappa^2}{2}(\nabla \times A) \cdot (\nabla \times \delta A) + (\nabla \varphi + A) \cdot \delta A = 0 \Rightarrow \]

\[ \frac{\kappa^2}{2} \nabla \times \nabla \times A + (\nabla \varphi + A) = 0 \]  
(1.24)

The last equation is essentially Ampere’s law. Taking the curl of it we obtain

\[ \frac{\kappa^2}{2} \nabla \times \nabla \times B + B = -\nabla \times (\nabla \varphi) \Rightarrow \]

\[ \frac{\kappa^2}{2} \nabla \times \nabla \times B + B = \Phi \delta(r). \]  
(1.25)

Next, we note that

\[ \nabla \times \nabla \times B = \nabla (\nabla \cdot B) - \Delta B. \]  
(1.26)

The magnetic field is divergence less and we thus have

\[ B - \frac{\kappa^2}{2} \Delta B = \Phi \delta(r). \]  
(1.27)

The solution to this is once again the modified Bessel function \( C_{II} K_0(\sqrt{2r}/\kappa) \). To obtain \( C_{II} \) we note

\[ \lim_{r \to 0} K_0(\alpha r) = -\ln(\alpha r), \]  
(1.30)

\[ \nabla (-\ln(\alpha r)) = -\frac{r}{|r|} \Rightarrow \]

\[ \Delta K_0(\alpha r) = -2\pi \delta(r). \]  
(1.31)

We thus obtain \( C_{II} \) from

\[ -\frac{\kappa^2}{2} (-2\pi) C_{II} = \Phi \Rightarrow C_{II} = \frac{\Phi}{\pi \kappa^2}. \]  
(1.32)

This readily gives us the magnetic field for a single vortex

\[ B(r) = \frac{\Phi}{\pi \kappa^2} K_0(\sqrt{2r}/\kappa). \]  
(1.33)
CHAPTER 1. GINZBURG LANDAU THEORY

Finally, we note that this diverges in the center of the vortex. This is a consequence of the fact that we have neglected the density suppression in the core, leading to infinite energy. Thus, we introduce a cut off that depends on the size of the core. In this case we have $\epsilon \sim K_0(2r)$ and so we estimate the core size to be $1/2$ and thus get

$$B(0) = \frac{\Phi}{\pi \kappa} K_0(1/\sqrt{2\kappa}). \quad (1.35)$$

Next, we return to the amplitude and recall that the variation of $F_I$ gives the asymptotic behavior

$$4\epsilon - \Delta \epsilon = 0 \Rightarrow \epsilon = C_I K_0(2r). \quad (1.36)$$

Once again, we have a function that is divergent at the origin. From the definition $\epsilon = \chi - 1$ it is also clear that $C_I < 0$ and that $\epsilon(0) = -1$ for a vortex solution. Also, we note

$$(4 - \Delta)C_I K_0(2r) = 2\pi C_I \delta(r). \quad (1.38)$$

Now, we can rewrite the energy as follows;

$$F_I = 2\epsilon^2 + \frac{1}{2}(\nabla \epsilon)^2 \quad (1.39)$$

$$= 2\epsilon^2 + \frac{1}{2} \nabla \cdot (\epsilon \nabla \epsilon) - \frac{1}{2} \epsilon \Delta \epsilon \quad (1.40)$$

Integrated over the entire space, the term $\nabla \cdot (\epsilon \nabla \epsilon)$ gives no contribution to the energy and we drop it to obtain

$$F_I = \frac{1}{2} (4\epsilon - \Delta \epsilon) \quad (1.41)$$

Similarly, for $F_{II}$ we have

$$\frac{\kappa^2}{4} B^2 + \frac{1}{2} (\nabla \varphi + A)^2 \quad (1.42)$$

$$= \frac{\kappa^2}{4} B^2 + \frac{\kappa^4}{8} (\nabla \times B)^2 \quad (1.43)$$

From standard vector calculus we have $(\nabla \times B)^2 = B \cdot \nabla \times \nabla \times B - \nabla \cdot (\nabla \times B \times B)$. The latter of the terms give no contribution to the total energy since

$$\int dV \nabla \cdot (\nabla \times B \times B) = \oint (\nabla \times B \times B) \cdot dS = 0 \quad (1.45)$$
as $B$ is exponentially localized. So we obtain

$$F_{II} = \frac{\kappa^2}{4} B \left( B + \frac{\kappa^2}{2} \nabla \times \nabla \times B \right)$$

(1.46) $$= \frac{\kappa^2}{4} B \left( B - \frac{\kappa^2}{2} \Delta B \right)$$

(1.47)

Using equations 1.29 and 1.38 we can write the energy of a single vortex as

$$E_{vI} = \int \frac{1}{2} \epsilon [2\pi C_I \delta(\mathbf{r})] = \pi C_I \epsilon(0)$$

(1.48)

$$E_{vII} = \int \frac{\kappa^2}{4} B \cdot \Phi[\delta(\mathbf{r})] = \frac{\kappa^2}{4} \Phi B(0)$$

(1.49)

Now, if we consider two interacting vortices and model them by a superposition we obtain

$$E_{2v}^{vI} = \int \pi C_I \epsilon[\delta(\mathbf{r} - \mathbf{r}_1) + \delta(\mathbf{r} - \mathbf{r}_2)]$$

(1.50)

$$E_{2v}^{vII} = \int \frac{\kappa^2}{4} B \cdot \Phi[\delta(\mathbf{r} - \mathbf{r}_1) + \delta(\mathbf{r} - \mathbf{r}_2)].$$

(1.51)

But here one of the pitfalls of linearized GL theory emerges: The interaction energy predicted by these expressions are

$$E_{I}^{\text{int}} = E_{2v}^{vI} - 2 E_{v}^{vI} = 2\pi C_I^2 K_0(2r)$$

(1.52)

$$E_{II}^{\text{int}} = E_{2v}^{vII} - 2 E_{v}^{vII} = \frac{\Phi^2}{2\pi \kappa^2} K_0(r\sqrt{2}/\kappa).$$

(1.53)

The latter of the two is qualitatively correct, while the former actually predicts that core interaction is repulsive. The reason for this is that we have approximated the solutions with two vortices by the superposition of two single vortex solutions. For the term $E_{II}$ this seems reasonable, as the magnetic field is quantized and each vortex carry one quantum. In contrast, the density suppression is not quantized at all, and considering a composite vortex it is pretty clear that the density in the center is zero just as for a single vortex.

Instead, we try to model the superposition as:

$$\chi^{2v}(\mathbf{r}) = \chi^{1v}(\mathbf{r} - \mathbf{r}_1) \chi^{1v}(\mathbf{r} - \mathbf{r}_2).$$

(1.54)

Denoting the perturbation of the vortex $i$ by $\epsilon_i$, we obtain

$$\epsilon^{2v}(\mathbf{r}) = \epsilon_1 + \epsilon_2 + \epsilon_1\epsilon_2 \Rightarrow$$

(1.55)

$$(4 - \Delta)\epsilon^{2v}(\mathbf{r}) = \delta(\mathbf{r} - \mathbf{r}_1)(1 + \epsilon_2) + \delta(\mathbf{r} - \mathbf{r}_2)(1 + \epsilon_1)$$

(1.56)

and thus
\[ E_{I_i}^{int} = \pi C_I \int d\mathbf{r} (\epsilon_1 + \epsilon_2 + \epsilon_1 \epsilon_2) \{ \delta(r - r_1)(1 + \epsilon_2) + \delta(r - r_2)(1 + \epsilon_1) \} \] (1.57)
\[ = \pi C_I \int d\mathbf{r} \{ \delta(r - r_1)(\epsilon_1 + \epsilon_2 + 2\epsilon_1 \epsilon_2 + \epsilon_1 \epsilon_2^2) \] (1.58)
\[ + \delta(r - r_2)(\epsilon_2 + \epsilon_1 + 2\epsilon_2 \epsilon_1 + \epsilon_1^2 + \epsilon_2^2) \} \] (1.59)

Subtracting the potential energy of two isolated vortices, i.e. \( \delta(r - r_i)\epsilon_i \) we obtain

\[ E_{I_i}^{int} = \pi C_I \int d\mathbf{r} \{ \delta(r - r_1)\epsilon_2(1 + 2\epsilon_1 + \epsilon_2 + \epsilon_1 \epsilon_2) \] (1.60)
\[ + \delta(r - r_2)\epsilon_1(1 + 2\epsilon_2 + \epsilon_1 + \epsilon_2 \epsilon_1) \} \] (1.61)

Keeping only the lowest order terms we obtain

\[ E_{I_i}^{int} \approx \pi C_I \{ \epsilon_2(r_1)(1 + 2\epsilon_1(r_1)) + \epsilon_1(r_2)(1 + 2\epsilon_2(r_2)) \} \] (1.62)
\[ = \pi C_I 2\epsilon(\Delta r)(1 + 2\epsilon(0)) = -2\pi C_I^2 K(2r) \] (1.63)

This gives a contribution to the interaction which is attractive and decays with the length scale given by the coherence length. It also suggests an intuitive interpretation of how fluctuation in the amplitude mediates inter-vortex interaction: The presence of vortices causes a reduction of the density of cooper pairs and thus an environment in which the energetic cost of an additional vortex core is reduced. At the same time, the energy contribution from currents and the magnetic field provides a repulsive contribution to the interaction.

For two well separated vortices, the interaction type with the longest range dominates. As it turns out however, the inter-vortex interaction in this model is monotonic and so this applies at any separation. Another way to formulate this is that the surface energy between superconducting and normal domains with magnetic flux is positive if \( \kappa < 1/\sqrt{2} \) and negative if \( \kappa > 1/\sqrt{2} \). This give rise to two classes of superconductors:

- Type-I superconductor when \( \kappa < 1/\sqrt{2} \).
- Type-II superconductor when \( \kappa > 1/\sqrt{2} \).

### 1.3 Magnetic response

Having explored the basic aspects of GL theory we now try to reconcile it with some of the properties of superconductors.

A fact that was mentioned in the introduction is that superconductivity is destroyed in the presence of sufficiently strong magnetic fields. Given the Meissner effect; that superconductors are perfect diamagnets, this is not surprising.Attributing a condensation energy \( F - f_n \) to the superconducting state, we should expect
It to be destroyed when the energetic cost of keeping out the magnetic pressure is sufficiently large. Thus, it seems reasonable to put

$$F - f_n = -\frac{H_c^2}{8\pi}$$

(1.64)

where $F$ and $f_n$ are the Helmholtz free energies per unit volume in the respective phases in zero field. This expression defines the critical field $H_c$ where the magnetic field enters the superconductor. The manner in which this occurs depends on whether it is a Type-I or Type-II superconductor. In the former of the two, it enters in the form of large normal domains that generally grow from the boundary and inwards. In the latter, there is a negative boundary energy between normal and superconducting domains, and so the normal domains split into the smallest units possible, quantum vortices carrying a single quantum of magnetic flux each.

Because vortices repel each other in Type-II superconductors, the energy cost per vortex increases with the density of vortices. A consequence of this is that magnetic penetration is gradual, rather than abrupt as is the case with Type-I superconductors. One can therefor define two critical magnetic fields for these systems: At $Hc1$ the magnetic field starts to penetrate in the form of vortices and at $Hc2$ superconductivity is destroyed.

Historically, the first superconductors discovered were of Type-I. This is no surprise, as many pure metals belong to this category. Ginzburgs and Landaus theory provided an intuitive model describing many of the basic properties of these. Initially, it was not realized that this theory predicts a second kind of superconductor, a discovery that was made in 1957 by Abrikosov [35]. At first, these were considered to be exotic materials, but from the early 1960’s, the vast majority of new superconductors discovered belong to this category [1].
Chapter 2

Multi-band superconductivity

Following the publication of the BCS theory in 1957 [8] it did not take long until it was realised that it is entirely possible for a material to have multiple gaps. In 1959, Suhl et al concluded that distinct fermi surfaces result in multiple gaps with potentially different transition temperatures [34].

More than four decades later, the first multi-gap material was found in magnesium diboride. In 2001 it was discovered to be a superconductor with a critical temperature of 39 K, at the time the highest for a non-copper-oxide bulk superconductor [26]. Its two-gap nature was established in 2001-2003 [36, 23, 32]. Since the discovery of iron based superconductors in 2008, the family of multi-gap materials have been growing steadily [20, 10, 16].

2.1 Properties of multi-component GL theory

In the context of GL theory, the implication of multiple gaps is a model with multiple complex wave functions. For a derivation and discussion of when GL theory is applicable to multi gap superconductors, see [31, 14]. We use the following free energy density to describe a multi-gap superconductor:

\[
F = \frac{1}{2} (\nabla \times A)^2 + \sum_i \left\{ \alpha_i |\psi_i|^2 + \frac{\beta_i}{2} |\psi_i|^4 + \frac{1}{2} (\nabla + eA)\psi_i |^2 \right\} + \frac{1}{2} \sum_{i \neq j} \eta_{ij} \psi^*_i \psi_j, \quad \text{where } \eta \text{ is hermitian.}
\]

Comparing this to the single component GL free energy 1.4, this expression obviously differs by having multiple order parameters. In addition to that, a factor \( \kappa^2 / 2 \) has been absorbed into \( A \), resulting in a parameter \( e \) that describes the coupling between the complex fields and the gauge field. The reason for doing this is that \( \kappa = \lambda / \xi \) is not generally well defined when there are multiple order parameters in the model. Finally, we have an entirely new term that was not present in the single
component theory: Josephson inter-band coupling, described by the terms $\eta_{ij}\psi_i^*\psi_j$. These terms originate from the Josephson tunnelling effect [19, 2]. Cooper pairs can tunnel between the two bands, and so a phase difference between the bands gives rise to a Josephson current. In time dependent theory, this gives rise to a type of excitations called Leggett modes, where the phase difference oscillates around the ground state value [21, 30]. Observation of the Leggett mode in MgB$_2$ was reported recently [9]. It should be stressed here that it is possible to have several other terms by which the complex fields interact besides the Josephson term.

A consequence of the Josephson coupling is that it is possible to have non-zero density of cooper pairs in a band even if $\alpha > 0$, a phenomena known as proximity induced superconductivity. Thus, if we imagine this band isolated from the other bands, then at the critical temperature, $\alpha$ changes sign, and there is a transition between a superconducting and a normal state. In the case with Josephson interband coupling it instead becomes a transition between proximity induced superconductivity ($\alpha > 0$) and active superconductivity $\alpha < 0$.

Multi-band GL theory is also relevant to several rather exotic physical systems. This includes for example neutron star interiors, consisting of a mixture of superfluid neutrons, and superconducting electrons [18]. These systems are generally modelled with two wave functions, of which only one is coupled to the gauge field.

Another application is the projected state of metallic hydrogen, which is predicted to be superconducting with a critical temperature in the range 200-400K under high pressure. If these predictions are correct, metallic hydrogen forms a two components superconductor with one band due to electrons, and one due to protons [3, 7]. A recent experiment suggest that hydrogen undergoes a transition to a metallic state at room temperature and a pressure of 260-270 GPa, although no observation of a superconducting state was reported [12].

This class of exotic multi band superconductors/superfluids differ from iron pnictides and MgB$_2$ in that the wave functions are associated with different types of particles. In the examples listed here, one of them is associated with electrons, and the other with nucleons. Since Josephson inter band coupling results due to tunnelling of cooper pairs between bands, it is clear that no such term can appear in a model of an electron and a nucleon condensate (as this would imply converting electrons to nucleons or vice versa).

### 2.2 Color charge

The fact that there are multiple wave functions in this model also implies that there are several types of singularities. A singularity with a phase winding of $2\pi$ in one of the order parameters is referred to as a fractional vortex, while a singularity in which all order parameters posses this same phase winding is referred to as a composite vortex. Thus, we can view the composite vortex as consisting of a number of fractional vortices.
2.2. COLOR CHARGE

There are two mechanisms in this model that binds together the fractional vortices. The first of them is the electromagnetic interaction, which derives from the fact that they all share the same vector potential \( A \). (The second is Josephson strings, which are treated below). In the London limit (constant density limit) the free energy of a multi-component superconductor in the absence of Josephson inter-band coupling is

\[
F_{\text{II}} = \frac{1}{2} \sum_i \chi_i^2 (\nabla \varphi_i + eA)^2 + \frac{1}{2} (\nabla \times A)^2. \tag{2.3}
\]

Taking the variation with respect to \( A \) gives

\[
\nabla \times \nabla \times A + e \sum_i \chi_i^2 (\nabla \varphi_i + eA) = 0 \Rightarrow \tag{2.4}
\]

\[
\nabla \times \nabla \times B + e^2 \sum_i \chi_i^2 B = -e \sum_j \chi_j^2 \nabla \times (\nabla \varphi_j) \Rightarrow \tag{2.5}
\]

\[
\nabla \times \nabla \times B = -\frac{1}{e^2} \sum_i \chi_i^2 \nabla \times (\nabla \varphi_i) \Rightarrow \tag{2.6}
\]

The solution to this is once again the modified Bessel function of second kind:

\[
B = C_{\text{II}} K_0 \left( r \sqrt{e^2 \sum_i \chi_i^2} \right) \tag{2.7}
\]

where \( C_{\text{II}} \) is determined from

\[
C_{\text{II}} \frac{2\pi}{e^2 \sum_i \chi_i^2} = -\frac{1}{e \sum_j \chi_j^2} \sum_j \chi_j^2 \nabla \times (\nabla \varphi_j) \Rightarrow C_{\text{II}} = -\frac{e}{2\pi} \sum_j \chi_j^2 \nabla \times (\nabla \varphi_j). \tag{2.8}
\]

The implication of this is that there is a fractional quantum of flux associated with each fractional vortex, and that this quantum is

\[
\Phi_{i,\text{frac}} = \frac{\chi_i^2}{\sum_j \chi_j^2} \Phi_{\text{comp}}. \tag{2.9}
\]

If we consider fractional vortices on a length scale larger than the penetration depth, then we can approximate the magnetic field by a delta function. This gives us the following approximation of the covariant phase gradient associated with a fractional vortex in the \( j \)th band located in \( r_v \)

\[
(\nabla \varphi_i + eA) = \left( \delta_{ij} - \frac{\chi_j^2}{\sum_k \chi_k^2} \right) \hat{z} \times \frac{(r - r_v)}{(r - r_v)^2}. \tag{2.10}
\]

Next, we introduce a ’charge’, which is associated with each band and denoted \( q_i \). The phase gradient

\[
\frac{\hat{z} \times (r - r_v)}{(r - r_v)^2} = \hat{z} \times \nabla \ln |r - r_v| \tag{2.11}
\]
is considered to be the unit charge. Hence, we can decompose a fractional vortex into a number of charges. For example, the $i$–type charge of a $\mu$–band fractional vortex is

$$q_{i,\mu} = \left(\delta_{i,\mu} - \frac{\chi_{\mu}^2}{\sum_k \chi_k^2}\right) \chi_i. \quad (2.12)$$

The interaction energy of a charge neutral set of fractional vortices can then be written

$$F = \sum_i \int dxdy \frac{1}{2} \left(\sum_{\mu} q_{i,\mu} \nabla \ln |\mathbf{r} - \mathbf{r}_\mu|\right)^2 \quad (2.13)$$

$$= \sum_i \int dxdy \frac{1}{2} \left(\sum_{\mu \neq \nu} q_{i,\mu} \nabla \ln |\mathbf{r} - \mathbf{r}_\mu| \cdot q_{i,\nu} \nabla \ln |\mathbf{r} - \mathbf{r}_\nu| + \sum_\gamma (q_{i,\gamma} \nabla \ln |\mathbf{r} - \mathbf{r}_\gamma|)^2\right). \quad (2.14)$$

The last term can be neglected, since it is independent of vortex/charge locations. Also, we note

$$\sum_{\mu,\nu} \int d^2r q_{i,\mu} q_{i,\nu} \left(\nabla \cdot [\ln |\mathbf{r} - \mathbf{r}_\mu| \nabla \ln |\mathbf{r} - \mathbf{r}_\nu|] - \ln |\mathbf{r} - \mathbf{r}_\mu| \Delta \ln |\mathbf{r} - \mathbf{r}_\nu|\right) \quad (2.16)$$

For a system that has finite energy and thus is charge neutral, the former of these terms disappears. The latter term is

$$= \sum_{\mu,\nu} \int d^2r q_{i,\mu} q_{i,\nu} \left( - \ln |\mathbf{r} - \mathbf{r}_\mu| \Delta \ln |\mathbf{r} - \mathbf{r}_\nu|\right) \quad (2.18)$$

$$= -2\pi \sum_{\mu,\nu} \int d^2r q_{i,\mu} q_{i,\nu} \ln |\mathbf{r} - \mathbf{r}_\mu| \delta(\mathbf{r} - \mathbf{r}_\nu) \quad (2.19)$$

and so we obtain, summing over all bands and charges

$$F = - \sum_{i,\mu \neq \nu} \pi q_{i,\mu} q_{i,\nu} \ln |\mathbf{r}_\mu - \mathbf{r}_\nu|. \quad (2.20)$$

Clearly, the set of vectors $\{\tilde{q}_\mu\}$ (containing the charges of the fractional vortex $\mu$) satisfy $\sum_{i=1}^N \tilde{q}_\mu = 0$, and so the dimension of the vector space spanned by $\{q_\mu\}$ is only $N - 1$, where $N$ is the number of bands. Thus, this model can be reduced to $N - 1$ charges, although generally at the cost of a more unwieldy expression. The
interaction between fractional vortices of various kinds can be obtained by simply computing a dot product:

\[-\pi \bar{u}_\mu \cdot \bar{u}_\nu \ln |\mathbf{r}_\mu - \mathbf{r}_\nu| = -\pi \left( \frac{\chi^2_\mu \chi^2_\nu}{\rho} - \delta_{\mu,\nu} \chi^2_\mu \right) \ln |\mathbf{r}_\mu - \mathbf{r}_\nu|.
\]

(2.21)

The interaction obtained here resembles a coulomb gas in 2D, except that there are now several types of charge, one for each band. Each type of fractional vortex is then made up by a set of such charges.

It should be stressed that this derivation was conducted in the London limit in the case when the vortices are well separated (|r_\mu - r_\nu| \gg \lambda) and can be treated as point particles.

The topic of fractional vortices and flux quantisation in multi band superconductors has attracted interest at least since the discovery of multi-band superconductivity in MgB_2. For an analytic treatment see for example [4]. While analytical treatment in the London limit does give the correct asymptotic interactions (i.e. the 2D coulomb gas) it does not accurately predict the structure of the magnetic field (and of course not the structure of a vortex core, since it is done in the constant density limit). Including density fluctuations in the treatment reveals that the magnetic field is not generally exponentially localised, although this requires the use of numerical methods [5]. It should be stressed that this treatment only is valid in the absence of Josephson inter-band coupling.

2.3 Josephson strings

The second mechanism that binds together fractional vortices into composite ones emerges from the Josephson coupling term in the GL functional. They are here treated in the context of a two-band model, although the generalisation to other models is straightforward. When \( \eta \neq 0 \), the potential attains a dependence on the phase differences which for a fractional vortex breaks the rotational symmetry. In Fig. 2.1 this effect is displayed in a two component superconductor with two fractional vortices. Because the energy is minimal for \( \phi_1 - \phi_2 = \pi \) this phase configuration is realized in most of the superconductor. But the winding of 2\( \pi \) in the phase difference implies \( \phi_1 - \phi_2 = 0 \) along some line that connects the vortices.

An estimate of the energy per unit length of the Josephson string can be obtained by treating the cross section of the string as a one-dimensional problem. We start by decomposing the kinetic energy of the two component GL functional in a charged and a neutral sector:

\[
\frac{1}{2} \sum_i \chi^2_i (\nabla \varphi_i + e \mathbf{A})^2 = \frac{1}{2} k (\nabla \varphi_1 - \nabla \varphi_2)^2 + w \left[ \sum_a \chi^2_a (\nabla \varphi_a + e \mathbf{A}) \right]^2
\]

(2.22)

\[
k = \frac{\chi^2_1 \chi^2_2}{\chi^2_1 + \chi^2_2}, \quad w = \frac{1}{\chi^2_1 + \chi^2_2}.
\]

(2.23)
CHAPTER 2. MULTI-BAND SUPERCONDUCTIVITY

Figure 2.1: Josephson string that connects two fractional vortices in different bands in a two band GL model. The vortices are located in $x = \pm 14$, $y = 0$. GL model parameters are $\alpha_{1,2} = -3$, $\beta_{1,2} = 1$, $\eta_{1,2} = -0.1$ and $e = 0.2$. The displayed quantity is $-\cos(\varphi_1 - \varphi_2)$. For a one-dimensional problem, the charged sector with pre factor $w$ is evidently zero. The string is then described by

$$F = \frac{1}{2}k(\nabla \varphi)^2 + \tilde{\eta}\cos(\varphi) + \sum_a \left(\alpha_a \chi_a^2 + \frac{1}{2} \beta_a \chi_a^4\right)$$

$$\varphi = \varphi_1 - \varphi_2 \quad \tilde{\eta} = \eta \chi_1 \chi_2. \quad (2.24)$$

In the general case, this can only be solved numerically. In the limit $\eta \to 0$ it is however tractable to treat this analytically, as the variation in amplitude then can be neglected. In that case we obtain the free energy

$$F = \frac{1}{2}k(\nabla \varphi)^2 + |\tilde{\eta}|\{1 - \cos(\varphi)\} = \frac{1}{2}k(\nabla \varphi)^2 + 2|\tilde{\eta}|\sin^2(\varphi/2), \quad \tilde{\eta} < 0. \quad (2.25)$$

This can be written

$$\frac{1}{2} \left\{ (\sqrt{k} \varphi' \pm \sqrt{\nabla})^2 \mp 2\sqrt{\nabla}\sqrt{k}\varphi' \right\}. \quad \sqrt{\nabla} = 2\sqrt{|\tilde{\eta}|}\sin(\varphi/2). \quad (2.26)$$

The first term is a quadratic form, and hence non negative. The second term therefore gives a lower bound for the energy. We can then write

$$\sqrt{\nabla} \varphi' = \frac{dw}{d\varphi} \frac{d\varphi}{dx} = w' \Rightarrow \frac{dw}{d\varphi} = \sqrt{\nabla} \Rightarrow w = \int d\varphi \sqrt{\nabla} = -4\sqrt{|\tilde{\eta}|}\cos(\varphi/2) \quad (2.27)$$
2.4 Phase frustration and broken time reversal symmetry

Figure 2.2: Analytically computed cross section of a Josephson string. The phase difference $\varphi_1 - \varphi_2$ of the two complex phases is plotted.

and so the energy of the string is

$$\pm \sqrt{k\eta} \left[ -4 \cos(\varphi/2) \right]_0^{2\pi} = \mp 8 \sqrt{k\eta}. \quad (2.28)$$

This is of course only physically relevant when the energy is positive. Thus, in order to obtain the corresponding solution we insert $-$ into the quadratic form and demand that is be zero everywhere. This gives the equation

$$\sqrt{k} \varphi' = -2 \sqrt{\eta} \sin(\varphi/2) \Rightarrow \varphi = 4 \arccot \left\{ \exp \left( \frac{x \sqrt{\eta}}{\sqrt{k}} \right) \right\}. \quad (2.29)$$

2.4 Phase frustration and broken time reversal symmetry

Yet another phenomena emerging from the model 2.2 is frustration with respect to the phase differences $\varphi_i - \varphi_j$ and, correspondingly, breakdown of the time reversal symmetry. This topic has sparked considerable interest lately in bulk superconductivity [33, 17] as well as in Josephson junctions with two-band superconductors [27].
In the context of GL theory, this phenomena can be understood from the Josephson coupling terms:

\[ \frac{1}{2} \sum_{i \neq j} \eta_{ij} \psi_i^* \psi_j = \sum_{i<j} \eta_{ij} \| \psi_i \| \| \psi_j \| \cos(\varphi_i - \varphi_j). \] (2.30)

These terms, depending on the sign of \( \eta_{ij} \) are minimal for either \( \varphi_i - \varphi_j = n2\pi \) or \( \varphi_i - \varphi_j = \pi + n2\pi \). Thus, if we consider a system with three bands, and \( \eta_{ij} > 0 \), then not all terms can be minimised simultaneously.

The ground state phase configuration of such a system can generally not be computed analytically, yet, some properties can be derived from qualitative arguments. In terms of the sign of the \( \eta \)'s, there are four principal situations:

<table>
<thead>
<tr>
<th>Case</th>
<th>Sign of ( \eta_{12}, \eta_{13}, \eta_{23} )</th>
<th>Ground State Phases</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>−−−</td>
<td>( \varphi_1 = \varphi_2 = \varphi_3 )</td>
</tr>
<tr>
<td>2</td>
<td>−−+</td>
<td>Frustrated</td>
</tr>
<tr>
<td>3</td>
<td>−++</td>
<td>( \varphi_1 = \varphi_2 = \varphi_3 + \pi )</td>
</tr>
<tr>
<td>4</td>
<td>+++</td>
<td>Frustrated</td>
</tr>
</tbody>
</table>

From the symmetry of the Josephson coupling terms in the energy density it is clear however that there are only two fundamentally different situations. Indeed, from Eq. (2.30) it is clear that the energy is invariant under the transformation with respect to component \( i \): \( \eta_{ij} \rightarrow -\eta_{ij}, \varphi_i \rightarrow \varphi_i + \pi \). Thus, the case 3 can be mapped onto 1, while case 4 can be mapped onto 2.

The situation (4), with \( \eta_{ij} > 0 \) can give a wide range of ground states, as can be seen in Fig. 2.3. As \( \eta_{12} \) is scaled, ground state phases change continuously from \((-\pi, \pi, 0)\) to the limit where one band is depleted and the remaining phases are \((-\pi/2, \pi/2, \pi/2)\).

An important property of the potential energy is that it is invariant under complex conjugation of the fields. That is, the potential energy does not change if the sign of all phase differences is changed, \( \varphi_{ij} \rightarrow -\varphi_{ij} \). Thus, if any of the phase differences \( \varphi_{ij} \) is not an integer multiple of \( \pi \), then the ground state posses an additional discrete \( Z_2 \) degeneracy. For example, in a system with \( \alpha_i = -1, \beta_i = 1 \) and \( \eta_{ij} = 1 \), there are two possible ground state given by \( \varphi_{12} = 2\pi/3, \varphi_{13} = -2\pi/3 \) or \( \varphi_{12} = -2\pi/3, \varphi_{13} = 2\pi/3 \). Thus in this case, the symmetry is \( U(1) \times Z_2 \), as opposed to \( U(1) \).

The term time reversal symmetry breakdown has its origin in the time reversal operator, under which wave functions transform as \( \psi \rightarrow \psi^* \). When taking the complex conjugate of a ground state with discrete symmetry \( Z_2 \), the resulting state is the other ground state allowed by the model.
2.5 Vortex structure formation in multi-band superconductors

As previously stated, superconductors are traditionally divided into two classes. This dichotomy can be described in terms of vortex interactions: If vortices attract, then it falls into the Type-I category, if they repel, it falls into the Type-II category. Alternatively, it may be described in terms of the energy of domain walls between normal and superconducting domains—If the domain wall energy is positive, then if falls in the Type-I regime, if it is negative, it falls into the Type-II regime. The repulsion between vortices in Type-II superconductors gives rise to a particular ordering; a triangular lattice that maximises the nearest neighbour distance, also known as the Abrikosov lattice [35].

In a paper from 2005 [6] it was demonstrated that non-monotonic vortex interaction with long range attraction and short range repulsion is possible in two band GL theory. Given that the formation of an Abrikosov lattice relies on vortex repulsion, it is natural to ask what kind ordering appears in multi-band systems. There are several natural approaches to this question. In a theoretical context one can compute vortex interactions and conduct molecular dynamics/MC simulations using the resulting interaction potentials, or determine the ground state of a group of vortices by minimising the GL free energy numerically. Experimental work addressing this question includes mapping out vortices in a superconducting sample by bitter decoration, SQUID interferometry and scanning Hall probe microscopy. While the details of these experimental techniques differ considerably, they are all based on determining where magnetic flux penetrates the superconductor, and hence where vortices are located.

In 2009 bitter decoration experiments conducted at a temperature of 4.2 K indicated a highly disordered distribution of vortices in a sample of MgB$_2$ [25]. The result was interpreted to be due to non-monotonic inter-vortex interaction, and the term 'Type-1.5 superconductor' was suggested to describe this class of materials.

A SQUID microscopy study published 2010 [28] and a report from 2012 on Scanning Hall probe microscopy gave similar results [15], and were accompanied by suggestions that it indeed results from non-monotonic vortex interaction emerging from the two band nature of MgB$_2$.

Disordered vortex patterns have also been seen in iron based superconductors, although the reason for this remains unclear. In 2011, a bitter decoration experiment conducted on BaFe$_{2−x}$Ni$_x$As$_2$, $x = 0.1$ (optimally doped) and $x = 0.16$ (overdoped) was published [22]. The experiment showed a tendency towards clustering of vortices, and in some cases also stripes forming. According to the report, this can be caused by defects in the sample, resulting in pinning of vortices in certain regions where the density of cooper pairs is slightly lower, and hence, vortices are energetically cheaper. Another mechanism discussed is the possibility of some novel form of inter-vortex interaction.

In conclusion, several new multi-band superconductors have been discovered
that last few years. Experiments on these materials show a variety of ordering patterns that should not be expected in regular Type-II superconductors. With this, we can state the set of questions that are the topic of this thesis:

1. What new types of inter-vortex interaction are possible in multi-band GL theory?

2. Under what conditions do they appear?

3. How does frustration and breakdown of the time reversal symmetry in the GL model affect vortex structure formation?

4. Are there novel multi-band phenomena that are immediately recognisable in experiments?
Ground state phases

Figure 2.3: Ground state phases of the three components as function of $\eta_{12}$ (where the gauge is fixed to $\varphi_3 = 0$). The GL parameters are $\alpha_i = 1$, $\beta_i = 1$, $\eta_{13} = \eta_{23} = 3$. For intermediate values of $\eta_{12}$ the ground state exhibits discrete degeneracy (symmetry is $U(1) \times Z_2$ rather than $U(1)$) since the energy is invariant under the sign change $\varphi_2 \rightarrow -\varphi_2$, $\varphi_3 \rightarrow -\varphi_3$. For large $\eta_{12}$ we get $\varphi_2 - \varphi_3 = \pi$ implying that $|\psi_3| = 0$ and so there is a second transition from $U(1) \times Z_2$ to $U(1)$ and only two bands at the point d). Here, the phases were computed in a system with only passive bands, though systems with active bands exhibit the same qualitative properties except for the transition to $U(1)$ and two bands only (i.e. active bands have non-zero density in the ground state).
Chapter 3

Methods

The work presented in this thesis relies to a large extent on numerical methods. These include a finite difference program, a finite element software kit and a program for mass spectrum analysis. The energy minimisation is conducted in 2D.

3.1 Energy minimisation with finite differences

One of the simplest ways of discretizing a model with continuous fields is by finite differences. The values of each function is then stored in a grid, and the functional to be evaluated then becomes a function of the values taken by the functions on the grid points. The specific discretization scheme used here, illustrated in Fig. 3.1 is as follows:

The complex fields are stored as a real and an imaginary part. The gradient part of the Hamiltonian then becomes

\[
\frac{1}{2} |(\nabla + ieA)\psi_j(r)|^2 = \frac{1}{2} |(\nabla + ieA)[R_j(r) + iI_j(r)]|^2
\]

\[
= \frac{1}{2} |\nabla R_j(r) - eA I_j(r) + i(eAR_j(r) + \nabla I_j(r))|^2
\]

\[
= \frac{1}{2} [\nabla R_j(r) - eA I_j(r)]^2 + \frac{1}{2} [eAR_j(r) + \nabla I_j(r)]^2
\]

(3.1)

(3.2)

(3.3)

where \(R_j\) and \(I_j\) are the real and imaginary parts of \(\psi_j\). This expression evidently includes contributions from the complex fields, their derivatives and the gauge field \(A\). These terms are then evaluated between all nearest neighbors:

\[
E_{\text{kin}} = \frac{1}{2} \sum_{j,(k,l)} \left\{ [\partial_{kl} R_{j,kl}(r) - eA_{kl} I_{j,kl}(r)]^2 + \frac{1}{2} [eA_{kl} R_{j,kl}(r) + \partial_{kl} I_{j,kl}(r)]^2 \right\}
\]

(3.4)

where \(\partial_{kl}\) is the gradient between two nearest neighbors and \(A_{kl}\) is the gauge field along the same direction. Since the values of the fields are stored on the grid points,
we use

\[ f_{j,k} = \frac{1}{2}(f_{j,k} + f_{j,l}) \]  

(3.5)

where \( f_{j,k} \) is the value of \( f_j \) in the gridpoint \( k \). Thus, we can imagine the gradient energy living on lines that connect the nearest neighbors on the grid. The energy contribution from the line depends on the values of the fields on the endpoints of the line, that is, the vertices. Likewise, there are 4 lines connecting a vertex and thus are dependent of it as can be seen in Fig. 3.1 (a). This also defines the value of the gauge field on a line. The magnetic flux can then be computed by integrating \( A \) along a placket, as shown in Fig. 3.1 (b). Compared to central derivatives, which is probably the most common scheme for discretizing derivatives, this has the advantage that it reduces the data dependency.

![Figure 3.1: Discretization scheme used in finite difference software, (a) gradients and (b) magnetic flux.](image)

Energy minimization is then conducted using a modified Newton-Raphson method. Let \( E_{ij} \) be the contributions to the total free energy that are dependent on the function values in the grid point \( i,j \). Also, let \( p_{ij,k} \) be the k’th function value in the grid point \( i,j \). Consider for example a two band model; there are 4 degrees of freedom due to the 2 complex fields, and two more degrees of freedom corresponding to the vector field \( A \). Thus, \( k \) runs over 6 indices. The procedure then becomes:

1. A grid point \( i,j \) is selected.
3.2. ENERGY MINIMIZATION WITH FINITE ELEMENTS

2. \( E_{ij}, \frac{\partial E_{ij}}{\partial p_{ijk}} \) and \( \frac{\partial^2 E_{ij}}{\partial p_{ijk}^2} \) are computed.

3. If \( \frac{\partial^2 E_{ij}}{\partial p_{ijk}^2} \neq 0 \), then an update \( \Delta p_{ijk} = \frac{-\left\{ \frac{\partial E_{ij}}{\partial p_{ijk}} \right\}}{\left\{ \frac{\partial^2 E_{ij}}{\partial p_{ijk}^2} \right\}} \) is proposed.

4. A new value of the free energy contribution \( E^\prime_{ij} \) is computed.

5. If \( E^\prime_{ij} < E_{ij} \), then the update is accepted.

This method differs from the standard NR method in that all off diagonal terms in the hessian \( \frac{\partial^2 E_{ij}}{\partial p_{ijk} \partial p_{ij'}^2} \) are neglected in order to avoid computing and inverting the full matrix. Also, the algorithm includes checking that the new solution in fact corresponds to a lower energy (step 5). This is necessary to obtain numerical stability.

This algorithm can easily be combined with successive grid refinements. When a solution is obtained for a grid with \( N_x \times N_y \) grid points, then it is interpolated to \( MN_x \times MN_y, M > 1 \) and a solution for this grid resolution is obtained by further iteration. This gives two types of convergence criteria:

- Convergence due to iteration: Defined by \( (E_n - E_{n+m})/(E_n) < \delta \) where \( E_n \) is the total free energy after \( n \) iterations. Thus, in \( m \) iterations, the relative change in energy should be smaller than \( \delta \).

- Convergence due to interpolation: Let \( E_M \) be the energy of a system that has been interpolated to a grid resolution of \( MN_x \times MN_y \) and has converged due to iteration. Then, \( (E_M - E_{2M}) < \epsilon \) is the criterion for convergence due to interpolation.

3.2 Energy minimization with finite elements

Some of the results reported in this thesis are obtained using energy minimization with finite elements, rather than finite differences. The software used for this is freeFEM, an open source software suit available at www.freefem.org. It allows minimization of nonlinear functionals using gradient methods like steepest descent and the nonlinear conjugate gradient method.

3.3 Mass spectrum analysis

One of the most useful tools for understanding the properties of the GL model is mass spectrum analysis. The central idea is to generate a set of differential equations from the GL free energy functional and linearize them around the ground state. In a single-band model this results in two length scales— the coherence length and penetration depth which in turn determine the superconductor class. In a multi-band model this method can give considerable insight into the qualitative properties of a system.
Writing out the free energy in polar form gives
\[ f = \sum_i \left\{ \frac{1}{2} (\nabla \chi_i)^2 + \frac{1}{2} \chi_i^2 (\nabla \varphi_i + e A)^2 \right\} + U (\chi, \varphi) + \frac{1}{2} (\nabla \times A)^2. \] (3.6)

The corresponding differential equations are
\[ \sum_i \left\{ \chi_i \delta \chi_i (\nabla \varphi_i + e A)^2 + \chi_i^2 (\nabla \phi_i + e A) \cdot \nabla \delta \varphi_i + \chi_i^2 (\nabla \varphi_i + e A) \cdot e \delta A \\
+ \frac{\partial U}{\partial \varphi_i} \delta \varphi_i + \frac{\partial U}{\partial \chi_i} \delta \chi_i + \nabla \chi_i \cdot \nabla \delta \chi_i \right\} + (\nabla \times A) \cdot (\nabla \times \delta A) = 0. \] (3.7)

Selecting a gauge where \( \nabla \cdot A = 0 \) we obtain \( (\nabla \times A) \cdot (\nabla \times \delta A) = -\Delta A \cdot \delta A \).

Introducing \( \chi_i = u_i + \epsilon_i \) where \( u_i \) is the field amplitude in the ground state and linearizing Eq. (3.7) close to the ground state we obtain
\[ \sum_i \left\{ u_i^2 (\nabla \varphi_i + e A) \cdot e \delta A - u_i^2 \delta \varphi_i \Delta \varphi_i - \Delta \epsilon \cdot \delta \epsilon \right\} = 0. \] (3.10)

The derivatives of the potential energy with respect to amplitudes and phases can be written \( H_{\gamma} \), where \( H \) is the hessian of the potential at the ground state, and \( \gamma \) is a vector containing the fluctuations of \( \chi_i \) and \( \varphi_i \) around the ground state. Collecting all terms we arrive at one equation for the gauge field:
\[ \sum_i e^2 u_i^2 (\nabla \varphi_i / e + A) = \Delta A \] (3.11)

which gives the mass
\[ m_A = e \sqrt{\sum_i \chi_i^2}. \] (3.13)

The equation for the wave functions becomes:
\[ \begin{pmatrix} K^\chi & 0 \\ 0 & K^\varphi \end{pmatrix} \begin{pmatrix} \Delta \epsilon \bar{\chi} \\ \Delta \epsilon \bar{\varphi} \end{pmatrix} = H \begin{pmatrix} \epsilon \bar{\chi} \\ \epsilon \bar{\varphi} \end{pmatrix}. \]

Here, \( \epsilon \) denotes small deviations from the ground state, \( \bar{\varphi}, \bar{\chi} \) are vectors with elements \( \chi_i, \varphi_i \) and
\[ K^\chi_{ij} = \delta_{ij}, \quad K^\varphi_{ij} = \delta_{ij} \chi_i^2. \] (3.14)
3.4. EMPLOYMENT OF NUMERICAL METHODS

It should be stressed here that strictly speaking, the ground state does not correspond to a single point in the configuration space, but rather, to some subspace whose dimension depends on the symmetry of the GL functional. Hence, the notion of a phase configuration that corresponds to the minimum can be confusing. One way of addressing this is by fixing some of the phases to eliminate the degeneracy of the vacuum, but as it turns out, this introduces constraints on the choice of gauge. Alternatively, one can retain all the degrees of freedom, which results in eigenvalues of the hessian $H$ which are zero. Rewriting Eq. (3.3) as

$$\Delta \gamma = K^{-1}H \gamma, \quad K = \begin{pmatrix} K^x & 0 \\ 0 & K^\varphi \end{pmatrix}$$

reveals some of the properties of a system. Denoting the eigenvalues and eigenvectors of $K^{-1}H$ by $\Lambda_k$ and $v_k$, we can expand any perturbation to the ground state $u$ in the basis $\{v_k\}$:

$$u = \sum_k c_k v_k.$$  \hfill (3.15)

The coefficients then decay as

$$c_k \sim e^{-r \sqrt{\Lambda_k}}.$$  \hfill (3.16)

Thus, the eigenvalues give all the length scales of the problem, while the corresponding eigenvectors give the modes corresponding to each length scale.

3.4 Employment of numerical methods

In the work that is presented in this thesis, energy minimization is used for two purposes. The first is to determine the ground state, or at least, some metastable state for a collection of vortices in a superconductor. This is done using finite elements. An initial configuration is created, and the energy is minimized without any constraints. The second one is to compute inter-vortex forces and potentials, or forces between clusters of vortices etc. This is done with finite differences. The reasons for this division of labor are the advantages and disadvantages of these methods. Finite element methods are much more computationally efficient than finite differences, and consequently are well suited for finding ground states, which can be computationally very demanding.

Finite difference methods with local update routines such as the one presented above are on the other hand much less complicated than finite elements. This makes it straight forward to introduce constraints of various kinds and hence makes the method attractive when computing inter-vortex potentials. Recall that the amplitude of the wave function is zero in the center of a vortex. If one places a vortex at some location $i, j$ in a grid, sets the amplitude there to zero, and omits updating that point, then this acts to pin the vortex in that location. This means
that the energy can be minimized subject to constraints such as the position of vortices, or indeed the position of fractional vortices, allowing inter-vortex forces to be computed. While finite difference methods are not computationally efficient compared to finite elements, it is possible to obtain acceptable performance by successive grid interpolations as described above. This also allows tracking of the numerical error due to discretization.

The software for finite difference energy minimization and mass spectrum analysis used for the work presented in this thesis was developed and run by me. The finite element calculations were conducted by Julien Garaud, a post doc in Egor Babaevs research group.
Chapter 4

Results

4.1 Type-1.5 Superconductivity

The term 'Type-1.5 superconductor' describes a material with properties that appear to be a mix of Type-I and Type-II behaviour in the form of inter-vortex interaction that is non-monotonic with with long range attraction and short range repulsion. The origin of this interaction is disparity in length scales in multi-band superconductors. The first claim of an experimental observation was done by Moshchalkov in 2009 [25].

Consider the analytical approximation to the vortex-interaction in single-component GL theory that was derived in the first chapter: According to Eq. (1.53) and Eq. (1.63), the super current and magnetic flux give an interaction of the form

$$\frac{\Phi^2}{2\pi\kappa^2} K_0(r\sqrt{2}/\kappa),$$  \hspace{1cm} (4.1)

while the wave function amplitude fluctuations give an interaction term of the form

$$-2\pi C_1^2 K_0(2r),$$  \hspace{1cm} (4.2)

though it should be stressed here that the exact coefficients of $r$ in the Bessel functions depends on the units used. If we instead consider a model with two wave functions and $\eta_{12} = 0$, then we obtain a second coherence length. In the analytical approximation, the interaction potential can then generally be written

$$F_I = c_A K_0(r/m_A) - \sum_{i=1}^{2} c_{\psi,i} K_0(r/m_{\psi,i})$$  \hspace{1cm} (4.3)

where $m_A$ is the mass of the gauge field, and $m_{\psi,i}$ is the mass of the amplitude of the field $i$. Consider now a system where $m_{\psi,2} \ll m_A \ll m_{1,\psi}$. The vortex core associated with the second band is the slowest decaying mode and gives an interaction term $-c_{\psi,2} K_0(r/m_{\psi,2})$ that dominates at large separation. On the other
CHAPTER 4. RESULTS

Figure 4.1: Interaction potential of two vortices in a two band GL model. The interaction energy is given in the units of $2E_v$, where $E_v$ is the energy of a single isolated vortex. The model parameters are $\alpha_1 = -1$, $\alpha_2 = -0.0625$, $\beta_1 = 1$, $\beta_2 = 0.25$ and $\epsilon = 1$. The Josephson coupling term $\eta_{12}$ is either 0 or 0.3.

hand, when the inter-vortex distance is small, there is a region where the second band is depleted. The interaction in this region is driven by the gauge field and the first band. From the relationship $m_A \ll m_{1,\psi}$ we see that the first band behaves as a type-II superconductor. Thus, we can think of this system as a Type-I (band 2) and a Type-II (band 1) superconductor that coexist in the same material. At large separation, the Type-I behavior dominates, giving long range attraction, and at short range, the Type-II behavior dominates, giving repulsion. Hence the name Type-1.5.

A numerical calculation of the interaction potential between two such composite vortices is shown in Fig. 4.1 ($\eta = 0$). The cross section plots (a-c) in Fig. 4.2 clearly illustrates the mechanisms behind the non-monotonic interaction: The longest length scale is associated with $\psi_2$, and at a sufficiently large separation, the overlap in $\psi_2$ is larger than the magnetic overlap (c). As the separation decreases, the magnetic overlap increases, until equilibrium is reached (b). At smaller separations the magnetic/kinetic interaction dominates, resulting in repulsion (a).
Figure 4.2: Cross section plots showing the vortex shapes obtained for two interacting composite vortices. The interaction potential is displayed in Fig. 4.1. The case $\eta = 0$ is shown in (a-c) while the case $\eta = 0.3$ is shown in (d-f). The top row (a,d) corresponds to vortex separation smaller than the binding distance, the middle row corresponds to the binding distance (i.e. energy minimum) and the bottom (c,f) corresponds to separation larger than the energy minimum where interaction is attractive.
Effects of inter-band couplings

Previous studies of vortex interaction in two-band GL theory have focused on the case where there is only electromagnetic interaction between the wave functions, and the symmetry is \( U(1) \times U(1) \) \([6, 25]\). However, in materials where (multi-band) superconductivity is due to cooper pairs of electrons, these can generally tunnel between bands. In the context of GL theory this gives rise to Josephson coupling terms in the hamiltonian, and consequently changes the symmetry to \( U(1) \). In addition to Josephson coupling, the two band GL model also allows symmetry altering mixed gradient terms. Finally we also consider density interactions, which complies with the \( U(1) \times U(1) \) symmetry. Including all these terms we obtain the GL free energy density \([13, 31]\)

\[
F = \frac{1}{2} (\nabla \times \mathbf{A})^2 + \sum_i \left\{ \alpha_i |\psi_i|^2 + \frac{\beta_i}{2} |\psi_i|^4 + \frac{1}{2} (\nabla + e \mathbf{A}) |\psi_i|^2 \right\} + \frac{1}{2} \sum_{i \neq j} \left\{ \eta_{ij} \psi_i^* \psi_j - \nu_{ij} ([\nabla + e \mathbf{A}] \psi_i) \cdot [\nabla + e \mathbf{A}] \psi_j^* + \frac{\gamma_{ij}}{2} |\psi_i|^2 |\psi_j|^2 \right\}
\]  

(4.4)

(4.5)

where \( \eta, \nu \) and \( \gamma \) are real and symmetric. In the presence of inter-band terms, it is generally not possible to ascribe a coherence length to each band. Despite this, there are generally multiple length scales associated with the wave functions, but a length scale is typically associated with a linear combination of several amplitudes as opposed to a single amplitude. A comparison between a system with, and without Josephson coupling is made in Fig. 4.1 (vortex interaction) and Fig. 4.2 (cross section of interacting vortices). In the case with Josephson coupling, the range of the attraction is reduced, indicating that the length scale associated with the amplitude is shorter. The mass spectrum shown in Fig. 4.3 (a) reveals that both the masses associated with amplitudes and the gauge field increases, yet \( m_A \) remains an intermediate mass, one of the provisions for Type-1.5 behavior. The mass of the phase difference (3) also reveals the change of symmetry from \( U(1) \times U(1) \) to \( U(1) \) that occurs when the Josephson coupling becomes non-zero.

Density coupling, which is due to

\[
\frac{1}{4} \sum_{i \neq j} \gamma_{ij} |\psi_i|^2 |\psi_j|^2
\]

(4.6)

can in some cases play a role similar to Josephson coupling. If \( \gamma_{ij} < 0 \), then it generally serves to lock fractional vortices together. Just like Josephson coupling, it also leads to mixed modes where a particular length scale corresponds to a linear combination of the amplitudes. An example of the mass spectrum is displayed in Fig. 4.3 (b). Unlike Josephson coupling however, it does not break the \( U(1) \times U(1) \) symmetry into \( U(1) \), as it exhibits no phase dependence.
4.1. TYPE-1.5 SUPERCONDUCTIVITY

Figure 4.3: Mass spectrum of a two band GL model with $\alpha_1 = -1$, $\alpha_2 = -0.0625$, $\beta_1 = 1$, $\beta_2 = 0.25$ and $c = 1$. $m_A$ is the mass of the gauge field, (1) and (2) correspond to fluctuations in the amplitudes, and (3) corresponds to fluctuations in the phase difference. a) The Josephson coupling is scaled from 0 to 0.3. b) The density coupling $\gamma_{12}$ is scaled from 0 to $-0.3$. In this case, the symmetry is $U(1) \times U(1)$ and the phase difference has no mass.
Finally, we consider mixed gradient terms. We have

\[ \frac{1}{2} \left[ \nabla + eA \right] \psi_i \cdot \left[ \nabla + eA \right] \psi_j^* + cc \]  

(4.7)

\[ = \text{Re} \left\{ e^{i\varphi} (i \chi_i [\nabla \varphi_i + eA] + \nabla \chi_i) \cdot e^{-i\varphi} (-i \chi_j [\nabla \varphi_j + eA] + \nabla \chi_j) \right\} \]  

(4.8)

\[ = \cos(\varphi_i - \varphi_j) \left[ \chi_i \chi_j (\nabla \varphi_i + eA) \cdot (\nabla \varphi_j + eA) + \nabla \chi_i \cdot \nabla \chi_j \right] \]  

(4.9)

\[ - \sin(\varphi_i - \varphi_j) \left[ (\chi_i [\nabla \varphi_i + eA] \cdot \nabla \chi_j - \chi_j [\nabla \varphi_j + eA] \cdot \nabla \chi_i) \right]. \]  

(4.10)

The effect of mixed gradient terms can not be derived analytically in most cases. However, if we consider two identical bands and impose that the fractional vortices that constitute the composite vortex are identical, then it is tractable to treat analytically. The GL functional may then be written

\[ F = \frac{1}{2} (D\Psi)^* M (D\Psi) + \frac{1}{2} (\nabla \times A)^2 + U(\Psi), \quad D = (\nabla + i eA) \]  

(4.11)

\[ M = \begin{pmatrix} 1 & -\nu \cos(\varphi_1 - \varphi_2) \\ -\nu \cos(\varphi_1 - \varphi_2) & 1 \end{pmatrix}. \]

The eigenvectors of \( M \) are \[1, 1]\] and \[1, -1\] with eigenvalues \(1 - \nu \cos(\varphi_1 - \varphi_2)\) and \(1 + \nu \cos(\varphi_1 - \varphi_2)\). Since we consider two identical vortices only the former of the two is relevant. The free energy is then

\[ F = \frac{1}{2} k |D\psi'|^2 + \frac{1}{2} (\nabla \times \mathbf{A})^2 + U(\psi') \]  

(4.12)

where \( \psi' = (\psi_1 + \psi_2)/\sqrt{2} \) and \( k = (1 - \nu \cos(\varphi_1 - \varphi_2)) \). Introducing the rescaling

\[ \nabla \rightarrow \frac{1}{\sqrt{k}} \nabla, \quad \mathbf{A} \rightarrow \sqrt{k} \mathbf{A} \]  

(4.13)

gives

\[ F = \frac{1}{2} |(\nabla + i e k \mathbf{A})|^2 + \frac{1}{2} (\nabla \times \mathbf{A})^2 + U(\psi'). \]  

(4.14)

Thus, the introduction of mixed gradient terms in this system is identical to rescaling the size of the system and the electric charge \( e \). If there are no phase dependent terms in the potential, then the system will attain a phase difference \( \varphi_1 - \varphi_2 \) so that \( k < 0 \), pushing the system towards a more Type-II like behavior. If there are Josephson coupling terms present that fix the phase difference to some other value, then it is possible to have \( k > 1 \).

While this derivation was conducted in the case where the two bands are identical, it shares qualitative properties with other systems as well. Fig. 4.4 shows a system where the disparity in length scale is \( \xi_2/\xi_1 = 4 \) in the absence of inter-band couplings (4). When Josephson coupling is introduced, then the binding distance
4.1. TYPE-1.5 SUPERCONDUCTIVITY

Figure 4.4: Intervortex interaction potential for a set of systems with two active bands. The systems share the parameters given in the table ‘common parameters’. The green curve (4) corresponds to the case where the bands are coupled by the vector potential only. In this case, the ratio of the coherence lengths is $\xi_2/\xi_1 = 4$. The curve (2) shows the effect of the addition of Josephson term, the curve (5) shows the effect of addition of mixed gradient term. The curves (1) and (3) show the effect of the presence of both mixed gradient and Josephson terms with similar and opposite signs.

decreases, and the binding energy increases (2). Mixed gradient terms on the other hand increases the binding separation and decreases the binding energy, similar to decreasing the electric charge (5). When $\mu = 0.025$ and $\eta = 0.05$, these effect cancel each other, and the binding energy and separation is similar to that with no coupling (3). Finally, $\mu = 0.025$ and $\eta = 0.05$ gives the largest binding energy (1).

Type-1.5 Superconductivity from intrinsic proximity effect in two-band superconductors

So far we only considered systems where $\alpha_i < 0$, i.e. where all bands are active. In multi component GL models it is however possible to have wave functions with non-zero amplitude even in the regime $\alpha > 0$, due to presence of inter-band couplings.
Figure 4.5: Inter-vortex interaction potential in proximity two-band GL model with one proximity induced band. The GL parameters are $\alpha_1 = -1$, $\beta_1 = 1$, $\beta_2 = 0.1$ and $\epsilon = 1.41$ while $\alpha_2$ and $\eta_{12}$ are scaled.

Just as in the case with active bands above, disparity in length scale is essential for non-monotonic vortex interaction. Fig. 4.5 shows the inter-vortex interaction potential in a GL model with two bands, one active (1) and one passive (2). The parameters $\alpha_2$ and $\eta_{12}$ are scaled according to:

<table>
<thead>
<tr>
<th>Curve</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\alpha_2$</td>
<td>2</td>
<td>1</td>
<td>0.5</td>
<td>0.25</td>
<td>0.1</td>
</tr>
<tr>
<td>$\eta_{12}$</td>
<td>2.82</td>
<td>1.41</td>
<td>0.7</td>
<td>0.35</td>
<td>0.14</td>
</tr>
</tbody>
</table>

As $\alpha_2$ and $\eta_{12}$ successively decrease, so does the condensation energy associated with the second band and thus the mass of one amplitude mode. This in turn implies that the range of the attractive force increases.
4.2 Multi-body inter-vortex forces

The current paradigm within which vortex matter in superconductors or superfluids is understood relies on the assumption that interactions in a system of vortices is a superposition of pairwise forces. Indeed, we used the force between two vortices to identify the superconductor types (I), (II) and (1.5).

Yet the inter-vortex forces in GL theory cannot be decomposed into only pairwise contributions. This is not surprising: While much of the analytical work on inter-vortex forces neglect amplitude fluctuations, the full GL model does exhibit variations in amplitude, especially near singularities. Consider two interacting vortices—In the GL functional, all terms except the magnetic energy exhibit a dependency on the amplitude on the wave function, and so variations in the amplitude due to a third vortex could potentially alter the interaction energy of the original pair.

The prevalence of multi-body forces was tested as follows: The energy of a single vortex is $E_v$. Thus, in a system of $N$ vortices, the interaction energy is $E_N - NE_v$, where $E_N$ is the total energy. The two body interaction is then determined from a pair of vortices separated by the distance $r$ according to

$$U_2(r) = E_2(r) - 2E_v. \quad (4.15)$$

The three body interaction is then

$$U_3(r_1, r_2, r_3) = E_3(r_1, r_2, r_3) - \sum_{i>j} U_2(|r_i - r_j|) - 3E_v. \quad (4.16)$$

Fig. 4.6 shows the interaction energy between a vortex pair and a single vortex in a system with proximity induced superconductivity. The total interaction energy between the pair and the vortex is displayed in (a), the pairwise contribution of this energy is shown in (b), while (c) gives the three body interaction

$$U([-0.75, 0], [0.75, 0], r_3). \quad (4.17)$$

This system is a likely candidate for structure formation that is influenced by multi body forces, because it meets the following set of criteria:

1. Two body interaction is long range attractive
2. The binding energy of two body forces is small
3. There are repulsive three body forces

Because of (1), we would expect that if it was only due to two body forces, the vortices would form a compact cluster. But due to (2), the energy required to break up the cluster should be small. Finally, (3) provides a mechanism that breaks clusters.
CHAPTER 4. RESULTS

To test this hypothesis, an initial configuration was prepared with a phase winding around the origin of $50\pi$ (corresponding to 25 vortices). Then, the free energy was minimized with respect to all degrees of freedom using finite elements. The resulting vortex configuration is displayed in Fig. 4.7. The two body forces hold the vortices together, yet the three body forces prevent the formation of a compact cluster. The result is an irregular vortex configuration. In this system, the resulting vortex configuration after energy minimization depends on the initial configuration. Yet all obtained configurations share two common features: Tightly bound vortices, but also vortex less voids. This is consistent with competition of attractive two-body forces, and repulsive multi body forces. The dependence on the initial configuration suggest the existence of either metastable vortex configurations, or a very flat energy landscape.
4.2. MULTI-BODY INTER-VORTEX FORCES

Figure 4.6: Interaction energy between a vortex pair and a single vortex. The pair is located in $r_1 = [-0.75, 0]$ and $r_2 = [0.75, 0]$ (marked by the black lines). A third vortex is then inserted, and the interaction energy is computed. The interaction energy between the pair and the third vortex as a function of $r_3$ is displayed in (a). The two body contribution to the interaction energy is displayed in (b). The three body interaction, resulting from subtraction of the two-body interaction energy from the total interaction energy is shown in (c). GL parameters are $\alpha_1 = -1$, $\beta_1 = 1$, $\alpha_2 = 3$, $\beta_2 = 0.5$, $\eta_{12} = 7$ and $\epsilon = 1.3$. 

\[
\text{Total energy} = \sum_{i=1}^{n} \left( E_i - E_{ij} \right)
\]
Figure 4.7: A bound state of an $N_v = 25$ vortices resulting from minimizing the free energy of the GL functional. Displayed quantities are magnetic flux \( \psi_1^2 \) (b), \( \psi_2^2 \) (c), \( \chi_1^2 |(\nabla \varphi_1 + eA)| \) (d), \( \chi_2^2 |(\nabla \varphi_2 + eA)| \) (e) and \( \text{Im}(\psi_1^* \psi_2) \). The GL parameters are $\alpha_1 = -1$, $\beta_1 = 1$, $\alpha_2 = 3$, $\beta_2 = 0.5$, $\eta_{12} = 7$ and $\epsilon = 1.3$. 
4.3 VORTEX MATTER IN FRUSTRATED SUPERCONDUCTORS WITH $U(1)$ SYMMETRY

4.3 Vortex matter in frustrated superconductors with $U(1)$ symmetry

As previously stated, the multi-band GL model Eq. (2.2) includes Josephson inter-band coupling terms that can give frustration with respect to phase differences. In a three band model, this can result in systems with either $U(1)$ symmetry, or $U(1) \times Z_2$ symmetry, see for example Fig. 2.3.

Fig. 4.8 shows the ground state, mass spectrum and corresponding eigen-modes of a frustrated three-band superconductor. Two of the bands, (1) and (2) are identical and active. The third band is passive (proximity induced by Josephson inter-band coupling). The plots show how the ground state and mass spectrum changes as $\eta_{1,3} = \eta_{2,3}$ varies. When $\eta_{1,3} < \eta_c \approx -3.69$, the symmetry is $U(1)$ and all phases are identical in the ground state. Then, at $\eta_c$ the symmetry changes to $U(1) \times Z_2$. Referring to the Josephson coupling terms in which the frustration originates, this should come as no surprise:

$$ F_{\text{Josephson}} = \frac{1}{2} \sum_{i \neq j} \eta_{ij} \chi_i \chi_j \cos(\varphi_i - \varphi_j). \quad (4.18) $$

In our case, the terms $\chi_i \chi_3 \eta_{i,3} \cos(\varphi_i - \varphi_3)$ are minimized by $\varphi_i = \varphi_j$, i.e. all phases identical. At the same time, the term $\eta_{2,3} \chi_1 \chi_2 \cos(\varphi_1 - \varphi_2)$ is minimal for $\eta_1 - \eta_2 = \pi$. When $\eta_{1,3} < \eta_c$, the former term dominates, and all phases are equal. When $\eta_{1,3} > \eta_c$, this is no longer the case. The mass spectrum analysis Fig. 4.8 does also reveal some other important properties of this system.

In the $U(1)$ region, all eigenvectors consist of either amplitudes, or phases. Thus, for a small variation from the ground state, the amplitudes and phases recover their ground state values independently.

In contrast, in the $U(1) \times Z_2$, all eigenvectors include both amplitude and phase components. In this case, all modes are mixed, and a perturbation to a the amplitude causes a response in the phase, and vice versa.

At the transition between the $U(1)$ and $U(1) \times Z_2$ regions, one of the masses drops to zero (5). From the corresponding eigenvector (5), we see that in the $U(1)$ region, this corresponds to a mode with fluctuations in $\varphi_1$ and $\varphi_2$. Thus, it is a Leggett modes which becomes mass-less at $\eta_{1,3} = \eta_c$.

The mass spectrum analysis also reveals another interesting phenomena present in this model, namely, chiral vortex clusters. Consider a system in the $U(1)$ region of Fig. 4.8. In the ground state, all phases are equal, but the system is still frustrated. Suppose that this superconductor was exposed to a magnetic field, so that vortices were formed. The Josephson inter-band coupling terms

$$ \eta_{ij} \chi_i \chi_j \cos(\varphi_i - \varphi_j) \quad (4.19) $$

are evidently depleted by vortices, because they depend on the amplitudes of the wave functions. According to the mass spectrum, the smallest mass of any amplitude state is (4). The corresponding eigenvector reveals that this is an amplitude
Figure 4.8: Ground state, masses and eigen-modes of a frustrated three band superconductor. The x-axis gives the two parameters $\eta_{13} = \eta_{23}$ while the other parameters are $\alpha_1 = -3$, $\beta_1 = 3$, $\alpha_2 = -3$, $\beta_2 = 3$, $\alpha_3 = 2$, $\beta_3 = 0.5$, $\eta_{12} = 2.25$. At $\eta_{13} = \eta_c \approx -3.69$ there is a transition between $(1)$ and $U(1) \times Z_2$ symmetry.
mode that is dominated by $\chi_3$. Apparently the vortices in the third band are the ones with the largest core. Consequently, the terms that depend on $\chi_3$ are depleted more than other Josephson terms due to vortices. The effect of this is similar to changing $\eta_3$, which we already saw, caused a change of symmetry.

Fig. 4.9 shows this effect in a system with two interacting vortex clusters. The vortex cores are noticeably larger in the third band (c) than in the other two bands (a,b) as predicted by the mass spectrum analysis. Consequently, the interaction terms that depend on $\chi_3$ are significantly depleted in the vortex cluster, and so the arrangement $\varphi_1 = \varphi_2 = \varphi_3$ is no longer preferable. The decay of this phase difference mode is determined by the mass (6) of Fig. 4.8, which is very small. Consequently, the phase difference, displayed in (d-f) decays at a much longer length scale than the amplitude. This provides a mechanism for long range inter-cluster interactions in frustrated superconductors.

4.4 Vortex matter in frustrated three band superconductors with broken time reversal symmetry

In the region with broken time reversal symmetry there are two ground states, and these related to each other by complex conjugation. This gives rise to a new object in these systems: Domain walls that interpolate between the two vacua. Such domain walls cost energy however, and omitting thermal fluctuations, we should
Figure 4.10: A skyrmion with two flux quanta. The GL parameters are $\alpha_1 = 1$, $\alpha_2 = 1$, $\alpha_3 = -2.75$, $\beta_1 = 1$, $\beta_2 = 1$, $\beta_3 = 1$, $\eta_{ij} = -3$ and $\epsilon = 0.08$. The displayed quantities are (A) magnetic flux, (B) $\sin(\varphi_1 - \varphi_2)$, (C) $\sin(\varphi_1 - \varphi_3)$, (D) $\chi_1^2$, (E) $\chi_2^2$ and (F) $\chi_3^2$. (G) shows the inter-skyrmion interaction potential computed according to the scheme (H): One skyrmion [A] is placed in the center of the system, the other [B] is placed at a distance $R$ and at an angle $v$. The separation and angle is varied. The plot (G) shows the potential as a function of the placement of the soliton [B].

expect the system to fall into one of the two ground states, much like the Ising model at low temperature. In the presence of vortices, the situation is a bit more subtle however. At a domain wall, the phase arrangement is not optimal, and there are also gradients in the phase differences. Both these factors contribute to decreasing the amplitude of the wave function (i.e. locally depleting the density of cooper pairs). But the energy of vortices greatly depends on the wave function amplitudes, and so they tend to be trapped on domain walls.

Consider a three-band GL model with broken time reversal symmetry and a large penetration depth, so that inter-vortex interaction is repulsive. Denote the two vacua $\uparrow$ and $\downarrow$. Suppose that the state in most of the system is $\uparrow$, and that there is a 'bubble' in which the state $\downarrow$ is realized. Then, if there are vortices trapped to the domain wall, the repulsion between these vortices can prevent the domain wall from shrinking. This gives rise to a so called skyrmion. Fig. 4.10 shows such an object, and some of its properties. The soliton solution displayed in (A-F) was obtained using finite element energy minimization. The interaction plot (G) was obtained from a finite difference computation where the positions of the fractional vortices that constitute the skyrmions were fixed. The skyrmion solution
also reveals another interesting phenomena generic to these objects: Recall the discussion of Josephson strings in chapter (2). Generally, Josephson coupling binds fractional vortices and gives rise to linearly divergent energy as fractional vortices are separated. But on the domain wall, the phase arrangement is unfavorable and the Josephson coupling gives rise to repulsion between fractional vortices. This leads to fractionalization— that the fractional vortices of different bands do not superimpose.
Chapter 5

Conclusions

In the end of the second chapter, the topic of this thesis was formulated in the form of a set of questions:

1. What new types of inter-vortex interaction are possible in multi-band GL theory?
2. Under what conditions do they appear?
3. How does frustration and breakdown of the time reversal symmetry in the GL model affect vortex structure formation?
4. Are there novel multi-band phenomena that are immediately recognisable in experiments?

The results presented here, do a least offer a glimpse of the many-faced phenomena that arise in these models.

The standard argument for the Type-I/Type-II dichotomy as presented in for example [35] relies on the notion of domain walls between superconducting and normal flux-carrying regions. These domain walls possess either negative or positive energy, determining the magnetic response (and class) of the superconductor. In multi-band models, this picture is misleading, as these generally possess several types of interfaces. One band can be completely depleted in a region, while the other band features well defined single quanta vortices in that same region.

In MCGL it is more fruitful to classify systems according to vortex-interaction. Both Type-I and Type-II SC is possible in this class of models, but as a consequence of additional length scales, Type-1.5 SC with non-monotonic vortex interactions is also possible. This allows other structure formations than the Abrikosov lattice. One possibility is clusters of vortices, surrounded by vortex-less voids, but the vortex structure formation can also be influenced by multi-body forces, giving rise to for example elongated branch-like structures.

Another major difference between single- and multi-band GL models lies in the notion of what a ground state is. In single-band models this merely means that the
amplitude has attained some value, $|\psi|^2 = -\alpha/\beta$. In MCGL it generally also implies a particular arrangement of the phases. In these models there are mechanisms by which vortex matter can induce variations in the phase differences, and this can mediate vortex interaction at length scales given by the masses of these modes. A throughout understanding of vortex interactions in these models generally requires identifying if such mechanisms are present, and at what length scale the variation in phase differences decay.

Finally, we also touched the concept of metastable skyrmions, which consist of vortices trapped on a domain wall that interpolates between degenerate ground states in systems with $U(1) \times Z_2$ symmetry. These exist for a wide range of parameter values, and can potentially provide means for identifying broken time reversal symmetry in experiments.

In conclusion, MCGL models exhibit several phenomena and behaviours that fall outside of the Type-I/Type-II dichotomy of single band theory. When this project started in 2009, Magnesium diboride was the main candidate for multi-band phenomena. Since then, the list of such materials has grown significantly with the discovery of iron-based superconductors. At the same time, computer resources for simulations and other numerical techniques are more accessible than ever. Thus, there seems to be every opportunity for a continued exploration of vortex physics beyond Abrikosov’s standard picture.
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Part II

Scientific Papers
Paper I

Type-1.5 superconducting state from an intrinsic proximity effect in two-band superconductors

Egor Babaev, Johan Carlström and Martin Speight,
Paper II

Type-1.5 superconductivity in multi-band systems: Effects of interband couplings.

Johan Carlström, Egor Babaev, and Martin Speight,
Paper III

Semi-Meissner state and nonpairwise intervortex interactions in type-1.5 superconductors.
Johan Carlström, Julien Garaud, and Egor Babaev,
Paper IV

*Length scales, collective modes, and type-1.5 regimes in three-band superconductors*

Johan Carlström, Julien Garaud, and Egor Babaev,
Paper V

*Topological Solitons in Three-Band Superconductors with Broken Time Reversal Symmetry*

Julien Garaud, Johan Carlström, and Egor Babaev,