Freezing of the Flux Liquid in High Temperature Superconductors

A thesis submitted for the degree of Doctor of Philosophy of the Australian National University

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The work contained in this thesis is my own original research, produced in collaboration with my supervisor — Dr M. P. Das. Any material taken from other references is explicitly acknowledged as such.

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Abstract

The work presented in this thesis is concerned with examining the freezing transition of the magnetic flux lines, and the effect of this transition on the critical current. It is believed that in the region of low magnetic field the freezing line corresponds well with the so called irreversible line that appears in the $H$-$T$ phase diagram of the HTcS materials. This therefore provides a useful reference to compare the results of this approach.

Chapter 1 presents a general introduction to the phenomenon of superconductivity of both the conventional and high temperature superconductors. It is argued that many of the more important properties of the HTcS materials, such as the critical current, are heavily dependent on the interactions of the flux lines, and therefore the real world usefulness of these materials relies on a good understanding of their properties.

In Chapter 2 a brief review of the ideas that have been put forward to explain the nature of the irreversible line is presented. Predictions made by these theories are then briefly compared with the results of recent experiments. This leads to the proposal of the irreversible line representing a freezing of the flux liquid into a flux solid.

To examine the freezing transition, a relatively straightforward theory has been developed, known as density functional theory. The basis for this theory is presented in Chapter 3, and the formalism developed. The freezing of the flux lattice can then be calculated using a phenomenological form for the interaction potential of the flux lines. The results obtained for the freezing line enable a comparison between experiment and theory.

In Chapter 4 an attempt to better understand the interaction potential of the flux lines is considered via a simple two-layer model. Such a model enables a better understanding of the nature of the full 3D interaction. Having calculated the interaction potential, it is then possible to repeat the calculation of Chapter 3, replacing the original phenomenological potential. The results are again compared with both experiment and earlier results.

Having calculated the freezing line, the case of low magnetic field and $T$ close to $T_c$ is examined in Chapter 5. In this region the existence of a vortex gas is postulated.
The approximate location of this state in the phase diagram is calculated, and its consequences discussed in terms of experimentally measurable effects.

Finally, Chapter 6 examines the critical current by using a model of a granular superconductor. The Josephson current is calculated by finding the Green’s functions for the system in the absence of magnetic field, and then using these in a linear response theory, valid for small values of applied field. While this work has not yet been completed, preliminary results show that the calculated form of the critical current is consistent with previously published results.

The work in Chapter 3 has been published as,


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Honi soit qui mal y pense.
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Introduction

Successful research impedes further successful research.

Prior to 1911, it was believed that there was nothing special to be found in the behaviour of the conductivity of metals. Their resistance to the flow of electrical current was to be expected, even if it was not particularly appreciated. This all changed when a Dutch physicist called Heike Kamerlingh Onnes decided to use his knowledge of liquefying Helium to study materials at very low temperatures. He found (Onnes, 1911) that when mercury was cooled to around 4K it lost all electrical resistance. This loss of resistance was quite sudden, and happened over a very small range of temperature.

Since the discovery of this effect in mercury, it has been found that many elements and compounds also possess similar behaviour when their temperature is lowered sufficiently. Superconductivity is mainly associated with this rather dramatic loss of electrical resistance, although there are many other effects that these materials manifest, some of which are mentioned below. While this phenomenon was well known and categorised by experimentalists, it took nearly 45 years for a satisfactory theory to emerge — the famous Bardeen-Cooper-Schrieffer (BCS) theory of superconductivity (Bardeen et al., 1957).

Just when theorists thought they had an understanding of superconductivity, another discovery in 1986 by Bednorz and Müller (Bednorz and Müller, 1986) turned everything upside down. This was the discovery of the so called high temperature superconductors (HTcS). Before these compounds were found, it was believed by many that the highest critical temperature had already been reached, and that new compounds would only change this by a fraction of a degree. This is not to say that the search stopped. The goal of a higher critical temperature led to the study of many different, exotic materials such as metallic alloys, intermetallics, nitrides and carbides, in addition to the standard metallics. The breakthrough was finally made with the synthesis of the new oxide materials. These new materials, therefore, produced quite a shock when they were found to have critical temperatures of around 1...
35K, compared with the conventional materials of around 23K.

Once again, these materials are one step ahead of the theorists. While many more materials are being found with higher and higher critical temperatures, and many HTcS materials are finding their way into real world applications, there is still no complete theory for this phenomena. This chapter will provide a brief introduction to both experimentally measurable effects of superconductivity and provide a tour of the theories that have been used to model them. The chapter ends with a discussion of the motivation for this work. This is in no way intended to be a rigorous introduction to the subject, which can be found in almost any book on the subject (Rickayzen, 1965; de Gennes, 1966; Schrieffer, 1964; Tinkham, 1975; Cyrot and Pavuna, 1992).

1.1 Properties of the Superconducting State

Conventional superconductors appear in two forms, known as type-I and type-II. A major difference is that type-I materials allow no magnetic flux to enter the sample interior as long as the temperature is maintained below the critical temperature, $T_c$. All the magnetic flux is expelled until the applied magnetic field reaches the critical field, $H_c$, when superconductivity is destroyed and the material reverts to its normal state. This total exclusion of magnetic flux is called the Meissner-Ochsenfeld effect, and in this regime the material exhibits perfect conductivity. These materials tend to have quite low values of both critical temperature and critical field.

Type-II materials have two distinct critical fields. The lower critical field, $H_{c1}$, and the upper critical field, $H_{c2}$, which plays a role analogous to the critical field in type-I materials in that it denotes the field at which superconductivity is destroyed. For magnetic fields between these values, the field penetrates the sample as lines of magnetic flux parallel to the applied magnetic field. For magnetic fields between $H_{c1}$ and $H_{c2}$ perfect conductivity is lost, for reasons that are discussed later. Each magnetic flux line contains a magnetic field of size equal to the magnetic flux quantum, $\phi_0 = \hbar c/2e$. These flux lines have a mutual repulsion due to their magnetic fields, and have been shown to combine to form a lattice of flux lines inside the material, known as an Abrikosov lattice (Abrikosov, 1957). A schematic is shown in Figure 1.1. The phase diagram for a typical conventional superconductor is shown in Figure 1.2. All the HTcS materials are of type-II, and only this type will be considered throughout this thesis.

Most of the discussion given here will be concerned with the magnetic properties of the superconducting state. While its other properties are important, it is the effect of an external magnetic field on these materials that is of direct relevance to this thesis.
1.1. Properties of the Superconducting State

Figure 1.1: A schematic drawing of the Abrikosov lattice. The flux lines (tubes) can be seen to form an hexagonal lattice in the $x$–$y$ plane, where the magnetic field is applied parallel to the $z$-axis.

1.1.1 Measurable Quantities for Conventional Superconductors

There are quite a few interesting properties exhibited by materials when they become superconducting. A brief description of a few of these properties is given below, and many more can be found in the references:

- As mentioned above, the Meissner-Ochsenfeld effect enables the material to exhibit both zero resistance and perfect diamagnetism.

- When the specific heat is measured, it is found to exhibit a jump at the transition temperature. As the temperature is raised, the specific heat starts to increase quite sharply. As it approaches $T_c$, it starts to curve over, and undergoes a rapid drop down to the value of the normal material, whose behaviour it then continues to follow.

- Microwave and infrared experiments can be used to show the existence of an energy gap in the excitation spectrum. It can be shown that this energy gap decreases with increasing temperature, until it vanishes at the critical temperature. The physical reason for the energy gap is discussed below in relation to BCS theory.

- When the isotopic mass of a compound is changed, a corresponding change is also found in the transition temperature of many materials, such that as the isotopic mass is increased, the transition temperature decreases. This
Figure 1.2: Typical magnetic phase diagram for a conventional low temperature superconductor.

The relationship between isotopic mass and transition temperature helped to point the way to phonon mediated electron-electron attraction.

- The wavefunction of the electron pair appears to be a spin singlet.

- The materials are found to possess a London moment of value $-2m\omega/e$, where $\omega$ is the angular frequency of the rotating superconducting disc.

These are just a few of the strange properties possessed by these materials. As it can be seen, there is a remarkable diversity of effects that would need to be explained by a theory of superconductivity.

1.1.2 Measurable Quantities for HTcS

Several of the properties of HTcS are identical to those of their low temperature counterparts. The pairing of electrons has been measured in these materials, as has the magnetic flux quantum which is found to have the same value as for conventional superconductors. Electron tunnelling experiments have shown the existence of an energy gap for temperatures less than the critical temperature, although the value of this gap is larger than it is for the conventional materials. The temperature dependence of the magnetic penetration depth has been found to behave quantitatively the same, though its magnitude is found to be larger in the HTcS. Figure 1.3 shows the corresponding phase diagram for a typical HTcS.
1.1. Properties of the Superconducting State

So while there is some similarity between conventional and HTcS materials, many of the properties of the HTcS are anomalous. In addition, there are several properties that are very hard to explain in terms of the theories that were developed for the conventional superconductors, some of which are listed below:

- The observed values of the critical temperature are found to be very high — of the order of 150K compared with around 20K. This is hard to explain within the framework of the electron-phonon interaction of the BCS model.

- The coherence length is very small and anisotropic, with the component parallel to the copper oxide planes being larger than the perpendicular component. In addition to this anisotropy, the core of the flux lines are also much thinner in HTcS materials, so they are less likely to get caught at pinning centres present inside the material. These small values also increase the effect of fluctuations on the physical properties. In addition, the magnetic penetration depth is found to be much greater than the coherence length while possessing the same anisotropy.

- When measuring the resistance as a function of temperature, it is found not to exhibit as rapid a decrease at the transition temperature. Instead there is greater structure in the shape of the line. This structure is thought to arise from the effects of the flux lattice. As the temperature is changed, this lattice undergoes one or more phase changes, which are detectable in measurements of the resistance.
• When plotting out the phase diagram in the $H-T$ plane, it is found that a new line appears between the upper and lower critical temperatures. This line is called the melting line, and marks the division between the flux liquid and flux solid phases. Experimentally, this line marks a distinction between phases of reversible and irreversible magnetic behaviour.

These are just a few of the features that are hard to explain with the theories for conventional superconductors. It would seem that both types of superconductors still have several properties in common, and so any theory put forward to describe HTcS might be expected to possess similarities to those for conventional materials. However, it is expected that in the HTcS materials the physics of the flux line lattice becomes much more important. Many of the measurable features of these materials derive from the behaviour of the flux lines. Therefore it would appear that a knowledge of the physics of the flux lines is just as important as a microscopic description.

As a first approximation it would seem to make sense to first try to apply conventional theories to these new materials, and to "tweak" them where required. If this is the case, what then are the theories used to explain conventional superconductivity?

### 1.2 Phenomenological Theories

There were many theories originally put forward in an attempt to explain superconductivity. This is in no way intended to be a thorough list, but only those that can be considered to have had a major impact on the evolution of the field.

#### 1.2.1 Two-Fluid Model

One of the first attempts to examine superconductivity as a two-fluid model was made by Gorter and Casimir (Gorter and Casimir, 1934). Their idea was that as the superconducting transition was a second order phase change, an order parameter could be introduced whose value would decrease gradually with increasing temperature until it vanished for $T > T_c$. This order parameter could be thought of as measuring the fraction of material that is in the superconducting phase. To find the behaviour of the order parameter the following form for the free energy was postulated,

$$F(T) = x F_s(T) + (1 - x)^{1/2} F_n(T),$$

where $x$ plays the role of the order parameter. These terms are chosen so that $x(T)$ can be determined in terms of $F_n(T)$ and $F_s(T)$ from the equilibrium condition

$$\left( \frac{\partial F}{\partial x} \right)_T = 0.$$
1.2. Phenomenological Theories

This choice is equivalent to having the two phases mutually dependent. After minimizing, one finds that

\[ x(t) = 1 - t^4, \]

where \( t \) is the reduced temperature, \( t = T/T_c \). Even though their choice for the free energy had little physical justification, the expression for \( x(T) \) gave a very good description of the temperature dependence of the penetration depth when substituted as the electron density in the London model.

1.2.2 London Theory

One of the most comprehensive of the early theories was that proposed by F. London and H. London (London, 1950). Their idea was that the local magnetic field was the factor that controlled the supercurrent. The total current inside a superconductor is the sum of the supercurrent, \( j_s \), and the normal current, \( j_n \). The equations used to describe this system are,

\[
\nabla \times (\Lambda j_s) = -\frac{h}{c} \\
\frac{\partial}{\partial t} (\Lambda j_s) = e \\
j = j_n + j_s \\
j_n = \sigma e,
\]

where \( \rho \) is the electric charge density, \( \sigma \) the electrical conductivity and \( \Lambda \) is a parameter to be determined. In addition to these expressions, Maxwell's equations are also required. By combining all the above equations, several of the variables can be eliminated. If, in addition, it is assumed that there is charge neutrality, the static case reduces to

\[
\nabla^2 h = \left( \frac{4\pi}{\Lambda c^2} \right) h,
\]

with similar expressions for \( e \) and \( j \). It can also be shown that the London equations imply perfect conductivity. The last equation is very important, in that it shows the existence of a magnetic penetration depth,

\[
\lambda = c \sqrt{\frac{\Lambda}{4\pi}}.
\]

This implies that the magnetic field is not discontinuous across the surface of a superconductor, but instead decays exponentially with distance. These equations can be solved analytically for many different situations to give the behaviour of the magnetic field within the superconductor.

Another important prediction of the London theory is that of flux conservation. It shows that the total magnetic flux inside a type-I superconductor is zero. To
achieve this, shielding currents are produced within a skin of depth $\lambda$ around the
edge of the superconductor that produce a field equal and opposite to the applied
magnetic field. However, if the superconductor contained a hole of some sort, the
magnetic flux would be able to pass through this hole, but still not penetrate the
superconductor itself.

The final part of the London theory of interest is the London kernel. In London
theory there is a connection between the current density and the vector potential
of the applied magnetic field,

$$A(r) = -c\Lambda j_s(r),$$

which can be written in Fourier space as

$$j_s(q) = -\left(\frac{1}{c\Lambda}\right)A(q).$$

Using both this relation, and the Maxwell relation between magnetic field and cur­
rent density, the following expression can be derived,

$$j_s(q) = -\left(\frac{c}{4\pi}\right)K_L(q)A(q),$$

where $K_L(q)$ is the London kernel, and is given by

$$K_L(q) = \frac{4\pi}{\Lambda c^2}.$$  

It can be seen that this kernel is in fact $q$-independent. To introduce a dependency
on $q$ into this expression leads to an examination of the Pippard kernel, $K_P(q)$.

1.2.3 Pippard Theory

While the London theory gave a good general description of the superconductors,
there was experimental evidence of behaviour not explainable within the London
framework, such as the variation of $\lambda$ with orientation, and the effect of impurities.
Pippard introduced the concept of the “range of coherence” (Pippard, 1953) to
describe the long range interactions of the electrons in these materials, and from
this produced a set of nonlocal relations.

Pippard measured the effect of impurities on the penetration depth and found
that it decreased exponentially with increasing impurity concentration. From this,
Pippard wrote down, in analogy with the anomalous skin effect, the following non­
local relation,

$$j_s = -\frac{3}{4\pi c\xi_0\Lambda} \int dr \frac{r \cdot A}{r^4} \exp(-r/\xi).$$

In spherical coordinates it is possible to integrate this expression, and so derive an
expression for the Pippard kernel in Fourier space,

$$K_P(q) = \frac{3\xi}{2\xi_0\lambda^2 L(q\xi)^3} \left[ (1 + (q\xi)^2) \tan^{-1}(q\xi) - q\xi + \ldots \right].$$
1.2. Phenomenological Theories

If this form is compared with the London kernel, the following relations can be shown,
\[
\lambda = \lambda_L \left( \frac{\xi_0}{\xi} \right)^{1/2} \quad \xi^3 \ll \xi_0 \lambda_L^2
\]
\[
\lambda = \lambda_L \left( \frac{\xi_0}{(2\pi)^{1/3}} \right)^{1/3} \left( \frac{\xi_0}{\lambda_L} \right)^{1/3} \quad \xi^3 \gg \xi_0 \lambda_L^2.
\]
In addition, the following form for $\xi$ was found to agree well with experiment,
\[
\frac{1}{\xi(\ell)} = \frac{1}{\xi_0} + \frac{1}{\alpha \ell},
\]
where $\ell$ is the mean free path and $\alpha$ is a fitting parameter. This model was then able to account for most of the behaviour not described by the London theory. Thus Pippard introduced the idea that any perturbation would not be a local effect, but would instead have its influence extended over a region of thickness $\xi$. This coherence length, along with the nonlocal nature of the theory, were the most important concepts introduced by Pippard. There were still some effects that had not been explained satisfactorily, such as the temperature dependence of the penetration depth. One such theory that sought to do so was that developed by Ginzburg and Landau.

1.2.4 Ginzburg-Landau Theory (GL)

This theory derives from work done by Landau on examining second order phase transitions. The central idea being that when a substance undergoes a phase change, there is some physical property of the system that differs between the two phases. If it is possible to identify this property, it can then be used to study the transition. Landau theory studies the phase transition through the change in symmetry that occurs between the two phases. This loss of symmetry can be measured by introducing the idea of an order parameter, which is a measure of the departure of the new configuration from the original, higher symmetry phase. In addition to the order parameter, the Landau free energy is also defined, from which physical properties can then be derived. The Landau theory of phase transitions has since been applied to many problems, and its foundations and applications are studied in detail in the book by Tolédano and Tolédano (Tolédano and Tolédano, 1987) as well as the original work of Landau (Ginzburg and Landau, 1950; Landau, 1965). It is important to note that the theory is a phenomenological theory, in that it assumes the existence of a phase transition and a change in symmetry, and no attempt is made to explain the microscopic origin.

A good starting point is the definition of the Landau free energy functional, which is given by
\[
F_s = F_{n0} + \alpha |\psi|^2 + \frac{\beta}{2} |\psi|^4 + \frac{1}{2m^*} \left| \left( -i\hbar \nabla + e^* \frac{A}{c} \right) \psi \right|^2 + \frac{\hbar^2}{8\pi},
\]
where \( \psi \) is an order parameter and \( \alpha \) and \( \beta \) are unknown coefficients, with \( \alpha \) chosen to be temperature dependent. The term linear in \( \psi \) can be shown to be zero through symmetry arguments. Both \( e^* \) and \( m^* \) represent effective electron charge and effective mass respectively. This is done to take into account possible electron pairing or some other mechanism. This functional will be discussed in much more detail in a later chapter.

By minimising the total free energy with respect to both \( \psi^* \) and \( A \) the following set of equations are generated,

\[
\frac{1}{2m^*} \left( -i\hbar \nabla + \frac{e^*}{c} A \right)^2 \psi + \alpha \psi + \beta |\psi|^2 = 0
\]
\[
\frac{c}{4\pi} \nabla \times h = -\frac{e^*}{2m^*} \left( \psi^* \nabla \psi - \psi \nabla \psi^* \right) - \frac{(e^*)^2}{m^*c} |\psi|^2 A,
\]

along with the following boundary conditions\(^1\),

\[
\hat{n} \cdot \left( -i\hbar \nabla + \frac{e^*}{c} A \right) \psi = 0
\]
\[
\hat{n} \times (h - H) = 0,
\]

where \( H \) is a uniform external field. It is possible to solve these equations in certain geometries, and doing so yields two important length scales — the penetration depth and the coherence length. Expressions for these quantities are respectively

\[
\xi(T) = \left( \frac{\hbar^2}{2m^*\alpha'(T_c - T)} \right)^{1/2}
\]
\[
\lambda(T) = \left( \frac{m^*c^2\beta}{4\pi(e^*)^2\alpha'(T_c - T)} \right)^{1/2},
\]

where the temperature dependence of \( \alpha \) has been chosen to be of the form \( \alpha'(T - T_c) \).

From these expressions the temperature dependence of these quantities is clearly visible. These lengths can be combined to form a temperature independent scaleless quantity, the Ginzburg-Landau parameter,

\[
\kappa = \frac{\lambda(T)}{\xi(T)}.
\]

This parameter can be shown to differentiate between the two types of superconductors. For \( \kappa < 1/\sqrt{2} \) the equations describe a type-I material, whereas for \( \kappa > 1/\sqrt{2} \) they describe a type-II material.

\(^1\) The boundary conditions are dependent on the nature of the boundary, such that different expressions are derived for a metal-superconductor junction compared with, say, an insulator-superconductor junction. For more details on this the reader is referred to the original work of Landau (Ginzburg and Landau, 1950; Landau, 1965).
Finally, it should be noted that this theory also nicely describes the quantisation of magnetic flux. If the order parameter is written in the form

$$\psi = |\psi|e^{i\varphi},$$

then when this is substituted into equation (1.1) and integrated around a closed curve, Stokes' theorem can be used to show

$$\int dS \cdot \mathbf{h} + \frac{m^*c}{(e^*)^2} \oint d\mathbf{l} \cdot \mathbf{j} = \pm \frac{\hbar c}{e^*},$$

where the fundamental flux quantum is defined as

$$\phi_0 = \frac{\hbar c}{2e},$$

(1.2)

where it has been assumed that $e^* = 2e$.

The beauty of this approach lies in its simplicity, which should not be confused with its usefulness. Some of the power of GL theory has been mentioned above, and more can be found in the references. The application of GL theory to type-II superconductors is covered in considerably more detail in the book by Saint-James (Saint-James et al., 1969). The theory gives the ability to step back from the microscopic nature of the problem, and attempt to make predictions based on a more macroscopic viewpoint. This means that even though no microscopic theory may be available, an understanding of some of the underlying mechanisms can still be attained through this approach. It can be particularly useful in examining the behaviour of the flux lines, which would be a daunting task starting from a microscopic theory (Das, 1989).

A microscopic theory is still needed, however, to explain, for example, the origin of electron pairing. Such a theory is available for conventional superconductors, and is presented next.

### 1.3 Microscopic Theory

#### 1.3.1 Conventional Superconductors

All of the above ideas are phenomenological in one sense or another. They all tend to view the problem from a macroscopic point of view. An attempt is made to explain the observable effects, but no assumption is made about the underlying microscopic mechanism that causes superconductivity. GL theory introduced the concept of effective electron charge and mass, which helped to take into account these effects. However it was not until the emergence of the BCS theory that all the ideas came together in one microscopic theory of superconductivity.
1. Introduction

One of the precursors to the formulation of this theory was the discovery by Cooper (Cooper, 1956) that it was possible for the normal state to be unstable to a certain kind of electron pairing. It was shown that the binding energy for a single pair of electrons could, under certain conditions, include negative values. This effect can be shown to be due to an over-screening of the Coulomb repulsion by the ions. The model that was considered consisted of pairs of electrons possessing equal and opposite momenta and so lying on opposite sides of the Fermi surface. The Hamiltonian for this model is given by,

\[ H = \sum_k 2\varepsilon_k b_k^+ b_k + \sum_{k'k} V_{k'k} b_{k'}^+ b_k, \]

where

\[ V_{k'k} = \langle k', -k' | V | k, -k \rangle \]

is the interaction potential describing the scattering of particles from one state \((k^\uparrow, k^\downarrow)\) to another with different momentum \((k'^\uparrow, k'^\downarrow)\), and

\[ b_{k'}^+ = c_{k'}^\uparrow \quad \text{and} \quad b_k = c_{-k^\downarrow} c_{k^\uparrow}. \]

To find a solution to this Hamiltonian the following trial wavefunction was used,

\[ |\psi_0\rangle = \prod_k \frac{1 + g_k b_k^+}{(1 + |g_k|^2)^{1/2}} |0\rangle. \]

When this is substituted into the Hamiltonian, the following expression is minimised,

\[ \delta \langle \psi | H - \mu N | \psi \rangle = 0, \]

where \(N\) is the total number of particles. After performing the minimisation, one finds that the energy required to create a quasiparticle of momentum \(k\) is given by

\[ E_k^2 = (\varepsilon_k - \mu)^2 + \Delta_k^2, \]

with \(\Delta_k\) being the "energy gap" which satisfies the relation

\[ \Delta_k = -\sum_{k'} V_{kk'} \frac{\Delta_{k'}}{2E_{k'}}. \]

Two approximations are generally made to solve these equations. One is that \(\mu = 0\), and the other is

\[ V_{kk'} = \begin{cases} -V & \text{for } |\varepsilon_k| \text{ and } |\varepsilon_{k'}| < \omega_c \\ 0 & \text{otherwise.} \end{cases} \]

These enable a solution both for zero and finite temperature. The finite temperature formalism is similar to that at zero temperature, but with the appearance
of the Fermi distribution function. The energy gap can be found as a function of temperature from the temperature dependent version of the earlier definition

\[
\frac{1}{N(0)V} = \int_0^{\omega_c} \frac{d\epsilon}{(\epsilon^2 + \Delta_0^2)^{1/2}} \tanh \left[ \frac{\beta}{2} (\epsilon^2 + \Delta_0^2)^{1/2} \right].
\]

In the weak coupling limit, several predictions are made by BCS theory,

\[
\frac{2\Delta_0}{k_B T_c} = 2\pi e^{-\gamma} \approx 3.52
\]

\[
\frac{T_c C_n(T_c)}{\hbar^2(0)V} = \frac{e^{2\gamma}}{6\pi} \approx 0.168
\]

\[
H_c(T) \approx H_c(0) \left[ 1 - 1.06 \left( \frac{T}{T_c} \right)^2 \right] \quad T \to 0
\]

\[
H_c(T) \approx 1.74 H_c(0) \left( 1 - \frac{T}{T_c} \right) \quad T \to T_c
\]

\[
\frac{[C_s - C_n]}{C_n} \bigg|_{T_c} = \frac{12}{7\zeta(3)} \approx 1.43
\]

\[
T_c = 0.85 \Theta_D e^{-1/N(0)V}.
\]

These predictions were found to be in reasonable agreement with many of the materials that were known to be superconducting. However certain materials such as lead and mercury were found to be in disagreement. For more details on the agreement between theory and experiment the reader is referred to the book by Parks (Meservey and Schwartz, 1969).

BCS theory has since been rewritten in the language of field theory (Abrikosov et al., 1963). While this obviously changes none of the results, it does allow for a more concise formulation of the theory. It should also be noted that it has been shown (Gorkov, 1959) that close to \( T_c \) the BCS and GL theories are equivalent. This work helps relate the GL functions to the parameters that appear in the BCS equation, for example the order parameter can be rewritten as

\[
\psi(r) \equiv \left( \frac{7\zeta(3)}{8\pi^2(k_BT)^2} \right)^{1/2} \Delta(r),
\]

and the GL phenomenological parameters \( \alpha \) and \( \beta \) as

\[
\alpha = -\frac{6\pi^2(k_BT)^2}{7\zeta(3)c_p^0} \left( 1 - \frac{T}{T_c} \right), \quad \beta = \frac{6\pi^2(k_BT)^2}{7\zeta(3)c_p^0 n}.
\]

This new formulation has also been a stepping stone for further extensions to the theory. A set of integral equations were derived (Eliashberg, 1960) in an attempt to introduce a frequency dependence for the energy gap — to help produce a retarded interaction that was dependent on the phonon velocity. The theory of the electromagnetic properties was also given a sounder footing (Rickayzen, 1959; Bogoliubov, 1959). These are just a few examples, and much more work has been done.
1.3.2 High Temperature Superconductors

Unfortunately, as of yet this section remains quite short. There still is no complete theory for HTcS in the sense that BCS theory was a complete theory for the conventional superconductors. As mentioned above, due to the similarities of several of the effects exhibited by the two types of materials, it was hoped that some form of extension of the BCS theory could be used. Some of the questions that must be answered by any such theory are:

- Are phonons the mediators of the interaction between electrons, or do other effects need to be considered, such as spin or charge fluctuations, or a combination of these effects?

- How important is the crossover from 2D to 3D that is present in these materials? This statement requires a little elaboration on the structural peculiarity of the oxide superconductors. In these materials it is believed most of the current flow occurs within the Cu-O layers. These layers are separated from their neighbours by a distance that is dependent on the chemical composition of the material. These systems can therefore be considered as a stack of \( N \) coupled layers, which in the limiting case of zero interlayer coupling reduces to a two dimensional problem.

- Is this a singlet spin state, or a triplet? This is a very important question, and has sparked much interest, both theoretically and experimentally. As of yet there is still no consensus of opinion one way or the other.

- Are all the novel normal state properties predicted? It is important that not only the superconducting phase of these materials be explained, but any such theory put forward must also provide an adequate description of the normal state.

These are of course just a few of the problems facing the theorists. This thesis does not have the space to go into detail about the current theoretical ideas, which can be found in many of the books dedicated to these fascinating materials (Kamimura and Oshiyama, 1988; Tunstall and Barford, 1991; Gupta and Multani, 1993; Maekawa and Sato, 1992; Wilczek, 1991; Lynn and Allen, 1990; Ashkenazi et al., 1991; Bedell, 1990; Das and Mahanty, 1994; Anderson, 1995; Plakida, 1995). From now on, little mention will be given to these theories, since the main topic of this thesis is an examination of the physics of the flux lattice. This will be discussed with no assumption about how superconductivity originates, or how the flux lines are formed.
1.4 Critical Values and Flux Dynamics

While there has been a large amount of work carried out in studying both the conventional superconductors and the HTcS from both the microscopic and phenomenological point of view, as far as practical use of these materials is concerned only a few properties are important: the critical temperature, $T_c$, the upper critical field, $H_{c2}$, and the critical current, $J_c$. It is known that in conventional type-I materials, both the critical temperature and upper critical field are low, but the critical current is quite high. For conventional type-II and HTcS the critical current becomes a function of the temperature and the applied magnetic field. For the HTcS, which are the main topic of this thesis, this critical value is very small, even though both critical temperature and magnetic field can be very large. This "relation of the criticals" is shown in Figure 1.4. The low value of the critical current density greatly restricts the use of the HTcS materials. To understand why the current is so low one needs to understand the physics of the flux lattice present inside these materials. It is part of the beauty of superconductivity that so much can be studied even when a microscopic theory is unavailable. The physics of the flux lines is very important for these critical values, and can be studied by itself, without the need for a theory of how these flux lines are produced — extensive reviews of the role of the flux lines in the HTcS materials have recently been presented by Blatter et
al. (Blatter et al., 1994) and Brandt (Brandt, 1995). Neglecting questions about mechanism, the behaviour of the critical current can be studied from the viewpoint of the flux lattice, if it is assumed that it is this phenomenon which has the greatest effect on the current.

It is known that each magnetic flux carries one flux quantum of magnetic field. This flux line can be thought of as a tube of normal material with a radius approximately equal to the coherence length. Around this core the supercurrent circulates forming a magnetic sheath extending out to a radius given by the magnetic penetration depth (Caroli et al., 1964). This model for the flux line is quite simple to picture, and useful for making predictions from theory. The exact nature of the core is very difficult to describe due to the nonlocality of the theory. Throughout this work, this qualitative description will be used for the flux lines, and the exact nature of the core and other details will be neglected.

The reason the flux lattice tends to suppress the critical current is simple to understand. If the flux lines are in a material which is relatively free of any form of pinning centres, then they are free to move around under the influence of an external force. This movement of the flux lines, along with the dissipation caused by their movement, has been examined by several authors (Anderson and Kim, 1964) and more details will be given in the next chapter. When the current starts to flow, there is an interaction between the current and the magnetic field of the flux line. This $J \times B$ force tends to move the flux lines perpendicular to the direction of current flow, and therefore scatter the electrons, hence reducing the maximum current that can flow. If, however, the material contains a lot of defects, then the entire lattice tends to become pinned as the flux lines become trapped inside pinning centres. This enables a much higher current to flow and helps to explain why the flux lattice is so important as regards the critical current. It would seem that to have as large a critical current as possible requires that the material used be able to effectively pin the flux lattice. One problem is that due to the small core and large magnetic “sheath”, the flux lines in HTcS are much more flexible than their conventional counterparts. This means that the concept of the rigid Abrikosov lattice is not really applicable, instead it is a more softer lattice, as shown schematically in Figure 1.5. Unfortunately this added flexibility introduces many complications, due to a higher probability of processes such as vortex cutting or entanglement, which are discussed in a little more detail in the next chapter.

Another problem has to do with the irreversible line mentioned earlier. This line is thought to mark some form of melting transition of the flux lattice into a flux liquid. Below this transition, at low temperatures and magnetic fields, the flux lines form an Abrikosov lattice, as in conventional superconductors, and the more effectively this is pinned, the higher the current. However, above this line the flux lattice melts into a flux liquid. The flux liquid is, by its very nature, much harder to pin, and so the current decreases quite drastically in this region. Therefore, to
1.5 Motivation of this Thesis

This thesis is therefore involved with the study of the flux liquid within a HTcS material. Most specifically it is concerned with examining the irreversible line. It is important to note that opinion is divided as to what the irreversible line actually represents. In the present author's opinion, this does represent some form of melting of the flux lattice, as it is hoped the following work will show. So as not to bias anyone's point of view, Chapter 2 is a brief review of the most recent theoretical ideas put forward to explain the origin of the irreversible line.

In Chapter 3 a density functional calculation is presented. This calculation uses a first principle approach to the examination of the melting/freezing transition. Using this method, the freezing point can be found as a function of both magnetic field and temperature and plotted out on the phase diagram to be compared with experiment. This is a first principle examination, requiring no free parameters to "fit the data."

In Chapter 4 a simple two-layer superconductor is examined from the viewpoint of Ginzburg-Landau theory of phase transitions. The nonlinear system is solved numerically to find both the inter and intralayer coupling between vortices. Also discussed briefly is the Berezinskii-Kosterlitz-Thouless transition, and its relation

Figure 1.5: In HTcS the flux lines are much more flexible, giving rise to a softer form of the Abrikosov lattice.

explain the behaviour of the current, an understanding of the irreversible line is required.
to the irreversible line.

In Chapter 5 the low density phase of the vortex liquid is studied. The existence of the vortex gas is postulated, and its position in the $H-T$ phase diagram calculated.

In Chapter 6 the critical current is examined in terms of the Josephson effect. A simple model of a granular superconductor is used, with each grain being considered as an island of superconductor in a sea of normal material. The grains are Josephson coupled, and this intergrain current is what determines $J_c$. Using the Gorkov formalism both the Green's function and anomalous Green's function are calculated, and then used to study the linear response of the system.

Finally, the conclusion attempts to bring all the information together to form a coherent picture about the irreversible line, and to suggest further work that should be carried out in this area.
The magnetic phase diagram for a conventional type-II superconductor has several important features, many of which were discussed in the last chapter. It was shown that a new feature appeared in the magnetic phase diagram of the HTcS materials. This new line is known as the irreversible line. Its name derives from the fact that on the lower side of this line, the magnetic behaviour of the material is reversible, but above the line it becomes irreversible. The effect is thought to be due to the melting of the Abrikosov lattice into a flux liquid. This melting transition can take place more easily in the HTcS materials due to the higher temperatures that are available for measurements. The transition is of great interest, as the critical current for a material is highly dependent on the state of the flux lines. If the Abrikosov lattice does undergo a melting transition, then the flux liquid will correspond to a lower $J_c$, due to stronger scattering. The following is a brief review of the current theories used to describe the nature of the irreversible line, starting with the early theory of flux creep of Anderson and Kim, and progressing to the newer theories put forward by Brandt, Nelson, Malozemoff and Fisher et al.

2.1 Anderson-Kim Flux Creep

For the flux lattice to be able to melt, it must be able to break away from any pinning centres, due to dislocations, vacancies, etc. To break free from the pinning centre, the flux line needs to overcome the potential barrier, which in the HTcS materials is possible due to the relatively high temperatures involved. Thermal activation also occurs in conventional superconductors, but due to the relatively low values of $T_c$ the effect is less pronounced. One of the first theories to exam-

\footnote{In the case of low magnetic field the melting line and the irreversible line are in very close proximity to each other. Therefore melting is sometimes considered as the cause of the irreversible line.}
ine this phenomenon for the conventional superconductors is due to Anderson and Kim (Anderson and Kim, 1964). The main idea behind their paper is to examine the thermal activation of flux lines past pinning centres. The pinning centres are used as a source for the potential barrier, and their exact nature was not important.

Their model consisted of a superconductor under a magnetic field, $H$, applied perpendicular to the material, and carrying a bulk current $J = (c/4\pi)\nabla \times H$. It can be seen that due to the presence of the current in the material, the density of the flux lines will be nonuniform. Because of the mutual repulsion of the flux lines, one can think of there being a magnetic pressure exerted by the flux lines on one another. This pressure is related to the magnetic energy per unit volume, $H^2/8\pi$. If there were no pinning sites, then this pressure would act so as to make the density of the flux lines uniform, which would then lead to $J = 0$. An assumption made in their derivation is that the internal and external magnetic fields are equal, i.e. $B = H$, which is valid for all but low fields.

To begin to calculate the rate of this thermally activated motion, knowledge of the driving force of the flux lines, due to the magnetic pressure, and of the nature of the potential barriers is required. The interaction energy between flux lines was calculated by Abrikosov (Abrikosov, 1957), and was written as

$$F_{\text{int}} = \left(\frac{1}{8\pi}\right) \mathbf{H} \cdot (\mathbf{H} - \delta^2 \nabla^2 \mathbf{H})$$

$$= \frac{H^2}{4\kappa^2} \sum_{i,j} K_0 \left(\frac{|r_i - r_j|}{\lambda}\right), \quad (2.1)$$

where $\kappa$ is the Ginzburg-Landau parameter defined in the last chapter and $K_0$ is a Bessel function. In most of the conventional superconductors the distance $|r_i - r_j|$ is usually less than $\lambda$, $\delta^2 \nabla^2 H$ is small, so the expression for free energy is simply given by the magnetic energy. This means that the force on the flux lines is just the Lorentz force, i.e. $\nabla F = J \times H/c$. The force per flux line per unit length is then just $J \times \phi_0/c$, where $\phi_0$ is given by equation (1.2).

Examining the long range behaviour of equation (2.1), i.e. $r \to \infty$, it can be seen that $K_0 \sim e^{-r/\lambda}$. Due to the long range nature of the interaction, perturbations of the flux density on a local scale are energetically unfavourable. Thus an irregular arrangement of flux lines is only allowable on a scale greater than $\lambda$, causing local variations to be spread out over a region of radius greater than $\lambda$. This means that although the pinning centres act on individual flux lines, for a line to escape the pinning centre it cannot move alone. Instead it must take a small bundle of surrounding flux lines, of radius $\lambda$, along with it. Therefore it is the force of the whole bundle of flux lines that act against the potential barrier. Because of the form of $K_0$ for small $r$, even though the flux bundles must have a uniform local density, the bundles are able to slide past one another quite easily, and need not have a regular geometrical structure.
To find the free energy of one of these bundles, a starting point is the Lorentz force equation shown above, which for a bundle containing \( n_b \) flux lines is given by

\[ J_0 n_b l/c, \]

where \( l \) is an effective interaction length, and can be taken as the distance between pinning centres. As a function of the bundle position the free energy can be written as

\[ F_{\text{force}} = \frac{J H \lambda^2 l \xi}{c}. \]

Taking the size of the potential barrier to be approximately \( \xi_0 \), then its energy scales as \( (H_0^2/8\pi)\xi_0^2 \). Assuming only a fraction \( p \) of this pinning force is acting, then the total barrier energy can be written as

\[ F_b = \left( \frac{p H_0^2 \xi_0^2}{8\pi} \right) - \left( \frac{J H \lambda^2 l \xi_0}{c} \right). \quad (2.2) \]

The rate of barrier penetration per second can then be written as

\[ R = \omega_0 e^{-F_b/k_BT}. \quad (2.3) \]

To find the rate of diffusion of flux density \( |B| \), the rate at which flux enters and leaves a small volume is required. This is given by

\[ \frac{d|B|}{dt} = -\nabla \cdot \left( \frac{\phi_0 R}{\lambda} \right), \quad (2.4) \]

where \( \nabla \) is a two dimensional gradient and \( R \) is the vector, whose magnitude is given by \( (2.3) \), in the direction of the gradient of magnetic pressure,

\[ \alpha = \nabla p = \nabla \left( \frac{H^2}{8\pi} \right) = J \times \frac{H}{c}. \quad (2.5) \]

However this simple idea will not be valid near the critical fields \( H_{c1} \) and \( H_{c2} \). Near the lower critical field the flux lines will have a separation greater than \( \lambda \), and as \( n_b \to 1 \) it would be expected that the force would become equal to that on a single flux line. Near the upper critical field, the flux lines are forced very close together, and under these conditions it is probable that the bundle idea may no longer remain valid, and that core interactions would be expected to become important. It is also suggested that the flux lattice may become rigid, and so the bundles would be unable to slip past one another.

Equation (2.4) can be used to derive both the critical current curve and the creep rate equation. The critical current is derived by assuming that the critical parameters are those for which the creep rate becomes immeasurably slow. If this rate is denoted by \( R_c \), then,

\[ k_BT \ln \left( \frac{R_c}{\omega_0} \right) = -(F_b)_{\text{crit}}, \]
or

\[ \alpha_{\text{crit}} = \frac{(JH)_{\text{crit}}}{c} = \frac{pH_0^2}{8\pi} \frac{c_0^2}{\lambda^2 l} + \frac{k_B T}{\lambda^2 l} \xi_0 \ln \left( \frac{R_c}{\omega_0} \right). \] (2.6)

To keep the derivation clear, redefine \( F_0 = pH_0^2 c_0^2 / 8\pi \) so that

\[ \alpha_{\text{crit}}(0) = \frac{F_0(0)}{\xi_0 \lambda^2 l}, \]

which is the critical magnetic force at \( T = 0 \). This means that the value of \( \alpha \) giving the minimum detectable creep can be defined as

\[ \frac{\alpha_{\text{crit}}(T)}{\alpha(0)} = \frac{F_0(T)}{F_0(0)} - \frac{k_B T}{F_0(0)} \ln \left( \frac{v_0}{v_{\text{min}}} \right), \] (2.7)

where \( v \) is the flux creep velocity. This is simply equation (2.6) written in a slightly different form, where it can be seen that the creep rate depends exponentially on \( \alpha \).

So from above, we have

\[ v = v_0 e^{\alpha/\alpha_1}, \]

with

\[ \alpha = \frac{JH}{c} = \frac{1}{4\pi} \frac{dH}{dr} \sim \frac{d}{dr} \left( \frac{H^2}{8\pi} \right), \]

where use has been made of

\[ J_\theta = \frac{c}{4\pi} \frac{dH}{dr} \]

and

\[ \alpha_1 = \frac{k_B T}{F_0(0)} \alpha_c(0). \]

If the derivation is restricted to one dimension, as in the flux line wall, one can write

\[ \frac{\partial \alpha}{\partial t} = \frac{H^2}{4\pi} v_0 \frac{\partial^2}{\partial x^2} e^{\alpha/\alpha_1}. \] (2.8)

It should be noted that the spatial derivatives of \( H \) have been neglected compared to those of \( v \). This is because the exponential dependence of \( v \) on the derivatives of \( H \) are of the order of \( \alpha_c(0)/\alpha_1 \) which is \( \sim 300 \) times larger than the direct dependence.

It is possible to solve equation (2.8) for \( \alpha \), giving

\[ \alpha = f(x) - \alpha_1 \ln t, \]

where \( f(x) \) is an unspecified function of distance. Using that fact that the creep rate is unobservably slow unless \( \alpha \sim \alpha_c \), then \( f(x) \sim \alpha_c \), so that

\[ \alpha = \alpha_c - \alpha_1 \ln t, \] (2.9)

showing the logarithmic dependence of the creep rate on time. It was this logarithmic dependence on time of the magnetisation that was initially measured for
2.2 Giant Flux Creep

2.2.1 Giant Flux Creep

Malozemoff used an idea based on the Anderson-Kim model, to try to describe the form of the irreversible line in HTcS. From experiments it is seen that the irreversible line can be characterised in the $H-T$ plane close to $T_c$ by $H \propto (1-t)^{3/2}$, where $t = T/T_c$. The work was motivated by the experiments of Worthington et al. (Worthington et al., 1987), who were able to measure a logarithmic dependence on time for the magnetisation of a YBCO sample. This dependence then suggested a flux creep picture, based on random pinning sites in the crystal. The model was based on equation (2.10), where $r$ was taken as half the sample dimension, with $H \parallel c$. They also derived a similar expression for a slab geometry,

$$\frac{dM}{dt} = \left( \frac{r J_c}{3c} \right) \left( \frac{k_B T}{U} \right),$$

(2.10)

where $U$ represents the pinning potential of the material. It is this equation that Malozemoff and Yeshurun (Yeshurun and Malozemoff, 1988) made use of in their giant flux creep model described below.

One important question to ask is how applicable this idea is to HTcS? The Anderson-Kim model of flux creep considers the flux line to be rigid along the $c$-axis, and so the system becomes basically 2D in nature. An obvious question is what would happen if the flux lines are allowed to be more flexible, giving the system a more 3D nature? By having the ability to flex, it is conceivable that the effect of the pinning centres could be altered. These types of effect are considered in more detail by the work of Brandt and Nelson discussed later.
et al., 1987), and in the geometry chosen, \( r > a \). This means that \( dM/d\ln t \) is larger for \( H \parallel c \), in agreement with experiment. Since a higher \( J_c \) corresponds to greater pinning, it is expected that this will lead to a weaker relaxation. But in the critical state model, a larger \( J_c \) corresponds to a larger flux gradient, and hence an increase in the rate of flux jumping.

To carry the calculation further, the following phenomenological forms were assumed. First, \( J_c = J_c(0)(1 - t)^n \), where the typical range in \( n \) is 1 to \( 5/2 \), and secondly \( U_0 \propto (1 - t)^{1/2} \). This means that the important quantity \( J_c/U_0 \propto (1 - t)^m \), where \( m = n - \frac{1}{2} \). These were then substituted into equations (2.10) and (2.11), and fitted to the experimental data. It is found that the best fit corresponds to \( m = 2 \) with \( U_0 = 0.6 \text{ eV} \) for \( H \parallel c \), and \( U_0 = 0.1 \text{ eV} \) for \( H \perp c \). It was mentioned that due to the fact that \( U_{0,||} > U_{0,\perp} \), twin boundaries will play an important role as pinning centres for \( H \parallel c \). The values found for \( U_0 \) are to be treated with “factor-of-two” accuracy, although their values seem reasonable if you consider the following argument. In the original Anderson-Kim model, the pinning potential was said to scale as \( H_c^2 \xi^3/8\pi \). If this is transferred over to the new superconductors, then one would expect \( \xi^3 = \xi_0^3 \xi_c \), and using published values for these coherence lengths one gets \( U_0 \approx 0.15 \text{ eV} \), which is consistent with the previously quoted values.

The calculation to parameterise the irreversible line starts with the following expression for the critical current density (Campbell and Everts, 1972),

\[
J_c = J_{c0} \left[ 1 - \left( \frac{k_B T}{U_0} \right) \ln \left( \frac{Bd\Omega}{E_c} \right) \right],
\]

where \( J_{c0} \) is the critical current density in the absence of thermal activation, \( d \) is the distance between pinning centres, \( B \) is the magnetic induction, \( \Omega \) is some oscillation frequency of a pinned flux line and \( E_c \) is a minimum measurement voltage per meter. For a conventional type-II superconductor, the logarithm term is small, and so the thermal activation contribution is negligible. But for the new HTcS, the term is a much larger correction, and should be taken into account. For this equation to be useful, a knowledge of the temperature dependence of \( U_0 \) is required. Malozemoff adopted a general scaling approach to obtain an order of magnitude estimate. To this end, it was considered that \( T \approx T_c \) and that the applied field was small, enabling the Anderson-Kim form for the pinning potential to be used. This is combined with the following Ginzburg-Landau expressions,

\[
H_c = 1.73 H_{c0} (1 - t)
\]

\[
\xi = 0.74 \xi_0 (1 - t)^{-1/2}.
\]

Substituting these expressions into the expression for \( U_0 \) gives,

\[
U_0 = \frac{1.21}{8\pi} H_{c0}^2 \xi_0^3 (1 - t)^{1/2}.
\]
2.3. Collective Pinning

When the flux lattice spacing becomes less than the penetration depth, then pinning due to collective effects becomes important. Assume for simplicity that this happens for $a_0 = f\xi$, where $a_0$ is the lattice spacing and is given by $a_0 = 1.075(\phi_0 / B)^{1/2}$. This means that for a field above that given by $a_0$, the potential is limited in the plane by $a_0$ and along the c-axis by $\xi$, so that $U_0$ is expected to scale as $H_c^2 a_0^2 \xi / 8\pi f^2$.

One can then substitute for both $H_c$ and $a_0$ to finally arrive at

$$U_0 = 2.56 \frac{H_c^2 a_0^2 \xi}{8\pi f^2 B} (1 - t)^{3/2}.$$ 

Using this expression for $U_0$ in equation (2.12), the condition for the critical current to vanish is

$$1 - t = \left( \frac{8\pi f^2 B k_B T_c \ln(B d_B / E_c)}{2.56 H_c^2 a_0^2 \xi} \right)^{2/3},$$

which reduces to

$$B \propto (1 - t)^{3/2},$$

as required. Thus it can be seen that by using as simple a model as flux creep, the main characteristics of the irreversible line can be derived.

One must suppose that similar arguments to before also remain valid in this case. This result draws heavily on the work of Anderson and Kim, along with other standard results for the conventional type-II superconductors. At some point in the phase diagram for the HTcS, a changeover from 2D to 3D behaviour is expected. This means that the 3D nature of the system will dominate part of the phase diagram. How accurately an inherently 2D theory can explain this region is open to question.

2.3 Collective Pinning

An idea similar to that of Anderson-Kim is one put forward by Larkin and Ovchinnikov (Larkin and Ovchinnikov, 1979). This is based on the phenomenon of collective flux creep. This occurs when the pinning in the system is weak, which leads to collective pinning. The early work on this idea was directed towards conventional superconductors, but has been extended to include the new HTcS (Feigel'man et al., 1989). The basic idea is that the flux lines do not jump between pinning sites individually, rather they jump in groups of several flux lines, and sometimes as a collection of such groups. The experimentally accessible predictions produced by this theory are similar to those produced from the vortex glass theory, which is discussed in more detail below.

It has been shown (Larkin and Ovchinnikov, 1979) that if a flux lattice is subjected to a random array of pinning sites, and the pinning force is short range, i.e. of the form

$$\langle U_{\text{pin}}(u, r) U_{\text{pin}}(u', r') \rangle = K(|u - u'|, |r - r'|),$$
where the function $K(x, y)$ decreases rapidly for $x, y > r_p$, with $r_p$ being some characteristic length of the system, then the long range order of the lattice breaks down beyond a certain distance, often denoted as $L_p$. It was also shown that the critical current was dependent upon both $R_c$ and $L_c$, pinning lengths along the $ab$ and $c$ direction respectively. A basis for this idea is in examining the current dependence of the pinning potential, that is, $U(J)$. The simplest case is for $B \sim H_{c1}$, with an isotropic medium where the elastic constants have approximately the same value, $C_{11} \sim C_{44} \sim C_{66} \sim C$, where $C_{11}$, $C_{44}$ and $C_{66}$ are the bulk, shear and tilt elasticity modulus respectively. Assuming also that $J \sim J_c$, the distance that a flux bundle hops is $u_{hop} \sim \xi$, giving $U_c \sim C(\xi / R_c)^2 V_c$, where $V_c = L_c R_c^2$.

A more interesting case is when $H \gg H_{c1}$, still for $J \sim J_c$. In this situation $C_{11} = C_{44} \gg C_{66}$, so shear and tilt deformations dominate $J_c$. It is shown (Feigel’man et al., 1989) that in this case

$$U_c \sim C_{66} \left( \frac{\xi}{R_c} \right)^2 R_c L_c^2.$$  

It is also shown that using $L_c \approx R_c(C_{44}/C_{66})^{1/2}$ and $R_c \approx C_{44}^{1/2} C_{66}^{3/2} \xi^2 / W$, this reduces to

$$U_c \sim C_{66}^{3/2} C_{11}^{3/2} \xi^4 W,$$

where

$$W = \int dr \left[ \frac{\partial K(u, r)}{\partial u^2} \right]_{u=\xi},$$

and $K(u, r)$ is the function defined earlier.

If this is compared with the earlier expression, it can be seen, upon substituting for $R_c$ and $L_c$, that the two expressions differ only by a factor of $(C_{11}/C_{66})^{1/2}$. The explanation for this difference is that in the second case, the flux jumps in the form of a bundle of approximately $(C_{11}/C_{66})^{1/2}$ subbundles of volume $V_c$. Due to the relatively large value of $C_{11}$, the flux lines prefer to jump in flux groups, and individual subbundle jumping is energetically unfavourable.

An interesting question arises when one considers $J \ll J_c$. Under this condition, the hopping distance of a bundle will be much larger than for $J \sim J_c$, and can be estimated as

$$J B u_{hop}(J) \sim C_{66} \frac{u_{hop}^2}{R_1^2(J)}$$  \hspace{1cm} (2.14)

where $R_1^2$ is the bundle size in the plane perpendicular to both the applied field and the hopping vector. This arises from the definition of $J_c$ (Larkin and Ovchinnikov, 1979).

It can also be shown that the fluctuations in a system of random pinning sites increase like

$$u(R) = \langle |u(r) - u(r + R)|^2 \rangle^{1/2} \propto R^\xi.$$  \hspace{1cm} (2.15)
2.3. Collective Pinning

This expression is also thought to be adequate to describe the relation between hopping distance and bundle size. Upon substituting equation (2.15) into equation (2.14), one finds the following relationships,

\[ u(J) \propto J^{-\zeta/(2-\zeta)} \]
\[ R_{\perp}(J) \propto J^{-1/(2-\zeta)} \]
\[ R_{\parallel} \approx L \approx (C_{11}/C_{66})^{1/2} R_{\perp} \]
\[ U(J) \propto J^{-\alpha}, \tag{2.16} \]

where \( \alpha = (d - 2 + 2\zeta)/(2 - \zeta) \) and \( d \) is the space dimension. The exponent \( \zeta \) has been calculated elsewhere (Halpin-Healy, 1989; Ioffe and Vinokur, 1987), and the details of the calculation can be found in the references. The expression for this exponent is

\[ \zeta_{d,n} = 2 \frac{(4 - d)}{(8 + n)} \tag{2.17} \]

where \( n \) corresponds to the dimensionality of the vector \( u(r) \) and \( d \) is the spatial dimension. One important assumption that is made in the calculation of this parameter is that \( \Delta E_{pin} \) is independent of the elastic module, but dependent on the volume involved.

If the applied magnetic field is small, then \( R_c \) becomes smaller than the lattice spacing \( a \). Under these conditions, the flux jumps as individual flux lines. This is the same mechanism found in the conventional superconductors. In this case the length scale is governed by \( L_c \), which is independent of the applied magnetic field. The case of collective line pinning occurs when \( \xi < L_c < a \). In this region it was shown that \( J_c \sim J_0 (\xi/L_c)^2 \) and \( U_c \sim H_c^2 \xi^3 (\xi/L_c) \), where \( J_0 \sim H_c/\lambda \).

For the region

\[ J_c > J > J_1 \sim J_c (L_c/a)^{2-\zeta_1} = J_c (L_c/a)^{7/5}, \]

the flux bundle becomes a section of flux line of length \( L_c < L < a \) with the value \( d = 1 \) substituted into equations (2.16) and (2.17). This gives the following expression for the potential,

\[ U(J) = U_c \left( \frac{J_c}{J} \right)^{(2\zeta_1 - 1)/(2 - \zeta_1,2)} \approx U_c \left( \frac{J_c}{J} \right)^{1/7}. \tag{2.18} \]

This expression can then be used to find the current density dependence by making use of (Geshkenbein and Larkin, 1989)

\[ U(J(t_{obs})) = T \ln \left( \frac{t_{obs}}{t_0} \right). \]
Using this, one obtains
\[ J(t) \approx J_c \left( \frac{U_c}{T \ln(t/t_0)} \right)^7. \] (2.19)

When \( J < J_1 \), the average flux line length \( L \approx a \). The fluctuation of a flux line in this region can be written as
\[ u = (|u(r) - u(r + R)|^2)^{1/2} \approx \xi^{1-2\xi^2} u_{LO}^{2\xi^2} = \xi^{3/5} u_{LO}^{2/5}, \]
with \( u_{LO} \) being given by the following expression, for \( u < \xi \),
\[ u_{LO}(R, L) \approx \xi \left( \frac{a}{L_c} \right)^{3/2} \left[ \left( \frac{R^2 + a^2 L^2}{\lambda} \right)^{1/2} + \ln \left( 1 + \frac{R^4 + a^2 L^2}{a^4} \right) \right]^{1/2}. \]

For the case where \( J_1 > J > J_2 = J_1 (a/\lambda)^2 \), flux creep occurs in bundles of approximate size \( \lambda \) in the ab plane. This regions suffers strong dispersion in the C's, as mentioned previously. In this case one can write
\[ U(J) \sim C_{66} \frac{u^2(J)}{R_1^2(J) R_\perp(J) L(J)} \sim U_1 \left( \frac{J}{J} \right), \] (2.20)
where
\[ U_1 \approx U_c \left( \frac{a}{L_c} \right)^{1/5}. \]

Finally for \( J < J_2 \), the bundle size is larger than the penetration depth, and there is no dispersion of the C's. From this one obtains,
\[ U(J) \sim U_2 \left( \frac{J}{J} \right)^{(2\xi^2+1)/(2-\xi^2)} \approx U_2 \left( \frac{J}{J} \right)^{7/9} \]
\[ U_2 \approx U_1 \left( \frac{\lambda}{a} \right)^3 \] (2.21)
\[ J(t) \approx J_2 \left( \frac{U_2}{T \ln(t/t_0)} \right)^{9/7}. \]

This expression is similar to that found in equation (2.16).

It can be seen that the above description is for the isotropic case only. The results show a strong dependence of the creep rate on the current density when \( J \ll J_c \). The above expressions show that as both time and temperature increase, then the current density, \( J(t) \), decreases rapidly.

2.4 Thermal Fluctuations and Flux Cutting

Theories like those by Anderson and Kim are inherently two dimensional in nature. The interaction between the vortex lines is considered as two dimensional,
2.4. Thermal Fluctuations and Flux Cutting

and vortex line self interaction is neglected. These types of theories obviously lack some of the important physics arising from the full three dimensional behaviour. Many processes that are thought unlikely in 2D become important in 3D, and can radically alter the behaviour of the flux lattice, for example see (Brandt, 1991). It is argued by Brandt that in the 3D case, flux lines are able to cross, cut through each other, and then reconnect. This is possible because if the two vortices are tilted as they approach one another, then their mutual interaction length is shorter. As they approach, the lines become more distorted, so that the cutting can occur at a large angle, and so minimise the magnetic repulsion. The expression for two rigid flux lines, at a separation \(d\) and an angle \(\alpha\), has the following form in 3D,

\[ F_{\text{int}}(d, \alpha) = \frac{\phi_0^2}{2\mu_0 \lambda \sin \alpha} \left[ \cos \alpha e^{-d/\alpha} - \frac{1}{\sqrt{2\pi}} e^{-d\sqrt{2}/\xi} \right]. \]

This expression is derived from the 3D Ginzburg-Landau energy functional (Brandt et al., 1979). It can easily be seen that this remains finite even for \(d = 0\). The barrier to flux line cutting is further reduced by the nonzero value of \(\xi\) and the curvature of approaching lines. For the 2D case, the corresponding expression for vortices of length \(L\) is given by

\[ F_{\text{int}}(d, 0) = \frac{\phi_0^2}{2\pi \mu_0 \lambda^2} \left[ K_0(d/\lambda) - K_0(d\sqrt{2}/\xi) \right]. \]

This differs from the 3D energy in that as \(\xi \to 0\), the energy diverges for \(d \to 0\), so that in 2D the flux lines are not able to cut. This helps to emphasise the point that there are many significant differences between assuming a 3D structure for the system, and assuming a 2D one. So if the system is considered to be a true 3D system, then the effect of this flux line cutting must be taken into effect, along with its consequences for the meaning of the irreversible line.

It is also believed that thermal fluctuations are important for an understanding of the irreversible line (Brandt, 1989). The melting of the flux lattice can be estimated from Lindemann’s criterion (Lindemann, 1910), which states that a lattice will melt when the root-mean-square vibrations \(~ 0.1a\), where \(a\) is the lattice spacing. To examine this effect, one must consider a nonlocal elastic theory.

The elastic energy of the eigenmodes of the lattice are given by

\[ \frac{1}{2} u_\alpha(k) \phi_{\alpha\beta}(k) u_\beta(k), \]

where \(\phi_{\alpha\beta}(k)\) are the elastic matrix elements of the lattice and \(u_\alpha(k)\) are the displacements. From this it can be seen that

\[ \langle u_\alpha(k) u_\beta(k) \rangle = k_B T \phi^{-1}_{\alpha\beta}(k), \]

and for \(V \to \infty\) this gives

\[ \langle u^2 \rangle = k_B T \int \frac{dk}{8\pi^3} \left[ \phi_{xx}^{-1}(k) + \phi_{yy}^{-1}(k) \right], \tag{2.22} \]
where \( k_z \) extends to \( \pm \infty \) and \( k_\perp \) extends from \( 0 \) to \( k_{BZ} \). The elastic matrix elements can be derived, but it is more convenient to use its continuum approximation

\[
\phi_{\alpha\beta}^{\text{cont}}(k) = k_\alpha k_\beta [C_{11}(k) - C_{66}] + \delta_{\alpha\beta} \left[ k_\perp^2 C_{66} + k_\parallel^2 C_{44}(k) \right],
\]

(2.23)

where

\[
C_{11}(k) = \hat{c} \left( 1 + \frac{k_\perp^2}{k_h^2} \right)^{-1} \left( 1 + \frac{k_\parallel^2}{k_\parallel^2} \right)^{-1} + C_{66}
\]

\[
C_{66} \approx \hat{c} (1 - b)^2 (8\pi k^2)^{-1} c_1 c_2
\]

\[
C_{44}(k) = \hat{c} \left[ \left( 1 + \frac{k_\perp^2}{k_h^2} \right)^{-1} + \frac{k_\parallel^2}{k_{BZ}^2} \right],
\]

with \( \hat{c} = \frac{B^2}{\mu_0} \approx \hat{C}_{44}, \ k_\parallel^2 = 2k_\perp^2k_h^2 \). These expressions become exact if \( k \ll k_{BZ} \).

The constants \( c_1 \) and \( c_2 \) can be approximated by \( 1 \). The expression (2.23) is then substituted into equation (2.22) to give

\[
\langle u^2 \rangle = \frac{k_B T}{2\pi^2} \int_0^{k_{BZ}} dk_\perp \int_0^{k_{BZ}} dk_z C_{66} k_\perp^2 \left( \frac{\hat{C}_{44} k_\parallel^2}{k_{BZ}^2} + k_\perp^2 + k_\parallel^2 \right)^{-1},
\]

(2.24)

plus an additional term with \( C_{66} \to C_{11}(k) \). The integration over \( k_z \) has been cut off at \( k_{BZ} \) by the constant term of \( C_{44}(k) \) in equation (2.23). The integral in equation (2.24) can be approximated by

\[
\langle u^2 \rangle \approx \langle u^2 \rangle_{\text{loc}} \left[ \frac{2 k_{BZ}^2}{\pi k_h^2} \left( \frac{C_{66}}{\hat{C}_{44}} \right)^{1/2} + \left( 1 + \frac{k_{BZ}^2}{4k_h^2} \right)^{1/2} \right]
\]

\[
\approx \langle u^2 \rangle_{\text{loc}} \left[ \left( \frac{2bc k_\parallel^2}{\pi^2} \right)^{1/2} + \left( 1 + \frac{bc^2/2}{1-b} \right)^{1/2} \right].
\]

(2.25)

The second term in this expression, \( \langle u^2 \rangle_{\text{nl}} \), is larger than \( \langle u^2 \rangle_{\text{loc}} \) by a factor of \( k_{BZ}^2/2k_h \). The major contributor to this nonlocal term is from \( k_\perp \leq k_{BZ} \), where one can write \( C_{44}(k) \approx \hat{C}_{44} k_\parallel^2/k_\perp^2 \). This shows that \( \langle u^2 \rangle \) is increased by the softening of the flux line lattice with respect to periodic tilt waves, whose momentum vector \( k \) is perpendicular to the flux lattice. If this is considered as the main term, then Lindemann’s criteria, \( \langle u^2 \rangle_{\text{nl}} = c^2 a^2 \), gives a melting temperature of

\[
T_m = 2k_B^{-1} c^2 a^2 n^{-1} k_h \left( C_{66} \hat{C}_{44} \right)^{1/2}
\]

\[
\approx T_m^* (1 - b)^{3/2} b^{-1/2} \frac{\lambda(0)}{\lambda(T_m)},
\]

(2.26)

where

\[
T_m^* = \left( \frac{2}{3} \right)^{1/2} \frac{c^2 \phi_0}{\mu_0 k_B \lambda(0) \kappa},
\]
2.5. Vortex Entanglement

along with \( b = \frac{B}{B_{c2}(T_m)} \). As a rough guide to the value of \( T_m \), for \( c = 0.1 \), \( \lambda(0) = 2500 \, \text{Å} \) and \( \kappa = 200 \), then \( T_m = 40 \, \text{K} \).

The value of \( T_m^* \) will be reduced in magnitude if the correct expression for the elastic matrix is used. Another effect which acts to change the melting temperature is plastic deformations which act to soften the lattice. This arises through the movement of screw dislocations through the lattice. If the lattice experiences strong pinning, then this will increase \( T_m^* \). So when examining the melting transition through thermal fluctuations, an accurate value of \( T_m^* \) will only arise after all the effects on the lattice are considered. It is important to note that the calculation based on the Lindemann criteria makes use of the values of the \( C \)'s. However, close to the melting temperature an anharmonic approximation no longer remains valid, and so the accuracy of the Lindemann calculation is open to question.

2.5 Vortex Entanglement

The idea of flux cutting is similar to the studies by Nelson (Nelson, 1988; Nelson, 1993). In his work he considers the entanglement of the flux lines. His ideas are based on the fact that due to the elevated temperatures in the new superconductors, flux lines are more able to move about inside a material, in contrast to the generally imagined rigid flux lattice.

Because the HTcS have \( \lambda \gg \xi \), they can be studied in the local London limit. The starting point for this is to examine the Gibbs free energy,

\[
G = \left[ \epsilon_1 - \frac{H\phi_0}{4\pi} \right] NL + \frac{\phi_0^2}{8\pi^2\lambda^2} \sum_{i<j} \int_0^L dz K_0(r_{ij}(z)/\lambda) + \frac{1}{2} \epsilon_1 \sum_{i=1}^N \int_0^L dz \left[ \frac{dr_i(z)}{dz} \right]^2,
\]

where \( L \) is the sample length, \( r_i(z) = (x_i(z), y_i(z)) \) where \( i = 1, \ldots, N \), \( r_{ij} = r_i - r_j \), \( \epsilon_1 \) is the flux line self energy per unit length and \( K_0(x) \) is the usual modified Bessel function. The calculation close to \( H_{c1} \) is then achieved by balancing the first two terms. The third term is set to zero, as at this field it is assumed that the flux lines form a lattice with constant density. This leads to the following for \( H \gtrsim H_{c1} \),

\[
B = \frac{2\phi_0}{\sqrt{3}\lambda^2} \left\{ \ln \left[ \frac{3\Phi_0}{4\pi\lambda^2(H-H_{c1})} \right] \right\}^{-2}.
\]

This expression will be altered by collisions, as the flux lines move through the sample. If a full treatment of this were to be attempted, it would require integrating the potential in equation (2.27) in the form \( \exp(-G/k_B T) \) for all trajectories \( \{r_i(z)\} \). It has been shown (Coppersmith et al., 1982) that the effect of collisions is to reduce the entropy by a factor \( k_B \ln q \), where \( q > 1 \), relative to the noninteracting system. It can be shown that the total number of collisions is of the order \( (L/l)N = \).
2. A Review of the Present Status of Flux Lattice Melting

\((LA)n^2k_BT/\epsilon_1\), with \(A\) being the cross sectional area. So that the Gibbs free energy per unit volume, when statistically averaged, becomes

\[
g(n) = g_0 + \left(\epsilon_1 - \frac{H\phi_0}{4\pi}\right)n + \frac{3\phi_0^2}{8\pi^2\lambda^2}nK_0(d/\lambda) + (k_BT)^2n^2\ln\frac{q}{\epsilon_1}, \tag{2.29}
\]

where \(g_0\) is a constant. If this expression is then minimised with respect to \(n\), then for small \(n\),

\[
B \approx c \left(\frac{\epsilon_1\phi_0^2}{(k_BT)^2}\right)(H - H_{c1}),
\]

with \(c\) being a geometrical constant. This constant can be estimated from a more careful treatment of the partition function.

If the boundary conditions in the \(z\) direction are assumed periodic, then the partition function can be written as

\[
Z = \sum_{N=0}^{\infty} \frac{1}{N!} \sum_P \int_{r_1(0)}^{P[n(0)]} dr_1(z) \cdots \int_{r_N(0)}^{P[n(0)]} dr_N(z) e^{-G/k_BT}, \tag{2.30}
\]

where there are sums both over \(N\) and \(P\), the permutations.

The form of the partition function is analogous to the Feynman path integral for the grand canonical partition function for a system of two dimensional interacting bosons (Feynman and Hibbs, 1965). Upon comparison, it can be shown that \(\epsilon_1\) maps onto the boson mass, \(k_BT\) maps to \(\hbar\), \(L\) maps to \(\beta\hbar\) in the imaginary time direction and the chemical potential is given by \(\mu = H\phi_0/4\pi - \epsilon_1\).

In the limit \(L \rightarrow \infty\), the problem is solved by finding the ground state of the interacting bosons. An approximate condition for the flux lattice to melt is for the vortex separation to exceed \(\lambda\). To calculate the field \(H_x\), below which the lattice melts, equation (2.28) is assumed to hold. The lattice spacing will equal the interaction range when \(B = \phi_0/\lambda^2\), giving

\[
H_x - H_{c1} \approx \left(\frac{3\phi_0}{4\pi\lambda}\right)\exp(-2^{1/2}/3^{1/4}).
\]

Combining this with the standard result, \(H_{c1} = \phi_0(\ln \kappa)/4\pi\lambda^2\), it was found that

\[
\frac{H_x - H_{c1}}{H_{c1}} = \left(\frac{3}{\ln \kappa}\right)\exp(-2^{1/2}/3^{1/4}) = 0.22,
\]

for \(\kappa = 100\). The chemical potential of the 2D Bose gas can be related to the particle density, and when the results are translated back to the superconducting system one finds

\[
B \approx \left[\frac{\epsilon_1\phi_0^2}{16\pi^2(k_BT)^2}\right](H - H_{c1}) \ln \left[\frac{\epsilon_1\phi_0\lambda^2}{(4\pi k_BT)^2(H - H_{c1})}\right]. \tag{2.31}
\]
2.5. Vortex Entanglement

The logarithmic term appears due to the ability of the flux lines to slide past one another, rather than colliding. It can also be seen that in comparison with the earlier expression, the value of the geometrical constant is given by \( c = 1/16\pi^2 \).

For the case when \( L < \infty \), interesting effects start to appear. For small \( L \) one has a "disentangled flux liquid", where the flux lines do not meander significantly as they move through the sample. An increase in \( L \), in the 2D Bose case, produces a probability of particles exchanging places, which transfers to the superconducting state as an entanglement of the flux lines. This effect has recently been observed in numerical solutions of the time dependent Ginzburg-Landau equations (Machida and Kaburaki, 1995). There is a critical length at which the lattice will change from disentangled to entangled, and this can be related to a critical density of flux lines. It can be shown that the critical density satisfies the following inequality,

\[
\lambda \lesssim n^{-1/2} \lesssim \left( \frac{32\pi^3 k_B T L}{\phi_0 \ln \kappa} \right)^{1/2} \lambda.
\]

This means that the phase diagram would pick up two extra phases, as shown in Figure 2.1. Phase A corresponds to an entangled flux liquid, and phase B to a disentangled flux liquid. The temperature where the phase changes from A to B is given by \( T_{ab} = \phi_0^2 (\ln \kappa)/32\pi^3 k_B \). For \( L \to \infty \), phase B disappears, and phase A becomes separated from the lattice phase by the dotted line.

In phase A, if there are pinning sites then one would expect flux flow to be suppressed. This is due to the fact that if one flux line is pinned, others will become tangled around it, leading to a reduced flux flow. In phase B, this entanglement
does not occur, and so the flux flow would be greater. If pinning were very strong, then both phases would be destroyed.

2.6 Vortex Glass Phase

In a paper published by Fisher et al. (Fisher et al., 1991), a new phase of the HTcS was considered, and was christened the vortex glass phase. The name derives from an analogy with the spin-glass phase of certain magnetic systems. When the lattice experiences random pinning, it was shown (Larkin and Ovchinnikov, 1979) that the long range order of the lattice is unstable for a dimensionality less than 4. Further, it is argued that this instability can give rise to a new phase, where there is a long range phase coherence beyond which the lattice correlations are destroyed. It can be shown in 2D that the “glass transition” temperature, $T_{vg}$, is zero, but that the effects of this new phase on the nonlinear $I-V$ characteristics are experimentally measurable.

If the length scale where pinning disorder is effective is denoted as $L_p$, then on length scales larger than this, the lattice description for the flux lines is not valid. In this new phase, the flux lines are considered to be frozen in place, which leads to a vanishing resistivity in the glass phase. Even though the flux lines are frozen into a random pattern, the pair wavefunction still possesses long range order. In the gauge $\nabla \cdot A = 0$, the correlation function that measures the long range order is given in terms of the pair wavefunction by,

\[
G_{vg}(r) = |\langle \phi^*(r')\phi(r' + r) \rangle|^2.
\]

This order is not directly measurable, but indirect measurements via electromagnetic response are possible, and are discussed below.

The phase transition can be examined by using general scaling arguments. The correlation length is assumed to diverge as $\xi_{vg} \sim |T - T_{vg}|^{-\nu}$, and the relaxation time as $\tau \sim \xi_{vg}^2 \sim |T - T_{vg}|^{-2\nu}$. This time is an approximate measure of the time taken for a fluctuation of size $\xi_{vg}$ to relax. For temperatures just above $T_{vg}$, the correlation length is very large, but it can be disrupted by the motion of vortex lines due to even a small current density, $J$. So near $T_{vg}$, the nonlinear resistivity is very sensitive to $J$. As a measure of this disruption, define a current density $J_{nl}$ as the current at which $\rho(J_{nl}) = 2\rho_l$, for $T > T_{vg}$. The result obtained by Fisher et al. was that this current scaled as the inverse square of the correlation length, $J_{nl} \sim \xi_{vg}^{-2} \sim (T - T_{vg})^{-2\nu}$. Experimental results have put $\nu \approx 2$. It is this prediction of the change in $J_{nl}$ that is in contrast to the thermal activation theories. These theories tend to predict no significant change in $J_{nl}$ over a range of temperatures.

This idea can also be used to predict the dependence of the electric field on the current density. For $T \geq T_{vg}$, and normalising the dissipation with respect to the
linear resistivity,
\[ \frac{\rho(J)}{\rho_l} \equiv \frac{E}{J \rho_l} \approx \mathcal{R}_+ \left( \frac{J}{J_{nl}} \right), \]
where \( \mathcal{R}_+(j) \) is a universal scaling function such that \( \mathcal{R}_+(j \to 0) = 1 \). Using the definition of \( J_{nl} \) from above, it can be seen that \( \mathcal{R}_+(1) = 2 \). As the temperature is lowered toward \( T_{vg} \), both \( \rho(J)/\rho_l \) and \( J/J_{nl} \) diverge. In order for \( E \) and \( \rho(J) \) to remain finite requires that \( \mathcal{R}_+(j) \sim j^{(v-1)/2} \) for large \( j \). At \( T_{vg} \), the power law relationship between voltage and current can be written in \( D \)-dimensions as
\[
\rho(J) \sim J^{(v-1)/(D-1)}
\]
\[ E \sim J^{(v+1)/(D-1)}. \]
(2.32)
For currents larger than \( J_{nl} \), the conductivity in 3D is given by the above, and tends to Ohmic behaviour at low currents for \( T > T_{vg} \), and exponentially small dissipation at low currents for \( T < T_{vg} \).

In the Meissner phase, no flux lines enter the sample. However for nonzero temperatures, fluctuations can appear. These fluctuations take the form of closed flux loops. If there is no applied current, the flux loop will tend to shrink, due to the line tension and curvature. However, if a current flows through the loop, the Magnus force that is produced may balance the line tension. For a loop of radius \( R \) in the plane perpendicular to the current, the free energy is given by
\[
F_{\text{loop}} \approx 2\pi R \epsilon_1 - J \frac{\phi_0}{c} \pi R^2,
\]
where \( \epsilon_1 \) is the flux line self energy per unit length. The radius at which the free energy is a maximum is given by \( R_c = \frac{\epsilon_1}{J \phi_0} \), resulting in a barrier height of \( \pi \epsilon_1^2 / J \phi_0 \). Loops with radii greater than \( R_c \) will tend to grow under the action of the current. The growth of the loop produces dissipation related to the probability of producing the flux loops, which behaves like the Boltzmann probability distribution. This means that the resistivity for small \( J \) is given by
\[
\rho = \frac{E}{J} \sim e^{-J_T/J},
\]
(2.34)
where \( J_T \approx \pi \epsilon_1^2 / \phi_0 T \). This indicates that even in the Meissner state, dissipation is present, but vanishes exponentially with \( J \).

The explanation of this effect for conventional superconductors is as follows. Before the flux line loops can be created, there is an energy barrier that must be crossed. This barrier becomes of the order \( k_B T \) for \( J = J_c \). This means that equation (2.34) is valid only for \( J > J_c \), and if \( J > J_c \), then the vortices are produced, and dissipation sets in. For the conventional superconductors, \( J_c \ll J_T \) except near the critical temperature, so loop production is very rare. This leads to
2. Review of the Present Status of Flux Lattice Melting

Figure 2.2: Plots of $E$ vs. $J$ for (a) conventional superconductors, where the dashed line represents the extrapolation of activation effects, and (b) the new HTcS.

...a very abrupt transition at $T_c$, as shown in Figure 2.2. The HTcS materials have $J_c \approx J_T$, and thermal fluctuations play a much greater role, tending to smooth out the $I-V$ curves. In anisotropic materials, the loops become more elliptical in shape and are associated with a current of the form $J_T \approx \pi c(\epsilon_{1\perp}\epsilon_{1z})/\phi_0T$, as would be expected for the anisotropic superconductors.

The vortex glass phase is therefore quite similar to the Meissner phase. Both phases have zero resistivity in the limit of $J \to 0$. In the Meissner phase, as the bulk current is increased, dissipation due to thermally activated flux creep becomes important. This has the same form for $E/J$ as for the vortex glass phase, as shown earlier. The vortex glass phase suffers dissipation from the creation of flux line loops.

2.7 What the Experiments Say

Having given a brief review of some of the theoretical ideas, it seems prudent to mention what the experiments indicate. Presented below is a brief review of some of the common experimental techniques, with a summary of what they each have to say about the irreversible line. Due to the vast literature on this subject, only one reference will be supplied for each type discussed. More recent experiments can be found in the appropriate section of (Wyder, 1994).

2.7.1 Decoration Experiments

It is possible to examine the magnetic flux structure at the surface of a HTcS sample using the Bitter pattern technique (Durán et al., 1995). The superconducting sample to be investigated is first cooled and placed in a magnetic field, then magnetic
“smoke” is blown over it. These small magnetic particles attach themselves to the surface of the sample, and preferentially decorate the regions of magnetic field. Once on the sample surface, the particles remain firmly fixed, and the sample can then be reheated, and the surface viewed in a scanning electron microscope.

When these samples are viewed at low temperatures it is found that a hexagonal flux lattice is clearly visible. However, when the experiment is repeated for higher temperatures it is found that this distinct lattice disappears. There are several explanations for this: one is that the structure of the flux lines is finer than the experimental resolution, or that a different type of state, with no visible correlations, is being measured. A flux liquid transition would certainly fit in with the results of this type of experiment. The explanation being that at the higher temperature, the experiment is actually attempting to pattern a liquid state, which would account for their null result. The main drawback with this type of experiment is that only the surface of the sample can be viewed. No clue is given as to what is happening deeper into the material, where it is expected that most of the interesting effects occur. A recent experiment (Yao et al., 1994) has been reported, whereby both surfaces were examined simultaneously using this method. The results show that the number of flux lines on both sides of the sample are not necessarily equal. This result is discussed further in Chapter 4.

2.7.2 Mechanical Measurements

A method that can be used to directly probe a melting of the flux lattice is that of the oscillating reed (Gammel et al., 1988). The idea behind the experiment is to attach a superconducting sample to a small silicon oscillator, in the presence of a magnetic field. The oscillator is set vibrating at its resonant frequency with the amplitude of the vibration being kept quite small. Small changes in the vibration frequency are then measured as a function of temperature for a fixed field. The flux liquid state can be identified by its small effect on the frequency, due to the rapid relaxation of the flux lines. In contrast, the lattice phase will have a much slower relaxation, and consequently produces larger frequency shifts.

This technique can then be used to directly probe the melting transition. It is seen that the melting temperature lies well below the critical temperature. While nothing is said about a possible mechanism, it is possible to plot out the experimental melting temperature on the $H-T$ diagram which can then be compared with theoretical predictions.

2.7.3 Resistivity vs. Temperature

When the resistance of a HTcS is measured as a function of temperature in an external magnetic field it is no longer found to exhibit such a rapid decrease at the
onset of superconductivity, rather the field acts so as to smooth out the transition. This has the side effect of making the determination of $T_c$ more difficult.

If this dependency is examined in more detail, several distinct phases can be seen (Palstra et al., 1988; Kwok et al., 1994a). Close to $T_c$ the resistance is seen to initially undergo a rapid drop, but the rate of decline then decreases. For low temperature the drop is seen to be approximately exponential. All of this has the effect of producing a "bump" in the resistivity for intermediate temperatures. So as the temperature is increased from zero, the resistance starts to increase until a certain temperature is reached, at which point it then increases at a slower rate. This slow increase continues until $T$ is close to $T_c$, at which point the resistance increases rapidly to its value in the normal state. So it would appear that at intermediate temperatures some change is taking place inside the material — possibly the melting transition or some form of flux creep.

2.7.4 Small Angle Neutron Scattering (SANS)

While SANS experiments have been performed on HTcS materials (Kleiman et al., 1992) it is worth mentioning a recent experiment has been carried out using SANS on single crystal Niobium (Lynn et al., 1994). This type of experiment produces very clear images of the Abrikosov lattice, which was found to be present for all temperatures. The data showed no evidence of a first order phase transition that could be associated with a melting transition. What is measured is a transverse broadening of the peaks, which is associated with a crossing of the irreversible line — although the lattice symmetry is still visible. This phase is dubbed a correlated flux liquid.

It is believed that the results do not point to a simple melting transition, but rather indicate a more complicated behaviour. It is speculated that as the temperature is slowly increased, the lattice passes through an intermediate orientationally disordered phase before entering the correlated flux liquid phase.

The application of these ideas from measurements on single crystal Niobium to the more complicated oxide materials might be considered questionable. More SANS measurements would really be needed on the HTcS before any conclusions could be drawn, but this is complicated by the higher temperatures involved.

2.7.5 Lorentz Microscopy

The last experiment to be mentioned is Lorentz Microscopy. This method produces images similar to those from Bitter patterns. The important difference in this technique is the possibility of observing the motion of the flux lines in real time (Harada et al., 1992). The method is based on bombarding a superconducting sample with a coherent electron beam. The sample is tilted at 45° and placed in a
magnetic field. The electrons are given enough energy to pass through the sample while still maintaining beam collimation. When they strike the sample, some electrons are affected by the field of the flux lines, so that when the Lorentz micrograph is produced, the flux lines are visible as small bumps on the sample surface. By varying the temperature it has been possible to observe effects such as flux creep, and the hopping of flux lines between pinning centres. However as the temperature is increased, due to the corresponding increase in the penetration depth, the vortices start to become smeared out and difficult to observe.

It would seem that if the resolution can be improved sufficiently, this technique will be one of the most effective methods of observing any melting transition in real time. It will hopefully at least be able to narrow down the possible theoretical ideas that have been presented in this chapter.

2.8 Summary

There is still quite a lot of interest in the origin of the irreversible line. The fact that it is considered as a marker for the melting of the flux line lattice is still a point of contention. While most ideas are based on this assumption, there are still some who doubt that this phase transition takes place. It has been shown by Malozemoff, that using a simple idea such as Anderson-Kim flux creep, one is able to generate the field dependence of the irreversible line. However, these ideas are inherently of a 2D nature, and their applicability to the case of HTcS are questionable.

The work done by Brandt and Nelson is quite similar in what it attempts to describe. Both consider a very complicated system, where the flux lines are able to flex and cut. This is very different to the case of conventional superconductors, where the flux lines are considered to be rigid along the c-axis. This idea strikes one as intuitively obvious, as in a full 3D system there is no reason for the lines to be rigid. The ability of lines to deform has quite dramatic effects on the physics of the system, and also the phase diagram. The work by Nelson explicitly predicts two new regions on the $B-T$ diagram, as shown in Figure 2.1. It should then be possible for these two regions to be verified experimentally.

The vortex glass model proposed by Fisher et al. is another idea that predicts a new phase for the HTcS. This idea is based on the spin glass phases of magnetic materials. It predicts another kind of long range order, beyond the Larkin-Ovchinnikov critical length. They use the idea of critical scaling to examine the effect of this new phase. It is found that the glass phase is very similar to the Meissner phase in the way that it behaves, in that both phases have zero resistivity in the limit that the bulk current density tends to zero.

All the above ideas make solid predictions, and quite remarkably are in good agreement with whatever experiment they have set out to reproduce. The prob-
lem with good, unambiguous experimental data is still an issue, and needs to be addressed. Once there is reliable, single crystal results, then it may be possible to perform a better comparison with experimental results. As it stands, all the current ideas are equally believable, and there is no real reason, other than personal preference, to favour one over the other.
CHAPTER 3

Density Functional Approach to Freezing

Having reviewed the current ideas on the origin of the irreversibility line, it is apparent that the idea of the flux lattice undergoing a melting transition is a possible explanation. Therefore, what is needed is a theory that is able in some way to describe such a transition. One such theory is that developed by Ramakrishnan and Yussouff (Ramakrishnan and Yussouff, 1979). In this method, a set of functionals that are dependent on the density are derived from the basis of statistical mechanics. This idea has been formulated into quite a powerful theory, called density functional theory. In this chapter it will be shown that this idea is also applicable to this new state of matter — the flux liquid.

The density functional method provides a convenient framework to examine the melting of the flux lattice. It is known that in the liquid phase, there are no long range correlations between particles, and so the calculation is simplified if it is performed in this phase, and the subsequent freezing transition examined. This is due in part to the solid phase, that the liquid freezes into, being a well characterised state. Generally, the distinction between melting and freezing is a semantic one, but in the case of HTcS this difference is real, as the symmetry between the two phases is broken by magnetic hysteresis. Physically, the difference arises due to the following effect: when the flux liquid freezes into a solid, this transition is quite abrupt, as large volumes of the liquid freeze simultaneously. However, when the temperature is raised, small volumes of the solid melt separately, and so the melting transition is less distinct. This behaviour has been very nicely measured by Kwok et al. (Kwok et al., 1994b) If the corresponding calculation, i.e. starting from the solid and melting into the liquid, were to be carried out, this effect should be observed.

This chapter will introduce the ideas of density functional theory, and apply them to the freezing of the flux lattice. The freezing line will be calculated as a function of temperature and applied magnetic field, and plotted out on the $H-T$ phase diagram for comparison with the experimentally measured irreversible line for two different HTcS materials.
3. Density Functional Approach to Freezing

3.1 Density Functional Theory

3.1.1 The Functional

The idea of density functional theory (DFT), as can be gathered from its title, is the use of a functional. To precipitate the use of these functionals, a few of their properties will be described. A functional can be written in the form

\[ F[\rho] = \int dr \, f(\rho(r)), \]

where it is said that \( F \) is a functional of \( \rho \). This functional depends on the value taken by \( \rho \) at each point in space, and so can be thought of as a function of a continuously infinite set of variables. The Taylor series of a functional is defined as

\[ F[\rho(r)] = F[\rho_0(r)] + \int dr \frac{\delta F}{\delta \rho(r)} (\rho(r) - \rho_0(r)) \]
\[ + \frac{1}{2} \int dr dr' \frac{\delta^2 F}{\delta \rho(r) \delta \rho(r')} (\rho(r) - \rho_0(r))(\rho(r') - \rho_0(r')) \]
\[ + \cdots, \]

where \( \rho_0 \) is some homogeneous density, usually taken to be the liquid density when examining the melting transition. Also, because a local functional is the sum of the contributions from each point in space, the functional derivative with respect to density at the point \( r \) depends only on the density at that point, and not on the entire functional, such that

\[ \frac{\delta F}{\delta \rho(r)} = f'(\rho(r)), \]

where

\[ f'(\rho(r)) = \frac{df}{d\rho} \]

is the conventional derivative of the function \( f(\rho) \) with respect to its argument. For systems that are nonlocal, there is an equivalent set of expressions that can be written down, based on adding a small perturbation to the local density,

\[ \rho(r) = \rho_0(r) + \delta \rho(r). \]

This form for the density is substituted into the nonlocal form for the functional,

\[ F[\rho] = \int dr \, dr' \, \omega(r, r') \rho(r)\rho(r'), \]

where \( \omega \) is the equivalent nonlocal function, and analogous expressions can be derived. So having briefly reviewed the basic idea of the functional, a start can be made on DFT itself.
3.1. Density Functional Theory

3.1.2 Basis of DFT

The theory as presented here will follow the work of Evans (Evans, 1979). Other excellent reviews of this material can be found in the references (Henderson, 1992; McDonald, 1989). To examine the phase transition, an order parameter is identified, which for melting can conveniently be taken as the finite \( k \) Fourier coefficient of the density. The phase transition is identified as the point where the condition \( \Omega_{\text{solid}} = \Omega_{\text{liquid}} \) holds, with \( \Omega \) being the grand potential. For a system like a solid, an energy functional based on statistical mechanics is required. The form of this energy functional is to be found by requiring that the energy of the system be a minimum. With statistical mechanics as the starting point, the following expression for the Hamiltonian can be written down,

\[
H = T + U + V
\]

\[
T = \sum_{i=1}^{N} \frac{p_i^2}{2m}
\]

\[
U = U(r_1, r_2, \ldots, r_N)
\]

\[
V = \sum_{i=1}^{N} V_{\text{ext}}(r_i),
\]

with \( T \) being the kinetic energy, \( U \) being the interaction of the particles between themselves and \( V \) being the interaction of the particles with an external potential. From this starting point, the following functional can be defined

\[
\Omega[f] = \text{tr}_{\text{cl}} f(H - \mu N + \frac{1}{\beta} \ln f),
\]

where \( \text{tr}_{\text{cl}} \) is the classical trace in the grand canonical ensemble, and is defined as

\[
\text{tr}_{\text{cl}} = \sum_{N=0}^{\infty} \frac{1}{N!} \int dr_1 \cdots dr_N \, dp_1 \cdots dp_N.
\]

The function \( f \) is dependent not only on the number of particles, but also their momenta and position coordinates. This trial distribution function also possesses the property that

\[
\text{tr}_{\text{cl}} f = 1.
\]

The equilibrium distribution function can be defined as follows,

\[
f_0 = \frac{1}{\Xi} \exp \left[ -\beta (H - \mu N) \right],
\]

where \( \Xi \) is the grand canonical partition function given by

\[
\Xi = \text{tr}_{\text{cl}} \exp \left[ -\beta (H - \mu N) \right].
\]
3. Density Functional Approach to Freezing

It is easily seen that

\[ \Omega[f_0] = \text{tr}_{c_\beta} f_0 \left( -\frac{1}{\beta} \ln Z \right) \]
\[ = -\frac{1}{\beta} \ln Z \]
\[ = \Omega, \]

and in the appendix, equation (A.1) shows that

\[ \Omega[f] > \Omega[f_0], \]

proving that \( f_0 \) is indeed the minimum of \( \Omega \). In addition, the appendix also shows that \( f_0 \) is determined uniquely by \( V_{\text{ext}}(r) \), and that this in turn is uniquely determined by the density \( \rho_0(r) \). This means that \( f_0 \) is in fact a functional of the density, and so for a given \( U \), two important functionals can be defined,

\[ \mathcal{F}[\rho] = \text{tr}_{c_\beta} f_0 (T + U + \beta^{-1} \ln f_0), \] (3.1)

\[ \Omega_V[\rho] = \mathcal{F}[\rho] + \int dr \rho(r)V_{\text{ext}}(r) - \mu \int dr \rho(r). \] (3.2)

If \( \rho(r) = \rho_0(r) \), then the first two terms of this expression combine to give the Helmholtz free energy, and the remaining term is just the Gibbs free energy. It is also shown in the appendix that this functional is minimised for \( \rho = \rho_0 \) just as in the case of the functional \( \mathcal{F} \). This information can be represented by the following equations,

\[ \left( \frac{\delta \Omega_V[\rho]}{\delta \rho(r)} \right)_{\rho_0(r)} = 0 \] (3.3)

and

\[ \Omega_V[\rho_0] = \Omega. \]

Upon combining equations (3.2) and (3.3) the following expression is obtained

\[ \mu_{\text{in}}[\rho_0, r] + V_{\text{ext}}(r) - \mu = 0, \] (3.4)

where the intrinsic chemical potential has been defined as

\[ \mu_{\text{in}}[\rho_0, r] = \frac{\delta \mathcal{F}[\rho]}{\delta \rho(r)}. \] (3.5)

As an example of the use of these equations, consider the case of a noninteracting fluid, i.e. \( U = 0 \). It is possible to find the exact form for \( \mathcal{F}[\rho] \), which can be shown to be of the form

\[ \mathcal{F}_{\text{ideal}} = \frac{1}{\beta} \int dr \rho(r) \ln(\lambda^3 \rho(r) - 1), \] (3.6)
where \( \lambda = (\hbar^2 \beta / 2m \pi)^{1/2} \) is the thermal de Broglie wavelength. This is identical in form to the standard statistical mechanics result, as would be expected. By making use of equation (3.4) it is possible to show that the density in this case is given by

\[
\rho_0(r) = z \exp[-\beta V_{\text{ext}}(r)],
\]

with \( z \) being a normalising factor. In the interacting case, things are not quite so simple. It is no longer possible to equate \( \mu_{\text{in}} \) directly with the chemical potential as was done above. The most interesting case is that for systems with large numbers of interacting particles. A method for approaching this problem will now be described.

One of the ways to include the effects of particle interaction is through the use of correlation functions. In addition, it also proves advantageous to separate the interacting and the noninteracting parts. To this end, define

\[
\mathcal{F} = \mathcal{F}_{\text{ideal}} - \Phi[\rho],
\]

(3.7)

where \( \Phi \) is a functional containing all the interaction parts. If \( U \) is known, then \( \Phi \) is a unique functional of \( \rho \). From this, it is possible to write the chemical potential as

\[
\beta \mu_{\text{in}}[\rho, r] = \ln(\lambda^3 \rho(r)) - c[\rho : r]
= \beta(\mu - V_{\text{ext}}(r)),
\]

where

\[
c[\rho : r] = \beta \frac{\delta \Phi[\rho]}{\delta \rho(r)}
\]

defines the one particle direct correlation function. It is then possible to again use equation (3.4) to solve for the density in the interacting case, giving

\[
\rho(r) = z \exp(-\beta V_{\text{ext}}(r) + c[\rho_0 : r]).
\]

The term \( c[\rho_0 : r] \) can be thought of as an effective external potential giving rise to a nonuniform density via a self-consistent processes. In addition, higher order correlation functions can also be defined,

\[
c[\rho : r_1, r_2] = \frac{\delta c[\rho : r_1]}{\delta \rho(r_2)} = \beta \frac{\delta^2 \Phi[\rho]}{\delta \rho(r_1) \delta \rho(r_2)}
\]

\[
c[\rho : r_1, r_2, r_3] = \frac{\delta^2 c[\rho : r_1]}{\delta \rho(r_2) \delta \rho(r_3)}, \text{ etc.}
\]

To show that \( c[\rho_0 : r] \) is the direct correlation function, start by defining

\[
u(r) = \mu - V_{\text{ext}}(r)
\]

(3.8)

so that

\[
\Omega_V[\rho] = -\int d\rho \rho(r)u(r) + \mathcal{F}[\rho].
\]

(3.9)
This expression can then be differentiated with respect to \( u(r) \) to give

\[
\frac{\delta \Omega_V[\rho]}{\delta u(r)} = -\rho(r) + \int dr' \frac{\delta \rho(r')}{\delta u(r')} \left( \frac{\delta F[\rho]}{\delta \rho(r')} - u(r') \right).
\]

From equation (3.4) it can be seen that if \( \rho(r) = \rho_0(r) \) then the final term in the brackets is equal to zero, and so

\[
\frac{\delta \Omega_V[\rho]}{\delta u(r)} = -\rho(r).
\]

It is now possible to define a further functional

\[
G(r_1, r_2) = -\frac{1}{\beta} \left( \frac{\delta^2 \Omega_V}{\delta u(r_2) \delta u(r_1)} \right)_{\rho_0(r)} = \frac{1}{\beta} \frac{\delta \rho_0(r_1)}{\delta u(r_2)},
\]

often referred to as the density-density correlation function. In the grand canonical ensemble this is given by

\[
G(r_1, r_2) = \rho^{(2)}(r_1, r_2) + \rho_0(r_1)\delta(r_1 - r_2) - \rho_0(r_1)\rho_0(r_2), \quad (3.10)
\]

where \( \rho^{(2)}(r_1, r_2) \) is the two-particle distribution function. If it is noted that

\[
c[\rho_0 : r_1] = \ln \left( \lambda^3 \rho_0(r_1) \right) - \beta u(r_1), \quad (3.11)
\]

then a simple differentiation with respect to \( \rho_0(r_2) \) gives

\[
c[\rho_0 : r_1 r_2] = c^{(2)}(r_1, r_2) = \frac{\delta(r_1 - r_2)}{\rho_0(r_1)} - \beta \frac{\delta u(r_1)}{\delta \rho_0(r_2)}
\]

\[
= \frac{\delta(r_1 - r_2)}{\rho_0(r_1)} - G^{-1}(r_1, r_2),
\]

where the inverse operator is defined by

\[
\int dr_3 G^{-1}(r_1, r_3)G(r_3, r_2) = \delta(r_1 - r_2). \quad (3.12)
\]

Now if equations (3.10) and (3.11) are substituted into equation (3.12) one obtains

\[
\rho^{(2)}(r_1, r_2) - \rho_0(r_1)\rho_0(r_2) = \rho_0(r_1)\rho_0(r_2)c^{(2)}(r_1, r_2)
\]

\[
+ \rho_0(r_2) \int dr_3 \left( \rho^{(2)}(r_1, r_3) - \rho_0(r_1)\rho_0(r_3) \right)c^{(2)}(r_3, r_2). \quad (3.13)
\]

This expression is simply the Ornstein-Zernike equation. If it is assumed the material is isotropic, such that \( c^{(2)}(r_1, r_2) = c^{(2)}(|r_1 - r_2|) \) and \( \rho^{(2)}(r_1, r_2) = \rho^2 g(|r_1 - r_2|) \), where \( g(r) \) is the radial distribution function, then equation (3.13) reduces to its more familiar form

\[
g(r) - 1 = c^{(2)}(r) + \rho_0 \int dr' (g(r') - 1)c^{(2)}(|r - r'|). \quad (3.14)
\]
This can be transformed into a more usable form by defining

\[ g(r) = h(r) + 1, \]

with \( h(r) \) being the total correlation function. Taking the Fourier transform gives

\[ h(k) = c(k) + \rho_0 h(k) c(k) \quad (3.15) \]

or

\[ \rho_0 c(k) = 1 - \frac{1}{S(k)}, \quad (3.16) \]

where \( S(k) \) is the structure factor, and is defined as

\[ S(k) = 1 + \rho_0 h(k) = 1 + \rho_0 \int dr \, e^{i kr} h(r). \]

The structure factor is useful in that it provides a link between the correlation function and the experimentally measurable properties of the system under study.

### 3.2 Equilibrium theory of Freezing

Having reviewed the formalism of DFT, it remains to show how the theory can be used in practice to calculate the freezing transition for a liquid. As mentioned earlier, the important quantity is the difference in free energy between the solid and liquid phases. When this difference is reduced to zero, both phases coexist, and it is this point that is said to mark the freezing of the liquid. So, to examine the irreversible line requires the calculation of the freezing transition in \( H-T \) phase space. This line can then be compared with the experimental line as a test of the theory.

To this end, a perturbation expansion is carried out around the density of a uniform liquid. This expansion is not of the full free energy, but only the part that contains the interactions, \( \Phi[\rho] \). The Taylor expansion of this quantity is given by

\[
\Phi[\rho] = \Phi[\rho_0] + \int dr_1 \left( \frac{\delta \Phi}{\delta \rho(r_1)} \right) (\rho(r_1) - \rho_0) \\
+ \frac{1}{2} \int dr_1 dr_2 \left( \frac{\delta^2 \Phi}{\delta \rho(r_1)\delta \rho(r_2)} \right) (\rho(r_1) - \rho_0)(\rho(r_2) - \rho_0) + \cdots
\]

It is only the minimum of the difference between the free energies that is important, and not their absolute values. The expression for this difference is

\[
\beta \Delta \Omega_V = \beta \Delta \Omega_V[\rho] - \beta \Delta \Omega_V[\rho_0] \\
= \beta \mathcal{F}_{\text{ideal}}[\rho] - \beta \mathcal{F}_{\text{ideal}}[\rho_0] - \beta \Phi[\rho] + \beta \Phi[\rho_0] - \beta \mu \int dr \, (\rho(r) - \rho_0),
\]
3. Density Functional Approach to Freezing

where equations (3.7), (3.8) and (3.9) have been used, and the external potential has been set equal to zero. Retaining only second order terms in the expansion of \(\Phi[\rho]\) and making use of equations (3.4), (3.5) and (3.6) shows that

\[
\left( \frac{\delta \Phi}{\delta \rho(r)} \right)_{\rho_0} = \ln(\lambda^3 \rho_0) - \beta \mu.
\]

Putting this all together for the isotropic case gives

\[
\beta \Delta \Omega_V = \int dr \rho_0 [\ln(\lambda^3 \rho(r)) - 1] - \int dr \rho_0 [\ln(\lambda^3 \rho_0) - 1]
- \int dr \ln(\lambda^3 \rho_0)(\rho(r) - \rho_0) + 2^{\text{nd}} \text{ order terms}
= \int dr \rho(r) \ln \left( \frac{\rho(r)}{\rho_0} \right) - \int dr (\rho(r) - \rho_0)
- \frac{1}{2} \int dr_1 dr_2 c(r_{12})(\rho(r_1) - \rho_0)(\rho(r_2) - \rho_0) + \cdots. \quad (3.17)
\]

This equation is the main result, and is used for the calculation of the freezing line. It is important to note that this expression is an expansion up to and including second order terms. The reader may well be wondering how important the higher order terms are. The reason for stopping at second order is simply that there is no standard way of calculating the three particle correlation function \(c^{(3)}\). There have been some attempts at including this term (Laird et al., 1987), but it is now generally believed (Haymet, 1993) that the effects of neglecting the \(c^{(3)}\) term are far outweighed by the difficulty of including it.

3.3 Calculation of the Freezing Line

To calculate the freezing line requires the solution that minimises equation (3.17). This equation requires several input parameters, such as a form for the solid density, \(\rho(r)\), and the two particle direct correlation function, \(c(r_{12})\). Once these quantities are known, they can be substituted for, and the energy minimised. The question is, therefore, what is a good choice for these parameters?

3.3.1 Choosing a Solid Density

There are two ways to choose the form of the solid density — one is using a real space formalism, and the other using a reciprocal space formalism. The real space formalism will be discussed first.

Real Space Formalism

In a solid the density is known to be periodic throughout the material, and this can be utilised in choosing a form. The density should not only be peaked around
the expected lattice site, but also allow for the particle to be found a small way from this expected position. This suggests the choice of a Gaussian function. This function provides a nice model of the probability distribution for finding particles around a mean point, and more importantly, has very nice mathematical properties. This Gaussian form has two free parameters associated with it: these are the height of the peak, and the width of the Gaussian. The width of the Gaussian determines how restricted the motion of the particles is, with a smaller width corresponding to the particles being held more firmly, and the height acts as a normalisation factor. With this in mind, the following choice for the density is made

$$\rho(r) = \left( \frac{A}{\pi^{d/2} \varepsilon^d} \right) \sum_R \exp \left[ -\left( \frac{r - R}{\varepsilon} \right)^2 \right],$$

where $A$ is constrained by the total solid density

$$\rho_s = \frac{1}{V} \int_V \, d^3 \rho(r) = \frac{A}{\Delta},$$

with $\Delta$ being the volume per lattice site of the crystal lattice. Both $\Delta$ and $R$ depend on the nearest neighbours lattice spacing $a$ through

$$\Delta = \delta a^3 \quad \text{and} \quad R = aT,$$

where both $\delta$ and $T$ depend on the underlying lattice type, which for the HTcS will be an hexagonal lattice. When using this representation there are three variational parameters that can be used to minimise the energy difference, the total solid density, $\rho_s$, the nearest neighbours lattice spacing, $a$, and finally the Gaussian width, or binding strength of the lattice, $\varepsilon$. The Gaussian width is actually constrained by $a$, as it can be assumed that $\varepsilon < a$.

Another advantage of using the Gaussian approach was mentioned earlier. This is the fact that it is well behaved mathematically. If this form for the density is substituted into equation (3.17), then the first two terms can be integrated analytically. In the general $d$-dimensional case it reduces to

$$\beta \Delta \Omega_V = 1 - \frac{\rho_s}{\rho_0} \left[ 1 + \ln \rho_0 - \ln(\delta \rho) - d \ln \left( \frac{a}{\pi^{1/2} \varepsilon} \right) + \frac{d}{2} \right]$$

$$- \frac{1}{2} \int d^3 \rho_1 d^3 \rho_2 c(r_{12}) \Delta \rho(r_1) \Delta \rho(r_2),$$

where for convenience the following definition has been made,

$$\Delta \rho(r_i) = (\rho(r_i) - \rho_0).$$

It can be seen that this equation still contains an integral term. This can be simplified by taking the Fourier transform of this term giving,

$$\beta \Delta \Omega_V = 1 - \frac{\rho_s}{\rho_0} \left[ 1 + \ln \rho_0 - \ln(\delta \rho) - d \ln \left( \frac{a}{\pi^{1/2} \varepsilon} \right) + \frac{d}{2} \right] - \frac{1}{2} \sum_G \rho_G \tilde{c}_G,$$

(3.18)
3. Density Functional Approach to Freezing

where $G$ is a reciprocal lattice vector and $\tilde{c}_R$ is the Fourier transform of the two particle direct correlation function. This expression raises an interesting question, how many terms should be kept in the summation to give an accurate result? When the calculation was first performed by Ramakrishnan and Yussouff they retained only the first term in the sum, and found their result to be quite good. When subsequent terms were included, it was found that the accuracy of the result was heavily dependent on the number of terms retained. For a graphic illustration of this effect see Figure 2 of Laird et al. (Laird et al., 1987). In this calculation, only the first term has been retained, for convenience. Selected results were compared with those generated when many terms were summed, and the difference was found to be negligible.

This shows that the choice of a real space formalism has several advantages. There are also disadvantages to this choice. As it stands, this function produces a density that is homogeneous. While this may be a good approximation for many systems, it is still just an approximation. This problem can be overcome by using the reciprocal space formalism. However, in this case the clarity of the physics in the real space formulation is lost.

Reciprocal Space Formalism

To overcome the homogeneous nature of the real space approach, it is possible to expand the density into its Fourier components. The expansion is carried out in terms of the reciprocal lattice vectors of the solid,

$$\rho(r) = \rho_0 (1 + \eta) + \rho_0 \sum_n \mu_n \exp(i\mathbf{k} \cdot \mathbf{r}),$$

where the coefficients $\mu_n$ are weights, and $\eta$ is the fractional density change on freezing,

$$\eta = \frac{\bar{\rho} - \rho_0}{\rho_0},$$

with $\bar{\rho}$ representing the average solid density. The difficulty with this method is apparent. In the real space model, the number of variational parameters was kept quite low. In this case each weight becomes, in effect, a variational parameter, making the solution much more difficult. It can be shown (Haymet and Oxtoby, 1981) that the solution for these weights is of the form

$$\mu_i = e^{\gamma_\eta V^{-1}} \int d\mathbf{r}_1 \exp \left( i\mathbf{k} \cdot \mathbf{r}_1 + \sum_n c_n \mu_n e^{i\mathbf{k}_n \cdot \mathbf{r}_1} \right).$$

This expression is analogous to equation (3.18) derived in real space with the exception of the number of variational parameters.

For this calculation a choice had to be made for the density. It was decided to use a real space representation, mainly for convenience. In practice there is little
difference between the results obtained by these methods, and as the real space density produces more tractable expressions, that form was finally chosen.

### 3.3.2 The Two Particle Correlation Function

Another important input to equation (3.17) is the two particle direct correlation function, $c(r_{12})$. There are two standard ways of obtaining this function. One is through measurements of the structure factor of the liquid in question. It has been shown in equation (3.16) that there is a direct connection between the structure factor and two particle correlation function, and this connection can be used to obtain $c^{(2)}$. The other method, and the method used for this calculation, is to obtain it theoretically. So far, only one expression has been presented that links both $c(r)$ and $h(r)$, and that is the Ornstein-Zernike equation (3.14). What is required is a second equation, such that we have two equations and two unknowns to enable a solution. There is, in fact, such an expression. There are two well known equations\(^1\), based on slightly different approximations, that are known to link these two functions. Their derivation from statistical mechanics is somewhat involved (McQuarrie, 1976), and the results will simply be quoted. The first is called the Percus-Yevick equation, and is of the form

$$c(r) = (1 + h(r))(\exp(-\beta V(r)) - 1),$$

and the other, that will be used for this calculation, is the Hypernetted Chain (HNC) equation

$$c(r) = \exp(-\beta V(r) + h(r)) - h(r) - 1.$$

The choice of approximation is motivated by the knowledge that for problems of this type, it is know that the HNC equation produces much better results, as a review of the DFT references quoted earlier will show. This now furnishes the two coupled equations that are required for a solution of the correlation function,

$$c(r) = \exp(-\beta V(r) + h(r)) - h(r) - 1$$

$$h(r) = c(r) + \rho_0 \int dr' c(|r - r'|)h(r')$$

where $c^{(2)}(r)$ has been written as $c(r)$ for convenience. If the Fourier transform is taken, these become

$$c(r) = \exp(-\beta V(r) + h(r)) - h(r) - 1$$

$$\tilde{h}(k) = \frac{\tilde{c}(k)}{1 - \tilde{c}(k)} - \tilde{c}(k),$$

\(^1\)Recent work (Rogers and Young, 1994) has produced an additional equation from a mixture of both approximations, whose results are in excellent agreement with Monte Carlo data.
along with the definitions,
\[
\tilde{c}(k) = \rho_0 \int dr \ c(r)e^{ikr} \\
\tilde{h}(k) = \rho_0 \int dr \ h(r)e^{ikr}.
\]

With these coupled equations, guessing an initial form for either \( h \) or \( c \) enables an iterative solution to be obtained. It should be noted that a modified form of these equations are required in this case. The above equations were derived for a three dimensional isotropic system, but examining a real HTcS requires a two dimensional system, with a discrete layer along the third dimension. It transpires that the HNC equation for such a system is equivalent, except for the addition of a layer index \( n \) and the Fourier transform being confined to the plane,
\[
c_n(r_\perp) = \exp(-\beta V_n(r_\perp) + h_n(r_\perp)) - h_n(r_\perp) - 1 \quad (3.19) \\
\hat{h}(k_\perp) = \frac{\tilde{c}(k_\perp)}{1 - \tilde{c}(k_\perp)} - \tilde{c}(k_\perp). \quad (3.20)
\]

These are the equations that are required to produce the two particle direct correlation function for input into the DFT calculation. The last remaining input needed for this calculation is the potential, \( V_n(r) \).

So far no mention has been made about the nature of the superconductor. The entire derivation to this point has been extremely generic. The expressions that have been derived have not been dependent on the type of material undergoing the melting transition, and so are equally applicable to almost any system. As mentioned at the start of this chapter, the calculation of the melting line is based on a theory that was originally developed for “classical” liquids, such as the hard sphere or Lennard-Jones systems. Here classical is used in the sense that the particles being modelled are known — in the first case they are just spheres of a given radius, while in the second they are the atoms or molecules that constitute the given substance. However if the HTcS material is considered as merely a background through which the flux lines can flow, then it is possible to draw an analogy between the flux lines and these classical particles. This is of course rather a gross oversimplification, but is nevertheless a good place to start.

Because of the two dimensional nature of the HTcS, the flux liquid is somewhat strange. The particles in the classical system now correspond to the pancake\(^1\) vortices present in each layer. These pancake vortices interact with other vortices in neighbouring layers, as well as vortices in the same layer. One of the most noticeable

\(^1\)The term derives from the fact that the vortices only exist in a superconducting region. In a HTcS the superconducting layers are quite thin, compared with the layer spacing. As the vortices are confined to these layers, they adopt a more 2D nature. These flattened vortices are known as pancake or Pearl (de Gennes, 1966) vortices. For more details see Section VIII of Blatter et al. (Blatter et al., 1994)
3.4 Determination of the Freezing line

The first step in the calculation is determining the correlation function. To aid this calculation the asymptotic form can be utilised. In the limit of large $r$, it is known that the correlation function behaves as

$$c(r) \sim -\beta V(r).$$

Making use of this knowledge, it is possible to expand both unknown functions into their long and short range parts,

$$c(r) = c^S(r) + c^L(r)$$
$$h(r) = h^S(r) + h^L(r).$$

Assuming a nearest neighbour interaction, it is possible to integrate out the effect of the layers, and reduce the problem to a single layer. The transformed versions of equations (3.19) and (3.20) become,

$$c^S_0(r_\perp) = \exp(y^L_0(r_\perp) + h^S_0(r_\perp)) - 1 - h^S_0(r_\perp) - y^L_0(r_\perp) \tag{3.21}$$

$$h^S(k_{\perp}) = \frac{d}{\pi} \int_{-\pi}^{\pi} dk_z \left( \frac{c^S(k_{\perp}) + c^L(k_{\perp}, k_z)}{1 - c^S(k_{\perp}) - c^L(k_{\perp}, k_z)} - c^S(k_{\perp}) - y^L(k_{\perp}, k_z) \right), \tag{3.22}$$

along with

$$c^L(k_{\perp}, k_z) = -\beta V(k_{\perp}, k_z)$$
3. Density Functional Approach to Freezing

Figure 3.1: Plot of the full two particle correlation function, $c^{(2)}(k_\perp)$. The dashed lines represent the first few reciprocal lattice vectors, based on the peak of $c^{(2)}(k_\perp)$ corresponding to the lattice spacing.

\[ h^L(k_\perp, k_z) = \frac{-\beta V(k_\perp, k_z)}{1 + \beta V(k_\perp, k_z)} + \beta V(k_\perp, k_z) \]
\[ y^L(k_\perp, k_z) = h^L(k_\perp, k_z) + c^L(k_\perp, k_z) \]
\[ y^L_0(r_\perp) = h^L_0(r_\perp) + c^L_0(r_\perp). \]

All the above expressions, although it was not explicitly shown, are dependent on both the temperature and applied magnetic field. The magnetic field dependence arises from the quantisation of magnetic flux. As all flux lines contain $\phi_0$ of magnetic flux, the number of flux lines is simply $\rho_0 = B/\phi_0$. The temperature dependence appears through the interaction potential. It is now possible to solve these equations to calculate the freezing line. The following steps were carried out:

- Values for both the temperature and magnetic field are chosen. In addition material dependent constants are assigned values from experimental data. These are the only inputs to the theory.

- The initial form for the function $h^S_0(r)$ is chosen and substituted into equation (3.21) to obtain a new form for $c^S_0(r)$. The effect of a bad choice for $h^S_0(r)$ is to increase the number of iterations required for stability. Initially the choice can be any function that smoothly decreases with distance with further choices
3.4. Determination of the Freezing line

being generated from the final form obtained in the previous solution. After the first iteration, the solution for $c_0^S(r)$ is then substituted into equation (3.22) to obtain a first iteration solution for $h^S(k_\perp)$. This process is carried out until the solution for the correlation function converges. This step can be speeded up by the use of a Newton-Raphson convergence scheme (Gillian, 1979), or some similar technique. A typical result for the correlation function, along with the associated reciprocal lattice vectors, is shown in Figure 3.1. These reciprocal lattice vectors are based on the peak of the correlation function giving the lattice spacing $a$.

- Having obtained the correlation function, it is then substituted into equation (3.17). This expression is minimised with respect to the variational parameters, and a value for the change in free energy is obtained. If this value is not found to be zero, the calculation is repeated at various temperatures, with the magnetic field fixed, until a zero is found. Once found, this point can then be plotted out in the $H$–$T$ plane of the phase diagram.

- The magnetic field is then changed to a new value, and the preceding steps are repeated until the freezing line is plotted out.

Figure 3.2: Calculated freezing curves for both BSCCO and HBCO compounds. The two dimensional freezing temperature is shown by the dashed line, as a reference.
3. Densities Functional Approach to Freezing

The final result of all the calculations is the plot of the freezing line. Figure 3.2 shows the results of the freezing line for two HTcS materials, Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ (BSCCO) and HgBa$_2$CuO$_{4+x}$ (HBCO). Also shown for comparison is the calculated freezing line for a purely two dimensional system, which was found to be constant for all magnetic fields examined. These numerical results can be compared with some recent experimental results for BSCCO and HBCO shown in Figures 3.3 and 3.4 respectively.

What is visible from the graph is that as the magnetic field increases, the freezing temperature of the flux lattice approaches that for the 2D system. A more detailed explanation of the reason is presented in the next chapter. There it will be shown that an increase in the field has the effect of reducing the effect of neighbouring layers, so that the system in effect becomes a set of independent layers of thickness $d$. This explains why the freezing temperature then starts to approach its two dimensional value. The results of this somewhat simplistic theory are in quite good agreement with experimental results for the BSCCO material (Supple et al., 1995), however the agreement is quite bad for the HBCO material (Estrela et al., 1994). The reason behind the similarity of the two calculated results is that the input parameters for both materials are very similar, $\lambda_{Bi} \approx 1500 \text{ Å}$, $d_{Bi} \approx 15 \text{ Å}$, $\lambda_{Hg} \approx 1170 \text{ Å}$, $d_{Hg} \approx 10 \text{ Å}$, and so it should be expected that the final results would be quite similar. A physical explanation for the difference present in the experimental results is that pinning will play a large role in determining the HBCO line. If the density of pinning centres is higher in the HBCO compound, then it would be expected that the melting temperature would undergo a corresponding increase, due to the higher temperatures needed to depin the flux lines from the pinning centres. While this simple argument may not explain the intricacies of what is really occurring, it does provide a plausible explanation for this discrepancy. The calculated results have no way to take into account this pinning force, and so there is nothing to distinguish the two systems from each other.

3.5 Summary

The density functional theory presented here is a simple, straightforward implementation. There has been much work put into improving the results, such as the weighted density approximation first examined by Tarazona (Tarazona, 1984) and the effective-liquid approximation developed by Baus and Colot (Baus and Colot, 1985). These sacrifice some of the simplicity of DFT to hopefully gain more accuracy in the final results.
3.5. Summary

Figure 3.3: Experimental irreversible line for BSCCO. The different lines represent different methods used for measuring the irreversible line. More details can be found in the original paper (Supple et al., 1995).

Figure 3.4: Experimental irreversible line for HBCO (Estrela et al., 1994).
When this theory is applied to the examination of the freezing of the flux line lattice, it is seen that it provides a reasonable description of this effect. So that with very little knowledge of any exact mechanism for the formation of superconductivity, it is still possible to examine more macroscopic properties. It has been shown that the results obtained for BSCCO are in quite good agreement with experiment, but HBCO is found to not exhibit such good agreement. It has been argued that this difference is possibly due to effects that are dependent on the properties of the material, that are not modelled in the theory. It also successfully models a crossover from a 3D to a 2D system with increasing magnetic field, which will be discussed in more detail in the next chapter. Attempts to incorporate the effect of the background material, such as pinning, into DFT have so far not been successful. It would certainly be interesting to examine its effect from a first principles approach, even though it can already be argued physically that such an effect should act to increase the freezing temperature.

In the next chapter, this problem will be reexamined from a slightly different viewpoint — that of Ginzburg-Landau theory. This will enable a self consistent determination of the interaction potential for both interlayer and intralayer coupling. Once found, they can be combined to produce the total 3D interaction potential which can then be substituted for \( V_n \).
In the previous chapter the freezing transition of a flux liquid was discussed. It has been shown that this effect has important consequences for the critical current, and hence the practical use of these materials.

In the earlier calculations, the interaction potential was obtained from a different theoretical basis. The system was also complicated by the fact that it was an $N$-layer problem. The behaviour of the freezing line was found to have some interesting properties, especially for large magnetic fields, which require an explanation.

To this end, a similar calculation will be performed, but on a slightly simpler system. What will be examined is a simple superconductor consisting of just two layers. The system is described by a set of Ginzburg-Landau equations, which will be solved numerically to obtain the interaction potential. The 2D, or pancake vortices, interact with those in the other layer by means of a coupling between the phases of the order parameters. Several other forms of coupling, both in the same layer and between different layers, are also considered. After the interaction potential is obtained, the freezing transition for this system is then examined.

Due to the relative simplicity of this system, it becomes possible to isolate the different forces between vortices, and, therefore, examine their effects on the freezing line. The effect of the background material is still not included, a shortcoming that remains to be overcome.

4.1 Ginzburg-Landau Energy Functional

As mentioned previously, Ginzburg and Landau (Ginzburg and Landau, 1950; Landau, 1965) applied the Landau theory of second order phase transitions to the phenomenon of superconductivity. This idea was based on the expansion of the free energy in powers of an order parameter. In this case, the order parameter, $\psi$, is taken as an effective wavefunction. As mentioned earlier, when Gorkov showed the equivalence of GL theory and BCS theory for temperatures close to $T_c$, it was found that this order parameter is related to the BCS energy gap. The order parameter is
taken as a complex number, and has the property that it can always be determined, up to a phase factor. This requires that only terms with equal an number of $\psi$ and $\psi^*$ can appear in the expansion.

So, for a uniform superconductor with zero applied magnetic field, it is possible to write down the free energy as

$$F_{so} = F_{n0} + \alpha |\psi|^2 + \frac{\beta}{2} |\psi|^4.$$  

In addition, the following conditions apply: $|\psi|^2 = 0$ for $T \geq T_c$, and $|\psi|^2 > 0$ for $T < T_c$. Putting all this together, it can easily be shown that for temperatures below the critical temperature,

$$|\psi|^2 \equiv |\psi_\omega|^2 = -\frac{\alpha}{\beta},$$

and

$$F_{so} = F_{n0} - \frac{\alpha^2}{2\beta},$$

where it has been assumed that the parameters $\alpha$ and $\beta$ satisfy

$$\alpha(T) = \left(\frac{d\alpha}{dT}\right)_{T_c} (T_c - T) = \alpha'(T_c - T) \quad \beta(T) = \beta.$$

If it is assumed that the system is no longer uniform, then another term must be added to the expansion of the free energy. This term can be thought of as opposing movement of the system from the uniform state, and is an expansion in terms of the gradient. The final term that must be added is an interaction with an external field. The full free energy per unit volume now becomes,

$$F_{so} = F_{n0} + \alpha |\psi|^2 + \frac{\beta}{2} |\psi|^4 + \frac{1}{2m} \left| -i\hbar \nabla + \frac{e}{c} A \right|^2 |\psi|^2 + \frac{\hbar^2}{8\pi}.$$ (4.1)

It is possible to obtain equations for both the order parameter and the vector potential by minimising equation (4.1) with respect to $\psi^*$ and $A$ respectively. Performing the functional differentiation with respect to $\psi^*$ leads to

$$\alpha \psi + \beta |\psi|^2 \psi + \frac{1}{2m} \left(-i\nabla + \frac{e}{c} A \right)^2 \psi = 0,$$ (4.2)

where $\hbar$ has been set equal to 1 for convenience, and an integration by parts has been performed. The equivalent expression for the vector potential is given by,

$$\frac{c}{4\pi} \nabla \times \mathbf{H} = \frac{ie}{2m} (\psi^* \nabla \psi - \psi \nabla \psi^*) - \frac{e^2}{mc} A |\psi|^2,$$ (4.3)
where another integration by parts has been performed, and use has been made of the identity $\mathbf{H} = \nabla \times \mathbf{A}$. These expressions are supplemented by the following boundary conditions,

$$\hat{n} \cdot \left(-i\nabla \psi - \frac{e}{c} \mathbf{A} \psi\right) = 0,$$

following from the derivation of equation (4.2), and

$$\hat{n} \cdot \mathbf{j} = 0$$

from the derivation of equation (4.3). Here $\hat{n}$ is the unit vector that is normal to the boundary.

While the above expressions are generally all that are required, it is instructive to continue a little further and derive several more expressions that help to show how powerful this idea can be. If a simple one dimensional geometry is considered, equation (4.2) can be written as

$$-\frac{1}{2m|a|} \frac{d^2 f}{dz^2} - f + f^3 = 0,$$  \hspace{1cm} (4.4)

where $f(z)$ has been defined through

$$f(z) = \frac{\psi(z)}{\psi_{\infty}},$$

and $\psi_{\infty}$ has been defined earlier. The constant factor of the derivative term in equation (4.4) has the dimension of a length squared, and so can be written as

$$\xi(T) = \left(\frac{1}{2m|a(T)|}\right)^{1/2}.$$

This temperature dependent length, $\xi(T)$, is known as the Ginzburg-Landau coherence length. The magnetic penetration depth can also be found from equation (4.3) if the order parameter is assumed to be approximately constant, such that

$$\mathbf{j}(r) = -\frac{e^2}{mc}|\psi|^2 \mathbf{A}(r),$$

and from this the penetration depth can be recognised to be

$$\lambda(T) = \left(\frac{mc^2 \beta}{4\pi e^2 |a(T)|}\right)^{1/2}.$$

Returning briefly to equation (4.4), the solution to this problem will quickly be examined and then made use of throughout the rest of this chapter. If the system considered is taken to be a flux line, whose centre is located at $z = 0$, it is known
that the order parameter is zero at the origin but will approach $\psi_\infty$ as $z$ increases. This leads to the following boundary conditions,

$$f(0) = 0 \quad (4.5)$$

$$\lim_{z \to \infty} f(z) = 1. \quad (4.6)$$

It is possible to obtain a first integral of (4.4) which takes the form

$$\xi^2 \left( \frac{df}{dz} \right)^2 = \frac{1}{2}(1 - f^2)^2,$$

where the constant has been determined from the condition $f' \to 0$ for $f^2 \to 1$. As $f$ is an increasing function of $z$, the positive square root is taken

$$\frac{df}{dz} = \frac{1 - f^2}{\sqrt{2\xi}}$$

and the final solution for the order parameter becomes

$$f(z) = \tanh \left( \frac{z}{\sqrt{2\xi}} \right). \quad (4.7)$$

This solution also helps to explain the role of the correlation length. From this form, it can be seen that $\xi$ can be thought of as a measure of the width of the normal core of a flux line. While this is a one dimensional solution, it can be used as a first order guess at the true solution for coupled layers, which will now be presented.

### 4.2 The Two-Layer Problem

Having reviewed the ideas involved in GL theory, it should now be possible to extend these ideas to the simple model of a two layer superconductor. This model consists of just two thin superconducting layers, each able to support pancake vortices. The layers are connected by Josephson coupling of the vortices. For this system, there are two order parameters, one for each layer. The form of the Ginzburg-Landau equations applicable to this kind of system is given by

$$F_\phi = \int dr \left\{ \alpha |\phi|^2 + \frac{\beta}{2} |\phi|^4 + \left| \left(-i\hbar \nabla + \frac{e}{c} A_\parallel \right) \phi \right|^2 ight.$$ \nonumber

$$+ \eta |(\phi \exp \left(-2ie \int_0^d A_\perp dz \right) - \psi)|^2 + \frac{(\nabla \times A)^2}{8\pi} \right\}$$

$$F_\psi = \int dr \left\{ \alpha |\psi|^2 + \frac{\beta}{2} |\psi|^4 + \left| \left(-i\hbar \nabla + \frac{e}{c} A_\parallel \right) \psi \right|^2 ight.$$ \nonumber

$$+ \eta |(\psi \exp \left(-2ie \int_0^d A_\perp dz \right) - \phi)|^2 + \frac{(\nabla \times A)^2}{8\pi} \right\}, \quad (4.8)$$
where the following conventions have been used: the subscript on the free energy corresponds to the layer, with \( \phi \) being layer 1 and \( \psi \) being layer 2. The strength of the Josephson coupling term is denoted by \( \eta \). In the simplest approximation, this factor can be assumed to be constant, although in reality it would have a more complicated dependency. For example, it might be expected that this would vary as the correlation length perpendicular to the layers,

\[
\eta(d) \sim e^{-\epsilon d},
\]

where \( \epsilon \) is some characteristic decay length. Finally, \( A_y \) represents the vector potential in the plane and \( A_z \) is the vector potential between the planes. For more details on the form of these equations, see for example Klemm et al. (Klemm et al., 1975)

This method, when generalised to many layers, is known as the Lawrence-Doniach model (Lawrence and Doniach, 1971).

To solve this system of equations, the same steps are performed as for the 1D GL energy functional, although they require a little more care. There are two distinct cases for their solution. The first is when vortices in different layers lie directly above one other. In this case, the system possesses rotational symmetry, and the equations can be numerically solved by some standard techniques. In the second case, when the rotational symmetry is broken, the system becomes quite difficult to examine, and new approaches need to be taken. These solutions will be presented in order. In addition, as can be seen from the expressions above, these solutions also require a knowledge of the form of the magnetic field surrounding the layers due to the presence of pancake vortices within the layers. This calculation is an extension of work by Clem (Clem, 1991), and is presented next.

### 4.2.1 Magnetic Field due to Pancake Vortices

The magnetic field of a pancake vortex in a superconducting layer was originally calculated in 1964 by Pearl (Pearl, 1964). The present calculation requires an extension of this due to the presence of a second superconducting layer which will affect the form of the magnetic field by generating shielding currents within the layer. Figure 4.1 shows the system under study and identifies the three regions of interest.

To calculate the magnetic field, it is possible to start by writing down a general expression for the angular component of the vector potential in cylindrical coordinates (Jackson, 1962),

\[
a_\varphi(\rho, z) = \int_0^{\infty} dq \, A(q) J_1(q\rho) Z(q, \rho),
\]

where \( J_1(q\rho) \) is a first order Bessel function and \( Z(q, \rho) \) is a function that depends on the boundary conditions of the system. It is quite easy to show that in the three
4. Properties of the Pancake Vortex Lattice

Figure 4.1: Schematic diagram of the system under study. The field lines must be calculated in the three different regions.

regions this function is given by,

Region-I  \[ Z(q, \rho) = \exp(-Qz) \]
Region-II \[ Z(q, \rho) = \frac{1}{\sinh(qd)} \left( e^{-Qd} \sinh(qz) + \sinh(q(d - z)) \right) \]
Region-III \[ Z(q, \rho) = \exp(qz). \]

The functions \( A(q) \) and \( Q \) can be derived by examining the sheet current density, which is defined as \( K = -n_{2D} e \nu_s \). This function can be obtained by two different approaches. The first is by substituting for the superconducting velocity, \( \nu_s \), which consists of contributions from both the current due to the magnetic field and due to the phase of the order parameter, \( \gamma \),

\[
K = -\frac{c}{2\pi \Lambda} \left( a + \left( \frac{\phi_0}{2\pi} \right) \nabla \gamma \right). \tag{4.10}
\]

Here, \( \gamma \) is chosen as zero for layers with no vortices and \( -\varphi \) for layers possessing a vortex, and \( \Lambda \) is the screening depth of the layer,

\[
\Lambda^{-1} = \frac{2\pi n_{2D} e^2}{mc^2},
\]

with \( n_{2D} = n_{3D} d \). The second approach is to examine the discontinuity in the magnetic field through the layers,

\[
K = \frac{c}{4\pi} \left[ b_\rho(\rho, 0^+) - b_\rho(\rho, 0^-) \right]. \tag{4.11}
\]
4.3. Single Layer Potential

Using equations (4.10) and (4.11), along with the identity

\[ b = \nabla \times a, \]  

it is possible to derive \( A(q) \) and \( Q \). The first is found by equating equations (4.10) and (4.11) for the layer containing the vortex, and the second by equating both expressions for the screening layer. These are given respectively by,

\[ -\frac{c}{2\pi \Lambda} \left( a_\phi - \left( \frac{\phi_0}{2\pi \rho} \right) \right) = \frac{c}{4\pi} \left[ b_\rho(\rho, 0^+) - b_\rho(\rho, 0^-) \right] \]

\[ -\frac{c}{2\pi \Lambda} a_\phi = \frac{c}{4\pi} \left[ b_\rho(\rho, 0^+) - b_\rho(\rho, 0^-) \right]. \]

After substituting for the magnetic field components from equation (4.12) and performing some simple algebra, it is easy to show that

\[ Q = -\frac{1}{d} \ln \left[ \frac{1 - e^{-qd} \sinh(qd)}{\cosh(qd) + \left( \frac{2}{q\Lambda} \right) \sinh(qd)} \right]. \]

The calculation of \( A(q) \) is almost identical but requires the use of the Hankel transform (Abromowitz and Stegun, 1972), which is given by

\[ \int_0^\infty d\rho \rho J_1(q\rho)J_1(q'\rho) = \frac{1}{q} \delta(q - q'). \]

Making use of this, similar algebra to that above shows that

\[ A(q) = \frac{\phi_0}{\pi} \left[ 1 + \frac{q\Lambda}{2} - \frac{q\Lambda}{2} \frac{e^{-qd}}{\sinh(qd)} + \frac{q\Lambda}{2} \frac{\cosh(qd)}{\sinh(qd)} \right]^{-1}. \]

It can be seen that in the limit \( d \to \infty \) this expression reduces to that calculated for the single layer, as required.

Having derived all the functions necessary for equation (4.9), it is possible to calculate the form of the magnetic field. It should be noted that if parameter values that are relevant to the HTcS materials are used, it is found that the effect of the screening layer on the field is small, and therefore it should be a reasonable approximation to neglect this layer. Having said that, the effect of the layer was considered for all the subsequent calculations, for completeness.

4.3 Single Layer Potential

The first interaction potential to be calculated is that due to vortices in the same layer, \( U_{11}(\rho) \). This potential can be found directly from the interaction of the magnetic field due to each vortex, and makes direct use of the results found above. The Lorentz force on a vortex due to another in the same layer is given by

\[ F_\rho(\rho) = \frac{K_\rho(\rho)\phi_0}{c}. \]
Figure 4.2: Plot of the intralayer interaction potential, $U_{11}(\rho)$, as a function of vortex separation.

where $K_\varphi$ is the sheet current density calculated earlier. The interaction potential can then be written as

$$U_{11}(\rho) = \int_\rho^\infty d\rho' F_\rho(\rho'),$$

and is shown in Figure 4.2. Several important properties should be noted: firstly if this potential is compared to that found for a single layer (Clem, 1991), it is seen that they are almost identical in form. This would be expected to be due to the small effect of the extra screening layer. The potential is seen to tend to infinity logarithmically as $r \to 0$ and to fall off approximately inversely with distance as $r \to \infty$. The logarithmic behaviour can be linked to a possible Berezinskii-Kosterlitz-Thouless transition (Berezinskii, 1971; Kosterlitz and Thouless, 1973) for vortices in a single layer when $\Lambda$ becomes sufficiently large, although this transition is not considered here.

Having calculated the intralayer potential, it now remains to find the interlayer potential. This calculation is split into two parts: the symmetric solution, and the antisymmetric solution. The symmetric solution is presented next.

4.3.1 Rotationally Symmetric Solution

The symmetric problem involves studying a system consisting of a pancake vortex in each layer aligned along the $z$-axis. It is then possible to use cylindrical
4.3. Single Layer Potential

coordinates to simplify the problem. As with the 1D functional, a minimisation is performed, but now with respect to three parameters: $\phi^*$, $\psi^*$ and $A_\parallel$. When this is carried out, the following coupled differential equations are produced,

$$
\frac{d^2 A_\parallel}{dr^2} - \frac{1}{r} \frac{dA_\parallel}{dr} - (1 - A_\parallel) f_\phi^2 = 0
$$

$$
\frac{d^2 f_\phi}{dr^2} + \frac{1}{r} \frac{df_\phi}{dr} - \frac{(1 - A_\parallel)^2}{r^2} f_\phi + f_\phi - f_\phi^3 + \eta \left( f_\phi \exp \left( -2i e \int_0^d A_z dz \right) - f_\phi \right) = 0
$$

$$
\frac{d^2 f_\psi}{dr^2} + \frac{1}{r} \frac{df_\psi}{dr} - \frac{(1 - A_\parallel)^2}{r^2} f_\psi + f_\psi - f_\psi^3 + \eta \left( f_\psi \exp \left( -2i e \int_0^d A_z dz \right) - f_\psi \right) = 0
$$

$$
\frac{d^2 A_\parallel}{dr^2} - \frac{1}{r} \frac{dA_\parallel}{dr} - (1 - A_\parallel) f_\psi^2 = 0.
$$

(4.13)

It can be seen from these equations that there is in fact a high degree of symmetry in the expressions, and therefore the solutions would be expected to possess a similar symmetry. In fact it would be expected that $f_\psi = f_\phi$, which is indeed observed. Therefore throughout this section, all references made to one of these functions will apply equally to the other. To obtain the equations in this form, the following forms were assumed,

$$
\phi(r) = e^{-in_\phi} f_\phi(r)
$$

$$
A_\parallel(r) = \hat{e}_\phi \frac{A_\parallel(r)}{r},
$$

along with a similar substitution for $\psi(r)$. In addition, the vector potential has also been scaled,

$$
A' = eA,
$$

where the prime has been removed from equations (4.13). Finally the convention $\hbar = c = 1$ has been adopted. The factor $n$ is the “strength” of a vortex, such that the magnetic flux through an individual vortex is $n\phi_0$, and in this case has been taken as 1. Finally, $\varphi$ denotes the azimuthal angle. The choice of the forms for the substitutions is guided by the known asymptotic behaviour of the functions. This leads to the following boundary conditions,

$$
\phi(0), \psi(0) = 0, \quad A_\parallel(0) = 0,
$$

$$
\phi(\infty), \psi(\infty) = 1, \quad A_\parallel(\infty) = -n.
$$

The solution to equations (4.13) has so far not been obtained analytically for the general case, so to obtain a solution requires a numerical approach. This type of solution is made somewhat more difficult by the form of the boundary conditions. It can be seen that one of these is set for $r \to \infty$, which is very hard to implement
in a numerical routine. To overcome this problem, a change of variable is required. The choice of
\[ \rho = \frac{z}{1-z}, \]
enables the infinite line of \( r \) to be shrunk to fit within the range 0 \( \rightarrow \) 1. If this change of variable is performed, equations (4.13) become,
\[
(1-z)^4 \frac{d^2 A_{\parallel}}{dz^2} - (1-z) \left( 2 + \frac{1}{z} \right) \frac{d A_{\parallel}}{dz} - (1 - A_{\parallel}) f_{\phi}^2 = 0
\]
\[
(1-z)^4 \frac{d^2 f_{\phi}}{dz^2} - (1-z)^3 \left( 2 + \frac{1}{z} \right) \frac{df_{\phi}}{dz} - (1-z)^2 \left( \frac{1 - A_{\parallel}}{z} \right)^2 f_{\phi} + f_{\phi} - f_{\phi}^3 + \eta \left( f_{\phi} \exp \left( -2ie \int_0^d A_{\parallel} \, dz \right) - f_{\phi} \right) = 0
\]
\[
(1-z)^4 \frac{d^2 f_{\psi}}{dz^2} - (1-z)^3 \left( 2 + \frac{1}{z} \right) \frac{df_{\psi}}{dz} - (1-z)^2 \left( \frac{1 - A_{\parallel}}{z} \right)^2 f_{\psi} + f_{\psi} - f_{\psi}^3 + \eta \left( f_{\psi} \exp \left( -2ie \int_0^d A_{\parallel} \, dz \right) - f_{\psi} \right) = 0
\]
\[
(1-z)^4 \frac{d^2 A_{\parallel}}{dz^2} - (1-z) \left( 2 + \frac{1}{z} \right) \frac{d A_{\parallel}}{dz} - (1 - A_{\parallel}) f_{\phi}^2 = 0.
\]
These equations were then solved numerically to find the functions \( \phi(r) \), \( \psi(r) \) and \( A_{\parallel}(r) \). Before this is possible, it is necessary to extend the calculation of Section 4.2.1 to include the presence of a pancake vortex in each layer. This turns out to be quite simple, as the required solution is merely a superposition of the single layer problem. Using this result it is possible to write the superposition vector potential along the z-axis as
\[
\tilde{\alpha}_{\phi}(\rho, z) = a_{\phi}(\rho, z) + \tilde{\alpha}_{\phi}(\rho, z + d),
\]
where \( \tilde{\alpha} \) is used to denote that unlike the multilayer case examined by Clem, more care needs to be taken when performing the addition for the case of two layers. Now it is possible to numerically solve equations (4.14) for the unknown functions. The form of these as functions of separation is shown in Figure 4.3. In this symmetric case the magnetic field along the superconducting layers, \( H_{\parallel}(r) \), is generated from the vector potential in the usual way,
\[
H = \nabla \times A_{\parallel} = -\frac{(1-z)^3}{z} \frac{d A_{\parallel}}{dz} \hat{e}_r.
\]
The magnetic field can be seen to decay away exponentially, which is in agreement with the 1D solution of equation (4.7). The form of the wavefunction can be also be shown to be very similar to the 1D solution. This would seem to imply that the results obtained from the numerical analysis are reasonably physical.

Generation of these solutions required values to be given for the parameters that appear in the GL functional. These parameters are the coherence length and the
4.3. Single Layer Potential

Figure 4.3: Plot of the typical form for the function $\phi(r)$ and the magnetic field for a vortex. Both are shown as a function of distance from the centre of the vortex.

magnetic penetration depth, values for which were given at the end of the preceding chapter, and were $\lambda \sim 1500$ Å, $\xi_\perp \sim 3$ Å, $\xi_\parallel \sim 15$ Å and $d \sim 5-8$ Å.

4.3.2 Non-Aligned Vortex Position

Once the rotational symmetry is lost, the method of solution used above is not applicable, and a new approach is needed. One of the simplest methods is to use a variational form for the wavefunction, substitute this into equation (4.8) and minimise. This requires a good initial guess for the form of the wavefunctions $\phi$ and $\psi$, as well as the vector potential. Initial approximations for these functions can be generated from the solutions obtained above. However, for ease of computation, it is possible to assume a simpler form as a first approximation for the wavefunctions. This first guess can be taken as a tanh function, which has the benefit of being analytical,

$$
\phi_{trial} = \tanh(ax + by)
$$

$$
\psi_{trial} = \tanh\left(\sqrt{(ax - r_0)^2 + b^2y^2}\right),
$$

where $a$ and $b$ are variational parameters used in the minimisation of the total free energy and $r_0$ is the separation between vortices along the $x$-axis. The use of the
two parameters enables any distortion of the flux line to be measured, although in practice it is found that the approximation \( a = b \) is valid, within numerical error, for all the vortex separations that were examined, which would tend to imply that the vortices retain their spherical symmetry, even as they are separated. If the numerical solution obtained for the symmetric case is used for the wavefunctions, it is found that the final solutions differ very little from the solutions obtained by using the above trial functions and therefore these functions were used to obtain the final solution.

So, having obtained useful functional forms for the parameters, they can be substituted into the free energy, which can then be minimised. The two vortices, \( \phi \) and \( \psi \), are separated by a distance \( \sqrt{r_0^2 + d^2} \), where \( d \) is the interlayer separation. By varying the inplane separation of the vortices, it is possible to obtain the interlayer potential as a function of distance. One assumption made is that there is no entangling of the flux lines. This means that the dominant interaction is that between the vortices that were originally aligned. A more detailed model would be required to take this more complicated behaviour into account. This approximation requires the maximum interlayer offset to be of the order of the vortex radius. As in the previous section, the vector potential between the vortices can be found from a superposition of the single vortex solution, but with the centre of one of the vortices offset by an amount \( r_0 \). An example of the form of this potential, denoted \( U_{12} \), is shown in Figure 4.4. The figure shows the potential for different values of the interlayer separation. It can be seen that as the separation increases, then the interlayer coupling decreases by an amount dependent on the ratio of the coherence length between the planes to the separation, as was discussed earlier. The opposite effect is observed as the separation decreases. A similar effect is also observed when the magnetic field is varied. Here it is found that as the field increases, the strength of the coupling decreases, and vice versa.

Having obtained the interaction potential, it remains to use this result in a calculation of the new freezing transition. It is possible to use the fact that the full potential is an addition of two separate functions to make a comparison with multicomponent systems. It is well known how to extend DFT to systems of more than one component, and so by relating each potential with a separate component of the system, it is possible to examine the freezing transition for the two-layer system.

### 4.4 Multi-Potential Density Functional Theory (MPDFT)

The two-layer system requires a small extension to the conventional DFT described in the last chapter. Here we can consider a kind of two-fluid model to help understand what is happening. In this type of model, there are different interac-
4.4. Multi-Potential Density Functional Theory (MPDFT)

Figure 4.4: Plot of the typical form of the interlayer potential, $U_{12}(r)$, shown as a function of total vortex separation for various values of $d$.

Figure 4.4: Plot of the typical form of the interlayer potential, $U_{12}(r)$, shown as a function of total vortex separation for various values of $d$.

Tions between the different particles making up the fluids. This is similar to the problem above, except there is only one type of particle, but two different types of interactions. Nevertheless it is possible to proceed in an analogous manner. The total interaction potential can be written as

$$U_{\text{tot}}(r, z) = U_{11}(r) + U_{12}(r)\delta(z - d),$$

where the definitions are as above. To calculate the freezing line in MPDFT requires two correlation functions, one for each component of the potential. These are calculated as before, by iterating the following equations,

$$c_{ij}(r) = \exp\{-\beta U_{ij}(r) + h_{ij}(r)\} - h_{ij}(r) - 1$$

$$\tilde{h}_{ij}(k) = \frac{\tilde{c}_{ij}(k)}{1 - \tilde{c}_{ij}(k)} - \bar{c}_{ij}(k).$$

The free energy functional used is a straightforward extension of the previous functional to include the different components, and can be written as (Rick and Haymet, 1989)

$$\Delta\beta\Omega = \sum_{i=1}^{\nu} \int dr \left\{ \rho_i(r) \ln \left[ \frac{\rho_i(r)}{\rho_i(0)} \right] - \rho_i(r) - \rho_0 \right\}$$

$$- \frac{1}{2} \sum_{i,j=1}^{\nu} \int dr_1 \int dr_2 c_{ij}(|r_1 - r_2|)[\rho_i(r_1) - \rho_0][\rho_j(r_2) - \rho_0],$$
4. Properties of the Pancake Vortex Lattice

where \( \nu \) is the number of components and \( \rho_{10} \) is the vortex density in layer \( i \). In this case, it can easily be seen that the density will be the same in each layer as the magnetic field is considered continuous, so \( \rho_{10} = \rho_{20} \). It is now possible to follow the procedure outlined in the last chapter to calculate the change in free energy. The result for the freezing line for the two-layered system, at a given layer separation of \( d = 5 \, \text{Å} \), is shown in figure 4.5.

It can be seen that the result is similar to that calculated earlier, which might be expected. As before, a calculation was performed for a pure two dimensional system, where it was found that the freezing temperature was again a constant. The freezing line for the full interacting system is seen to approach that for the 2D system for large applied fields, although it is seen that the form of the line differs from that obtained earlier, in that for lower temperatures the freezing line increases more rapidly. However, the form of the freezing line is in reasonable agreement with recent experimental results (Estrela et al., 1994) obtained for HgBa₂Ca₃Cu₄O_{10+\delta}. The exact position of the freezing line in the phase diagram is dependent on the

---

1It is worth mentioning a recent Bitter pattern experiment where both the upper and lower surfaces of the sample were measured simultaneously (Yao et al., 1994). Their results show that the number of vortices on each side of the sample were not, in general, equal. The implications of these measurements has been recently discussed by Cristina Marchetti and Nelson (Cristina Marchetti and Nelson, 1995).
interlayer spacing, due to the dependence of $U_{12}$ on $d$, as well as the extent of pinning centres inside the material. The final result shown is that for a value of $d = 5 \, \text{Å}$, a value chosen merely for convenience. As is evident from the derivation given, no attempt has been made to include pinning effects in the calculation, a shortcoming that was discussed at the end of Chapter 3, although it would be expected that the presence of pinning sites would raise the freezing line, due to the higher temperatures required for thermal depinning of the flux lines. No result has be presented for BSSCO, however, by comparison with the earlier calculation, it can be assumed that the two results would again be similar for reasons also discussed at the end of Chapter 3. As these two materials are known experimentally to exhibit different forms for their melting lines, it would appear that a more detailed model is required. Such a model must obviously be more dependent on the properties of the materials than the one presented here.

4.5 Summary

The results obtained from the analysis of the freezing transition for a two-layer system remain in general agreement with those from the last chapter. There are, however, some slight differences, such as a more rapid increase in the freezing line for lower temperatures. Adopting this rather simple model enables all the individual parts that make up the total force to be examined in isolation. When this is done, what is seen is that as the applied magnetic field is increased, the Josephson coupling between the layers starts to decrease. This means that higher fields tend to decouple the layers, and this would explain the approach to a 2D freezing temperature. At low temperatures, even with a very weak Josephson coupling, the magnetic interaction between the vortices still acts to align the vortices in different layers. However, as this magnetic force is very weak, the high values of temperature associated with these materials causes thermal fluctuations to destroy this magnetic alignment.

The MPDFT calculations predict a crossover in dimensionality which differs from that predicted for the BKT transition (Pierson, 1994). The crossover produced from the freezing transition can be seen to be a smooth changeover. The dimensionality is dependent on the applied magnetic field, where for a large enough field, say for example $H^*$, the system behaves like a 2D system. Of course, as mentioned above, $H^*$ would itself depend on the material properties. In contrast, the RG calculations predict a more abrupt change in dimensionality, occurring at a specific temperature. The exact role of the dimensional change would seem to require further study.

Some recent Monte Carlo calculations have been reported, also based on the Lawrence-Doniach model (Šášik and Stroud, 1995). These calculations shown that in a highly anisotropic layered superconductor, such as BSCCO, the 3D flux solid undergoes a smooth transition to a 2D solid, which then undergoes a melting tran-
sition to a flux liquid. If the system is only mildly anisotropic, like YBCO, then the 2D solid no longer appears in the phase diagram, and the liquid freezes directly into the 3D solid phase. It is thought that such a transition may explain effects observed in neutron scattering data from BSCCO materials.

One problem with the analysis presented above is that the effect of fluctuations has been ignored. It is possible to examine these effects through G-L theory as well as by measurements of the specific heat (Loram et al., 1992). It is seen that the effects of fluctuations can become quite large for a 2D system, and that as the interlayer correlation increases and the system generates a more 3D nature, the fluctuation effects decrease. Thus examining the 2D region would require the theory to take these fluctuations into account, going beyond the simple Gaussian approximation.

While the freezing transition may help to explain some of the observable effects, it is still quite a simple model. The effects of the material have not been taken into account, nor the complexities of the flux lines themselves. However for all its simplicity, it still explains in a general way what is observed and helps to conceptualise some of the subtleties of the interactions.

In the next chapter, the region of low magnetic field and $T$ close to $T_c$ will be examined. In this region the intervortex spacing is much larger than the penetration depth, and so interaction between the particles is much weaker than in the solid and liquid phases. Under these circumstances the system acts more like a gas of vortices.
Existence of the Vortex Gas

The last two chapters have put forward a possible explanation for the irreversible line. It was argued that due to the higher temperatures involved, along with other properties of the HTcs, it is possible for the usual Abrikosov lattice of flux lines to undergo a melting transition, to the flux liquid. It was shown that by examining this transition with the help of density functional theory, that the calculated freezing line was in reasonable agreement with experimental results for the irreversible line.

However, the freezing line was examined only over an intermediate temperature range. For temperatures closer to $T_c$ it is possible that more complicated behaviour occurs. In this region, the magnetic field is quite small, which in turn implies that the density of vortices is very low. In this region the intervortex separation is very much greater than the coherence length. Under these circumstances it is more appropriate to describe the system as a "vortex gas"\textsuperscript{1}. This short chapter will calculate the region of the magnetic phase diagram where this gas phase is speculated to exist. The consequences of this phase on the measurable properties of these materials will then be discussed.

5.1 The Vortex Gas Phase

The possibility of the existence of this phase can be easily demonstrated with the aid of a quick calculation. As mentioned earlier, the density of flux lines is proportional to the applied magnetic field,

$$\rho = \frac{B}{\phi_0}.$$ 

If the flux lines are considered to form an hexagonal lattice, then the lattice spacing, $a_0$, is given by

$$a_0 = \left(\frac{\sqrt{3} \phi_0}{4 B}\right)^{1/2},$$

\textsuperscript{1}se non è vero, è ben trovato
from which it can be seen that $a_0 \sim B^{-1/2}$. It is instructive to examine the value of $a_0$ for selected magnetic field values. For a field of 2.65 T, the lattice spacing is approximately 300 Å, while for a field of 0.0265 T, $a_0$ is approximately 3000 Å. The first value is within the range of the penetration depth, and therefore the vortices continue to mutually interact. The second value of $a_0$ is larger than the penetration depth, and so this region of low field is a good candidate for the gas phase.

A good test of this prediction would be to examine the form of the pair distribution function introduced in Chapter 3, $g(r)$, either side of the predicted crossover. This is performed by calculating $g(r)$ for two different magnetic fields, while the temperature is kept constant. The magnetic field values are chosen to be either side of the crossover line, as discussed above. In the gas phase there are no long range correlations between particles, resulting in the pair distribution function tending to unity as the separation of particles increases. An example of the distribution function for a HTcS in both the liquid and gas phases is shown in Figure 5.1. In the low field region the function clearly shows a lack of structure, and therefore an absence of correlation, and so can be argued to be evidence of the gas phase. In the higher field region the distribution function clearly shows the liquid structure found earlier, and so this can be assumed to be in the liquid phase. Therefore, at some intermediate field, a crossover between the two phases has taken place.
5.2. Experimental Consequences

Figure 5.2: The $H-T$ phase diagram for a HTcS showing the region of vortex gas close to $T_c$. The solid line marks the original freezing line, while the dashed line represents the predicted solid-gas crossover.

It is possible to calculate the position in the magnetic phase diagram of this crossover. However, because the transition to the gas state is continuous, an accurate identification of the crossover is very difficult to identify precisely, and so the position of the crossover shown in the phase diagram of Figure 5.2 should be treated only as approximate. This figure shows the phase diagram calculated earlier, but on an expanded scale close to $T_c$. The original freezing line is displayed, along with the predicted crossover line. It can be seen that this line bends back under the freezing line, implying a gas phase lying below the Abrikosov lattice phase.

If this gas phase does exist, the question is what effect does this have on the properties of these materials that can be verified experimentally?

5.2 Experimental Consequences

In the gas state, the average intervortex separation is large, and the interaction between vortices is much weaker than in the corresponding liquid state, which has important consequences for the effect of pinning centres. In the liquid state, when an individual vortex becomes pinned it is possible that it may depin due to the interactions of neighbouring vortices. In the gas state, because of the lower density of vortex lines, as well as the greater separation, there is a lower probability of such
an effect and therefore the pinning sites tend to be more effective. The consequence of this is that the critical current in this phase should be higher than the liquid phase, but lower than the lattice phase. Such an effect has indeed been observed in conventional superconductors, and is known as the Peak Effect (Pippard, 1969).

This effect derives its name from the peak in resistivity that is seen to arise for fields close to the upper critical field. In this model, this peak would occur when the system passes through the gas phase. The reason being that as the field is decreased, at a constant temperature below that at which the freezing line bends back, the system passes from the zero resistance Abrikosov lattice phase to a resistive gas phase. As the field is further lowered, the system then passes into the zero resistance Meissner phase. It is possible to measure the conductivity/resistivity of the material as a function of magnetic field at fixed temperature. If the temperature is chosen sufficiently close to $T_c$, it should be possible to pass through these different phases, and a corresponding peak in the resistivity should be observable. Such measurements have been performed on single crystal HTcS materials which have been found to exhibit this effect, see note added of Bhattacharya and Higgins (Bhattacharya and Higgins, 1994).

5.3 Summary

If the Peak Effect is indeed a measurable property of the HTcS, then the existence of the vortex gas phase would seem a viable explanation. The gas phase itself is a straightforward low density consequence of the vortex liquid. While there are obviously other explanations of this effect, the gas phase seems consistent with the melting hypothesis, and it would seem that the idea of the melting of the Abrikosov lattice is gaining a wider acceptance. An unfortunate consequence is that such a phase is not directly measurable, unlike, for example, the solid phase. Therefore it may be almost impossible to decide between alternate mechanisms put forward to explain this effect.
CHAPTER 6

Critical Current in a Granular Superconductor

The last chapter considered a model system for a layered superconductor whose layers were coupled via the Josephson effect. This chapter will extend the idea of Josephson coupling a little farther. The system under study consists of grains of superconducting material embedded in a “sea” of normal, non-superconducting, material — the so called granular superconductor. Each grain couples to its neighbours by means of Josephson coupling. Using such a model it is possible to examine the dependence of the maximum Josephson current as a function of both applied magnetic field and temperature. The behaviour of the current between the grains can then be used to make predictions about the critical current within HTcS materials.

There are several methods with which to approach this problem, however the one chosen is that of the Green’s function. As was mentioned in Chapter 1, the BCS theory has since been rewritten in terms of the Green’s function, and this will act as the basis for this calculation. The next section starts with a brief introduction to field theory of use to condensed matter physics, which will then lead to the definition of the Green’s function. BCS theory is then put into this language, and an expression for the Josephson current is derived. Finally, the Green’s functions for the system under study are calculated, from which the current can be found. For more details on the derivation the reader is referred to the references (Abrikosov et al., 1963; Fetter and Walecka, 1971).

6.1 Second Quantisation

Second quantisation is based on the definition of field operators, which can be expressed in terms of the standard wavefunctions,

\[ \psi(\xi) = \sum_i \phi_i(\xi) a_i \]
\[ \psi^+(\xi) = \sum_i \phi_i^*(\xi) a_i^+ \]
6. Critical Current in a Granular Superconductor

where $\phi$ is the usual wavefunction and $a (a^\dagger)$ is the usual destruction (creation) operator. The functions $\psi$ act as creation/destruction operators for particles in \( \xi \)-space. The usual commutation rules can be written down in terms of the field operators,

\[
\begin{align*}
\psi(\xi)\psi^+(\xi') \mp \psi^+(\xi')\psi(\xi) &= \delta(\xi - \xi') \\
\psi(\xi)\psi(\xi') \mp \psi(\xi')\psi(\xi) &= 0 \\
\psi^+(\xi)\psi^+(\xi') \mp \psi^+(\xi')\psi^+(\xi) &= 0,
\end{align*}
\]

where the upper sign is for Bose statistics and the lower for Fermi. In these variables it is possible to write down the standard Hamiltonian as,

\[
H = \int \left[ \frac{1}{2m} \nabla \psi^+_a(r) \cdot \nabla \psi_a(r) + U(r)\psi^+_a(r)\psi_a(r) \right] \, dr \\
+ \frac{1}{2} \int \psi^+_a(r)\psi^+_\beta(r)U_2 \psi_\beta(r)\psi_a(r) \, dr \, dr' + \cdots,
\]

with $\alpha$ and $\beta$ representing the spin degrees of freedom and $U$ representing the interaction potentials.

Having defined the field operators, it now remains to choose the most appropriate representation to work in. The usual representation used is the Schrödinger representation, where it is assumed that the operators contain no time dependence, all of which is taken into the wavefunctions. It is possible to define another representation, called the Heisenberg representation. This can be seen to follow directly from the Schrödinger equation, 

\[
i \frac{\partial \Psi}{\partial t} = H \Psi.
\]

The solution for $\Psi$ can be written down directly as,

\[
\Psi(t) = e^{-iHt}\Psi_H,
\]

where the subscript $H$ represents the Heisenberg representation. It can be seen that the Heisenberg wavefunction is now independent of time. It is now possible to write the operator in terms of this new representation,

\[
\hat{O}_{nm}(t) = \langle \Psi^*_n(t)\hat{O}\Psi_m(t) \rangle = \langle \Psi^*_n e^{iHt}\hat{O} e^{-iHt}\Psi_m \rangle,
\]

from which it is possible to identify the operator in the Heisenberg representation as

\[
\hat{O}_H(t) = e^{iHt}\hat{O} e^{-iHt}.
\]

So it can be seen that the time dependence has now been transferred from the wavefunction to the operator. The time dependence of the operator can be found from the useful identity,

\[
\frac{\partial \hat{O}}{\partial t} \equiv i[H, \hat{O}],
\]
6.1. Second Quantisation

which can quite easily be shown from above. It should be noted that this merely represents a different viewpoint for examining the problem, and both methods will produce the same results. Having said that, due to the shift in the time dependency, the commutation rules for wavefunctions at different times will not, in general, be equal.

Having presented the Heisenberg representation, the representation most useful in the Green’s function approach will now be presented. This new representation is called the interaction representation. The reason behind the name is derived from the process of separating the Hamiltonian into interacting and noninteracting parts,

\[ H = H_0 - H_{\text{int}}. \]

Then, in analogy with above, we can define the wavefunction in this representation to be

\[ \Psi_i = e^{iH_0 t} \Psi. \]  

If this form is substituted into the Schrödinger equation, it can be easily shown that,

\[ i \frac{\partial \Psi_i}{\partial t} = H_{\text{int}}(t) \Psi_i, \]

where

\[ H_{\text{int}}(t) = e^{iH_0 t} H_{\text{int}} e^{-iH_0 t}. \]

In the interaction representation, the wavefunctions are given by equation (6.1) and the operators are given by,

\[ \frac{\partial \hat{O}}{\partial t} = i[H_0, \hat{O}(t)], \]

which can be seen to be equivalent to the noninteracting Heisenberg picture. This means that in the interaction representation, the operators can be obtained from the noninteracting Heisenberg operators, while the wavefunctions can be obtained from the Schrödinger equation with Hamiltonian \( H_{\text{int}} \).

However not everything has been determined, there still remains the time dependence of the wavefunction, which is complicated by the fact that \( H_{\text{int}}(t) \) at different times does not commute. The way around this is as follows: if it is assumed that we know \( \Psi \) at some time \( t_0 \), then a solution for arbitrary \( t \) can be found from

\[ \Psi_i(t) = \Psi_i(t_0) - i \int_{t_0}^{t} H_{\text{int}}(t') \Psi_i(t') \, dt', \]

where the differential equation has now been converted to an integral equation. Using perturbation techniques, the solution to this equation can be written down in the form,

\[ \Psi_i(t) = \Psi^{(0)}_i + \Psi^{(1)}_i + \cdots, \]
where $\Psi_i^{(n)}$ is used to represent $\Psi_i(t_n)$. It can be easily shown that the solution for the $n$'th term takes the form,

$$\Psi_i^{(n)} = (-i)^n \int_{t_0}^{t} H_{\text{int}}(t_1) \, dt_1 \int_{t_0}^{t_1} H_{\text{int}}(t_2) \, dt_2 \cdots \int_{t_0}^{t_{n-1}} H_{\text{int}}(t_n) \, dt_n \, \Psi_i(t_0).$$

The whole solution can now be written down quite neatly by defining a function $S(t,t_0)$, such that

$$S(t,t_0) = 1 - i \int_{t_0}^{t} H_{\text{int}}(t_1) \, dt_1 + \cdots + (-i)^n \int_{t_0}^{t} H_{\text{int}}(t_1) \, dt_1 \cdots \int_{t_0}^{t_{n-1}} H_{\text{int}}(t_n) \, dt_n \, \Psi_i(t_0) + \cdots,$$

so that the wavefunction is given by

$$\Psi_i(t) = S(t,t_0) \Psi_i(t_0).$$

One thing to notice from the expression for $S(t,t_0)$ is that operators taken at later times are always on the left of those for earlier times. The expression can be made more symmetrical by a simple permutation of the time variables. While performing this permutation the time ordering of these products must be maintained. To achieve this it is possible to define a time ordering operator $T$, such that

$$T(\hat{A}(t) \hat{B}(t')) = \begin{cases} \hat{A}(t) \hat{B}(t') & t > t' \\ \pm \hat{B}(t') \hat{A}(t) & t < t' \end{cases},$$

so that the operator with the later time is always on the left. If the operators obey Fermi statistics a minus sign is introduced for each pair of operators exchanged. Using this, $S(t,t_0)$ can be simplified to,

$$S(t,t_0) = \frac{(-i)^n}{n!} \int_{t_0}^{t} \cdots \int_{t_0}^{t} T(H_{\text{int}}(t_1) \cdots H_{\text{int}}(t_n)) \, dt_1 \cdots dt_n,$$

or more concisely

$$S(t,t_0) = T \exp \left\{ -i \int_{t_0}^{t} H_{\text{int}}(t') \, dt' \right\}.$$

It is possible to use this result to derive the relationship between the interaction and Heisenberg representations. This relationship is derived under the assumption of the "adiabatically switched on" interaction. This means that at $t = -\infty$ there is no interaction, but afterwards it is turned on infinitely slowly. This, along with the relation

$$S(t_2,t_1)S(t_1,t_0) = S(t_2,t_0) \quad t_2 > t_1 > t_0,$$

can be used to show that

$$\Phi_i(t) = S(t)\Phi_H,$$
where
\[ S(t) = S(t, -\infty). \]
The relationship between operators can be shown to be of the form,
\[ \tilde{F}(t) = S^{-1}(t)F(t)S(t). \]

By making use of all the above, it is possible to rewrite the time ordered average of operators over the ground state,
\[
\langle \Phi_H^0 T(\tilde{A}(t)\tilde{B}(t')\tilde{C}(t'')\cdots)\Phi_H^0 \rangle = \langle \Phi_H^0 S^{-1}(t)A(t)S(t)S^{-1}(t')B(t')S(t')\cdots\Phi_H^0 \rangle
= \langle \Phi_H^0 S^{-1}(\infty)S(\infty,t)A(t)S(t,t')B(t')\cdots\Phi_H^0 \rangle
= \langle \Phi_H^0 S^{-1}(\infty)T(A(t)B(t')C(t'')\cdots S(\infty))\Phi_H^0 \rangle.
\]

It is still necessary, however, to determine
\[ \Phi_H^0 S^{-1}(\infty) = [S(\infty)]\Phi_H^0. \]

It follows from earlier definitions that
\[ \Phi_H^0 = \Phi_i(-\infty) \quad S(\infty)\Phi_H^0 = \Phi(\infty), \]
which shows that \( \Phi_i(\infty) \) is the function obtained from \( \Phi(-\infty) \) by turning on the interaction adiabatically. However, from quantum mechanics it is known that a system in a non-degenerate ground state cannot undergo a transition to a different state under the action of an infinitely slow perturbation. This means that the functions \( \Phi_i(\infty) \) and \( \Phi_H^0 \) can differ only by a phase factor,
\[ S(\infty)\Phi_H^0 = e^{i\omega} \Phi_H^0, \]
which in turn implies that,
\[
\langle \Phi_H^0 T(\tilde{A}(t)\tilde{B}(t')\tilde{C}(t'')\cdots)\Phi_H^0 \rangle = \frac{\langle \Phi_H^0 T(A(t)B(t')C(t'')\cdots S(\infty)\Phi_H^0 \rangle}{\langle \Phi_H^0 S(\infty)\Phi_H^0 \rangle}.
\]

This final expression remains valid only over the ground state, as the argument used above are not valid for excited states.

It is now possible to define, making use of the above ideas, the one particle Green’s function,
\[ G_{\alpha\beta}(x, x') = -i\langle T(\bar{\psi}_\alpha(x)\psi_{\beta}(x')) \rangle, \]
where \( x \) and \( x' \) represent the position and time coordinates and \( \alpha \) and \( \beta \) are spin indices. The notation has been simplified by using \( \langle \cdots \rangle \) to represent the average over the ground state given in equation (6.2). It is now possible to make direct use of this definition to rewrite the BCS Hamiltonian.
6.2 Green’s Function Approach to Superconductivity

Having reviewed the basis of the Green’s function, it seems appropriate to discuss its usefulness in describing superconductivity, and more importantly the intergrain Josephson current. To do this, the standard BCS Hamiltonian needs to be rewritten in the language of the Green’s function. The BCS Hamiltonian, in the Schrödinger representation, can be written as

\[ H = \int \left[ - \left( \psi^+ \frac{\nabla^2}{2m} \psi \right) + \frac{\lambda}{2} (\psi^+ \psi) \right] \, dr, \]

where the wavefunctions obey the usual commutation rules. It is possible to write this in the Heisenberg representation as

\[
\begin{align*}
\left( i \frac{\partial}{\partial t} + \frac{\nabla^2}{2m} \right) \psi_\alpha(x) - \lambda (\psi^+(x)\psi(x))\psi_\alpha(x) &= 0 \\
\left( i \frac{\partial}{\partial t} - \frac{\nabla^2}{2m} \right) \psi_\alpha(x) + \lambda \psi^+_\alpha(x)(\psi^+(x)\psi(x)) &= 0.
\end{align*}
\] (6.4)

By using the earlier definition of the Green’s function at zero temperature, equation (6.3), this reduces to expressions of the form,

\[
\left( i \frac{\partial}{\partial t} + \frac{\nabla^2}{2m} \right) G_{\alpha\beta}(x, x') + i\lambda \langle T((\psi^+(x)\psi(x))\psi_\alpha(x)\psi^+_\beta(x')) \rangle = \delta(x - x').
\]

It is possible to make use of Wick’s theorem to decompose the term consisting of four operators into pairs of operators. If the effects of scattering of particles by each other are neglected, it is possible to write these products such that the first two terms give a correction to the chemical potential, and thus can be ignored, and the other terms are of the form,

\[
\langle N | T(\psi^+ \psi) | N + 2 \rangle \langle N + 2 | T(\psi^+ \psi^+) | N \rangle.
\]

For a little more detail on this expansion see Section 34.1 of (Abrikosov et al., 1963). From here it is possible to define an anomalous Green’s function,

\[
\begin{align*}
\langle N | T(\psi_\alpha(x)\psi_\beta(x')) | N + 2 \rangle &= e^{-2i\mu t} F_{\alpha\beta}(x, x') \\
\langle N + 2 | T(\psi^+_\alpha(x)\psi^+_\beta(x')) | N \rangle &= e^{2i\mu t} F_{\alpha\beta}^+(x, x').
\end{align*}
\]

The exponential term arises from the definition of the time derivative of a quantum mechanical operator, and the chemical potential arises from \( \partial E/\partial N \), such that \( 2\mu = E_{2N} - E_N \). With the final definition that

\[ F_{\alpha\beta}(0+) = e^{2i\mu t} \langle N | T(\psi^+ \psi) | N + 2 \rangle \equiv \lim_{t \to +\infty} F_{\alpha\beta}(x, x'), \]
6.2. Green’s Function Approach to Superconductivity

It is possible to write the set of equations (6.4) as matrix equations of the form,

\[
\begin{pmatrix}
(i \frac{\partial}{\partial t} + \frac{\nabla^2}{2m}) G(x, x') - i\lambda \hat{F}(0+) \hat{F}^+(x, x') & = \delta(x - x') \\
(i \frac{\partial}{\partial t} - \frac{\nabla^2}{2m} - 2\mu) \hat{F}^+(x, x') + i\lambda \hat{F}^+(0+) \hat{G}(x, x') & = 0
\end{pmatrix}
\]

where the system is assumed to be homogeneous and the matrix elements are of the form \(G_{\alpha\beta}, F_{\alpha\beta}\) and \(F_{\alpha\beta}^+\).

The above derivation was given for zero temperature. What is actually required is a finite temperature version of these equations. It can be shown that the same arguments used above can be used for finite temperature. This means that the above derivation can be repeated again for \(T \neq 0\), which yields the following temperature expressions,

\[
\begin{aligned}
\left(-\frac{\partial}{\partial \tau} + \frac{\nabla^2}{2m} + \mu\right) \hat{G}(x, x') + \Delta \hat{F}^+(x, x') & = \delta(x - x') \\
\left(\frac{\partial}{\partial \tau} + \frac{\nabla^2}{2m} + \mu\right) \hat{F}^+(x, x') - \Delta \hat{G}(x, x') & = 0,
\end{aligned}
\]

where \(\tau\) is the imaginary time, \(it\), and the energy gap, \(\Delta\), has been defined through,

\[
\Delta = |\lambda| \hat{F}(0+), \quad \Delta^* = |\lambda| \hat{F}^+(0+).
\]

These expressions can easily be extended to account for an external magnetic field by making the substitution

\[
\nabla \to \nabla - i e A \quad \text{or} \quad \nabla \to \nabla + i e A,
\]

depending on which operator the differential acts. Ideally these expressions should be gauge invariant, however if the standard gauge test is performed, i.e. \(A \to A + \nabla \chi\), then the Green’s functions transform as,

\[
\begin{aligned}
\hat{G}(x, x') & = \hat{G}(x, x') \exp \left[i e (\chi(r) - \chi(r'))\right] \\
\hat{F}(x, x') & = \hat{F}(x, x') \exp \left[i e (\chi(r) + \chi(r'))\right] \\
\hat{F}^+(x, x') & = \hat{F}^+(x, x') \exp \left[-i e (\chi(r) + \chi(r'))\right].
\end{aligned}
\]

It is obvious that none of these functions are invariant under a change of gauge, which has some important ramifications that are discussed later. The set of equations (6.5) will serve as a starting point to examine the intergrain current as a function of small applied field.
6. Critical Current in a Granular Superconductor

6.3 Current in a Small External Field

All that remains to be done is to find an expression for the current in the presence of an external field. Unfortunately it is only possible to examine the system under the assumption that the external field is small compared with the critical field. For large fields, there are other effects that need to be taken into account, such as the "tunnelling" of flux lines between different grains for example. Under these conditions the problem is extremely difficult to solve, therefore expressions will be derived that are valid only for small fields.

The starting point is the second quantisation form for the current in an external field,

\[ j(x) = \frac{ie}{2m} (\nabla_{r'} - \nabla_r)_{r' \rightarrow r} (\tilde{\psi}(x')\tilde{\psi}(x)) - \frac{e^2}{m} A(x)(\tilde{\psi}(x)\tilde{\psi}(x)). \]

From the work above it is seen that this can easily be written down in the language of the Green's function,

\[ j(x) = 2 \left( \frac{ie}{2m} (\nabla_{r'} - \nabla_r) G(x, x') - \frac{e^2}{m} A(x) G(x, x') \right)_{r' \rightarrow r, r' \rightarrow r+0}. \]  

(6.8)

The next step involves finding the first order correction to the Green's functions due to the external field. This is made slightly easier by using the fact that in a constant field the Green's functions depend only on the difference in \( \tau_1 \) and \( \tau_2 \), so it is possible to take the Fourier transform with respect to these variables. This reduces equation (6.5) to

\[ \left( i\omega + \frac{1}{2m} (\nabla - ieA(r))^2 + \mu \right) G_\omega(r, r') + \Delta(r) \mathcal{F}^+(r, r') = \delta(r - r') \]
\[ -i\omega + \frac{1}{2m} (\nabla + ieA(r))^2 + \mu \right) \mathcal{F}^+_\omega(r, r') - \Delta^*(r) G_\omega(r, r') = 0, \]

(6.9)

where the subscript \( \omega \) represents the imaginary time Fourier transform. Linear in the field correction, the Green's functions become

\[ G = G_0 + G^{(1)}, \quad \mathcal{F} = \mathcal{F}_0 + \mathcal{F}^{(1)}, \quad \mathcal{F} = \mathcal{F}_0^+ + \mathcal{F}^{+(1)}, \]

and when substituted into equation (6.9) produce the following expressions,

\[ \left( i\omega + \frac{\nabla^2}{2m} + \mu \right) G_\omega^{(1)}(r, r') + \Delta^{(0)} \mathcal{F}^{+(1)}_\omega(r, r') = -\Delta^{(1)}(r) \mathcal{F}^{+(1)}_\omega(r - r') + \frac{ie}{2m} (\nabla \cdot A(r) + A(r) \cdot \nabla) G_\omega(r - r') \]
\[ \left( -i\omega + \frac{\nabla^2}{2m} + \mu \right) \mathcal{F}^{+(1)}_\omega(r, r') - \Delta^{(0)} G_\omega^{(1)}(r, r') = \Delta^{*(1)}(r) G_\omega(r - r') - \frac{ie}{2m} (\nabla \cdot A(r) + A(r) \cdot \nabla) \mathcal{F}^{+(1)}_\omega(r - r'). \]

(6.10)
Equations (6.9) and (6.10) are both gauge invariant, this means that in this linear approximation the current can only depend on the transverse part of the vector potential. But equation (6.7) showed that the Green's functions are not gauge invariant, and so therefore from equation (6.6) neither is \( \Delta^{(1)} \). In the general case, \( \Delta^{(1)} \) is an unknown function of the vector potential. However, in the homogeneous case \( \Delta^{(1)} \) is a scalar, and therefore depends only on \( \nabla \cdot A \). So if the gauge is chosen so that the divergence of \( A \) is zero, then the problem becomes much simpler. In the inhomogeneous case this argument no longer holds and \( \Delta^{(1)} \) will now be dependent on both the longitudinal and transverse components of the vector potential. It is possible, however, to choose the longitudinal component of the form \( A_1(r) = \nabla \chi \), such that \( \Delta^{(1)} \) is again zero. The function \( \chi \) that achieves this is found from the condition that \( \nabla \cdot j = 0 \). It should be noted that the problem of gauge invariance in superconductivity has received much attention and more details can be found on this problem in Schrieffer (Schrieffer, 1964), where the gauge invariance of the BCS theory is discussed in detail.

So if the vector potential is chosen with sufficient care, it is possible to express the first order change in the Green's functions in terms of the zero field solutions. This expression makes use of the matrix form of equation (6.5),

\[
\begin{pmatrix}
-\frac{\partial}{\partial r} + \frac{v^2}{2m} + \mu \\
-\Delta^* 
\end{pmatrix}
\begin{pmatrix}
\Delta \\
-\frac{\partial}{\partial r} + \frac{v^2}{2m} + \mu 
\end{pmatrix}
\begin{pmatrix}
G(x, x') \\
F(x, x')
\end{pmatrix}
= \hat{i},
\]

which can be written as

\[
\hat{G}^{-1} \hat{G} = \hat{i}.
\]

Making use of this, it is possible to write the solution for \( G^{(1)} \) from equation (6.10) as,

\[
G^{(1)}(r, r') = \frac{ie}{m} \int \left\{ G_{\omega\ell}(r, \ell) [A(\ell) \cdot \nabla_{\ell} \nabla_{\ell}] G_{\omega\ell}(\ell, r') + F_{\omega\ell}(\ell, r) [A(\ell) \cdot \nabla_{\ell} F^+_{\omega\ell}(r', \ell)] \right\} \, d\ell.
\]

Once this expression has been obtained, it is sufficient to substitute it back into equation (6.8) to enable the current to be calculated in terms of the Green's functions calculated in the absence of the magnetic field,

\[
j(r) = \frac{e^2}{m^2} T \sum_{\omega} (\nabla_r - \nabla_{r'}) \int \left\{ G_{\omega\ell}(r, \ell) [A(\ell) \cdot \nabla_{\ell} \nabla_{\ell}] G_{\omega\ell}(\ell, r') + F_{\omega\ell}(\ell, r) [A(\ell) \cdot \nabla_{\ell} F^+_{\omega\ell}(r', \ell)] \right\} \, d\ell - \frac{Ne^2}{m} A(r).
\]

Therefore to calculate the current, the zero field Green's functions are first required, and their calculation is presented next.
6. Critical Current in a Granular Superconductor

6.4 Zero Field Green's Functions

To calculate the Josephson current between superconducting grains, it is useful to introduce a rather simple model. This model consists of three regions: region-I covers from $-\infty < z < -d/2$, region-II covers $-d/2 \leq z \leq d/2$ and region-III covers $d/2 < z < \infty$, the system is assumed homogeneous along the $x$ and $y$ directions. Regions-I and III are superconducting, and sandwich region-II which is normal. This is shown diagrammatically in Figure 6.1. There are several ways of examining this type of junction, such as by use of the Bogoliubov-de Gennes equation (Furusaki and Tsukada, 1991), but the method that will be used here is that of the Green's function. The following method of obtaining the zero field Green’s function is taken from Golub and Horovitz (Golub and Horovitz, 1994). As it is only the final expressions for the Green’s functions that are required, the final solution will simply be quoted, those interested in the derivation are directed to the original publication. The Green’s functions can be written in each of the regions as:

Region-I

$$F_{0\omega}^+(z, z') = a_1 e^{i\lambda z} + a_2 e^{-i\lambda z},$$

$$G_{0\omega}(z, z') = -\frac{i}{\Delta} \left[ a_1 \omega_+ e^{-i\lambda z} - a_2 \omega_- e^{i\lambda z} \right]$$

Region-II

$$F_{0\omega}^+(z, z') = c_1 e^{i\kappa z} + c_2 e^{-i\kappa z}$$

$$G_{0\omega}(z, z') = d_1 e^{i\kappa z} + d_2 e^{-i\kappa z} \quad z < z'$$

$$= e_1 e^{i\kappa z} + e_2 e^{-i\kappa z} \quad z > z'$$

Figure 6.1: Schematic diagram illustrating the regions of superconducting and normal materials used to model a granular superconductor.
Region-III \[ F_{\alpha\omega}^+(z, z') = b_1 e^{i\lambda_\alpha z} + b_2 e^{-i\lambda_\alpha z} \]
\[ G_{\alpha\omega}(z, z') = -i \frac{e^{i\kappa_\alpha}}{\Delta} \left[ b_1 \omega_+ e^{i\lambda_\alpha z} - b_2 \omega_- e^{-i\lambda_\alpha z} \right], \]
where in addition it has been assumed that \( m \equiv m_\alpha = m_\kappa \) for simplicity. The definition of the various functions are as in Horovitz. It can easily be shown that these functions satisfy equation (6.9), as required. At the boundary between the inner and outer regions it is possible to make use of the continuity of the functions to solve for the unknown coefficients \( a-d \). The delta function in the first of equations (6.9) introduces a discontinuity in the derivative of \( G_{\alpha\omega} \) at the boundaries, such that
\[ \frac{\partial}{\partial z} G_{\alpha\omega}(z, z') \bigg|_{z \to z' + (\pm d/2)} - \frac{\partial}{\partial z} G_{\alpha\omega}(z, z') \bigg|_{z \to z' - (\pm d/2)} = 2m. \]
These continuity equations can be used to show that it is possible to express \( e_i \) in terms of \( d_i \),
\[ e_1 = d_1 + \beta(z') \]
\[ e_2 = d_2 - \tilde{\beta}(z'), \]
where
\[ \beta(z) = \frac{m}{\iota k_\kappa} e^{-i\kappa_\alpha z} \]
\[ \tilde{\beta}(z) = \frac{m}{\iota k_\kappa} e^{i\kappa_\alpha z}. \]
What remains are eight equations enabling a solution for the eight unknown coefficients \( a_1, \ldots, d_2 \). It is possible to express this system in terms of matrices, where the multiplication factors of the unknowns are denoted by the \( 8 \times 8 \) matrix \( M \), whose components are of the form \( m_{11} = \exp(-i\lambda_\alpha/2) \), and the right hand side values are denoted by the 8-dimensional vector \( C \). It can be shown that \( C \) has a simple form, with all the components except \( c_7 \) and \( c_8 \) being identically zero. The solution matrix for the coefficients is given by,
\[ S = M^{-1} \times C. \]
The expressions for these components are quite lengthy, although quite straightforward to calculate, and so for brevity they will be referred to as \( s_{ij} \). Once the forms of the coefficients are known, it is possible to substitute the full expressions for \( F_{\alpha\omega} \) and \( G_{\alpha\omega} \) into equation (6.11). Before performing this step, it is important to note that the limits on the integral over \( \ell \) (or in this simplified geometry, \( \bar{z} \)) is not infinite. Once the superconducting regions are penetrated by a distance greater than the coherence length, knowledge of the existence of this region is lost. Therefore it would seem that a reasonable approximation would be to replace the upper and
lower limits by ±(d/2 + ξ). The equation to be solved for the current along the
z-axis then simplifies to,

\[ j_z(z) = \frac{e^2}{m^2} T \sum_\omega \left( \frac{\partial}{\partial z} - \frac{\partial}{\partial z'} \right) \int_{z'-z} \int_{-(d/2 + \xi)}^{d/2 + \xi} dp \, dz \left\{ G_{0w}(z, \bar{z}) \mathcal{A}_y(\bar{z}) G_{0w}(\bar{z}, z') + \mathcal{F}_{0w}(\bar{z}, z) \mathcal{A}_y(\bar{z}) \mathcal{F}_{0w}^*(\bar{z}', \bar{z}) \right\} - \frac{Ne^2}{m} \mathcal{A}_y(\bar{z}), \] (6.12)

where a choice of gauge has been made and a Fourier transform has been performed
with respect to both the x and y coordinates.

6.5 Simplification of the Current Expressions

Having set up the expression for the current in terms of the zero field Green’s
functions, it is possible to simplify the expressions further by analytically performing
the integral over \( \bar{z} \) as well as the derivatives with respect to \( z \) and \( z' \). It is necessary
to perform the integral separately in each of the three regions, taking extra care
with \( G_{0w}(z, z') \) to handle the separate cases of \( z < z' \) and \( z > z' \). The calculation
will be presented for just a single term of the integral in just one of the regions, due
to the similarity of the steps performed for the other terms.

The calculation of the first term in region-I starts by expressing \( a_1 \) and \( a_2 \) in
terms of the solution matrix, \( S \),

\[ a_1 = s_{17} \beta(z)e^{ikn d/2} + \beta(z)e^{-ikn d/2} + s_{18} \left( ik_n \beta(z)e^{ikn d/2} - ik_n \beta(z)e^{-ikn d/2} \right) \]
\[ = \beta(z) \left( s_{17} e^{ikn d/2} + ik_n s_{18} e^{ikn d/2} \right) + \beta(z) \left( s_{18} e^{-ikn d/2} - ik_n s_{17} e^{ikn d/2} \right) \]
\[ = \delta_{11}^a \beta(z) + \delta_{13}^a \tilde{\beta}(z) \]
\[ a_2 = \delta_{31}^a \beta(z) + \delta_{32}^a \tilde{\beta}(z). \]

In these expressions the forms for the coefficients \( c_i \) have been substituted for ex­
plicitly. Expanding the Green’s functions gives,

\[ G_{0w}(z, \bar{z}) A_y(\bar{z}) G_{0w}(\bar{z}, z') = -B_0 \bar{z} \left[ g_1(a(z, z') a_1(\bar{z}) e^{i\lambda_s z} + g_2(a(z, z') a_2(\bar{z}) e^{i\lambda_s z} \right. \]
\[ + g_3(a(z, z') a_1(\bar{z}) e^{-i\lambda_s z} + g_4(a(z, z') a_2(\bar{z}) e^{-i\lambda_s z} \right] \],

where the dependence on \( z \) and \( z' \) has been hilighted by making the definitions,

\[ g_1(z, z') = \gamma^2 a_1(z'), e^{i\lambda_s z} \]
\[ g_2(z, z') = \gamma \gamma^2 a_1(z') e^{-i\lambda_s z} \]
\[ g_3(z, z') = \gamma \gamma^2 a_2(z') e^{i\lambda_s z} \]
\[ g_4(z, z') = \gamma^2 a_2(z') e^{-i\lambda_s z}. \]
and
\[ \gamma_2 = -\frac{i\omega_+ e^{i\varphi_2}}{\Delta}, \]
\[ \tilde{\gamma}_2 = \frac{i\omega_- e^{i\varphi_2}}{\Delta}. \]

It is now possible to substitute for \( a_1 \) and \( a_2 \) to give,
\[ G_{\omega_0}(z, \bar{z}) A_{\omega_0}(\bar{z}) G_{\omega_0}(\bar{z}, z') = -B_0 \bar{z} \left[ \Gamma_{12}^a(z, z') \beta(\bar{z}) e^{i\lambda_+ z} + \Gamma_{34}^a(z, z') \beta(\bar{z}) e^{-i\lambda_+ z} \right. \]
\[ + \Gamma_{12}^a(z, z') \beta(\bar{z}) e^{i\lambda_- z} + \Gamma_{34}^a(z, z') \beta(\bar{z}) e^{-i\lambda_- z} \],

where
\[ \Gamma_{12}^a(z, z') = \delta_{12}^a g_1^a(z, z') + \delta_{21}^a g_2^a(z, z') \]
\[ \Gamma_{34}^a(z, z') = \delta_{13}^a g_3^a(z, z') + \delta_{24}^a g_4^a(z, z') \]
\[ \Gamma_{12}^a(z, z') = \delta_{12}^a g_1^a(z, z') + \delta_{22}^a g_2^a(z, z') \]
\[ \Gamma_{34}^a(z, z') = \delta_{13}^a g_3^a(z, z') + \delta_{24}^a g_4^a(z, z'). \]

So the integral over \( \bar{z} \) for the first region can be written as,
\[ -\frac{B_0}{ik_n} \int_{-\xi}^{-\xi} d\bar{z} \left\{ \Gamma_{12}^a(z, z') \bar{z} e^{i(\lambda_+ - k_n)z} + \Gamma_{34}^a(z, z') \bar{z} e^{-i(\lambda_+ + k_n)z} \right. \]
\[ \left. - \Gamma_{12}^a(z, z') \bar{z} e^{i(\lambda_+ + k_n)z} - \Gamma_{34}^a(z, z') \bar{z} e^{-i(\lambda_+ - k_n)z} \right\}, \]

and after some simple algebra, this reduces to,
\[ \int_{-\xi}^{-\xi} G_{\omega_0}(z, \bar{z}) A_{\omega_0}(\bar{z}) G_{\omega_0}(\bar{z}, z') = \eta_1^a \Gamma_{12}^a(z, z') + \eta_2^a \Gamma_{34}^a(z, z') \]
\[ + \eta_3^a \Gamma_{12}^a(z, z') + \eta_4^a \Gamma_{34}^a(z, z'), \]

along with the definitions,
\[ \eta_1^a = -\frac{B_0}{ik_n(\lambda - k_n)^2} \left[ e^{-i(\lambda - k_n)d/2} (1 + i(\lambda - k_n)\frac{d}{2}) - e^{-i(\lambda - k_n)\xi} (1 + i(\lambda - k_n)\xi) \right] \]
\[ = -\frac{B_0}{2ik_n} \left( \frac{d^2}{4} - \xi^2 \right) \quad \text{for} \ \lambda = k_n \]
\[ \eta_2^a = -\frac{B_0}{ik_n(\lambda^* + k_n)^2} \left[ e^{i(\lambda^* + k_n)d/2} (1 + i(\lambda^* + k_n)\frac{d}{2}) - e^{i(\lambda^* + k_n)\xi} (1 + i(\lambda^* + k_n)\xi) \right] \]
6. Critical Current in a Granular Superconductor

\[
\eta_2^a = \frac{B_0}{ik_n(\lambda_s + k_n)^2} \left[ e^{-i(\lambda_s + k_n)d/2} (1 + i(\lambda_s + k_n)\frac{d}{2}) - e^{-i(\lambda_s + k_n)\xi} (1 + i(\lambda_s + k_n)\xi) \right]
\]

\[
\eta_4^a = \frac{B_0}{ik_n(\lambda_s - k_n)^2} \left[ e^{i(\lambda_s - k_n)d/2} (1 + i(\lambda_s - k_n)\frac{d}{2}) - e^{i(\lambda_s - k_n)\xi} (1 + i(\lambda_s - k_n)\xi) \right]
\]

\[
\eta_4^a = \frac{B_0}{2ik_n} \left[ \frac{d^2}{4} - \xi^2 \right] \quad \text{for} \quad \lambda_s = -k_n
\]

The derivation of the other terms is analogous, and will not be presented. Having carried out the integration over \( \bar{z} \), there still remains the derivative. Taking the derivative is a two stage process: first the individual derivatives are taken, with respect to \( z \) and \( z' \), and then the limit \( z' \to z \to 0 \) is taken. The first step is to perform the \( z' \) derivative,

\[
\frac{\partial}{\partial z'} \Gamma_{12}^a = \frac{\partial}{\partial z'} \left[ \delta_{11}^a \gamma_1^a(z', z') + \delta_{21}^a \gamma_2^a \right]
\]

\[
\frac{\partial}{\partial z'} \Gamma_{34}^a = -m \left[ \delta_{11}^a \gamma_2^a \gamma_2^a e^{i(\lambda_z - k_z)z'} + \delta_{11}^a \gamma_2^a \gamma_2^a e^{i(\lambda_z + k_z)z'} + \delta_{21}^a \gamma_2^a \gamma_2^a e^{i(\lambda_z + k_z)z'} + \delta_{21}^a \gamma_2^a \gamma_2^a e^{i(\lambda_z - k_z)z'} \right]
\]

The derivative with respect to \( z \) is less involved, and gives,

\[
\frac{\partial}{\partial z} \Gamma_{12}^a = \frac{i \lambda_s}{2} \left[ \delta_{11}^a \gamma_2^a \lambda_s - \delta_{21}^a \gamma_2^a \lambda_s \right]
\]

\[
\frac{\partial}{\partial z} \Gamma_{34}^a = \frac{i \lambda_s}{2} \left[ \delta_{11}^a \gamma_2^a \lambda_s - \delta_{21}^a \gamma_2^a \lambda_s \right]
\]
6.6 Calculation of the Current

\[
\begin{align*}
\frac{\partial}{\partial z} \Gamma_{12}^a &= i a_1(z') \left[ d_{12}^a \gamma_2^2 \lambda_s - d_{22}^a \gamma_2^2 \lambda_s^* \right] \\
\frac{\partial}{\partial z} \Gamma_{34}^a &= i a_2(z') \left[ \delta_{12}^a \gamma_2 \lambda_s - \delta_{22}^a \gamma_2 \lambda_s^* \right].
\end{align*}
\]

The final result is achieved by taking the limit \( z' \to z \) followed by the limit that \( z \to 0 \). It is quite straightforward to calculate this limit from the expressions given by making use of,

\[
a_1 \to \frac{m}{ik_n} (\delta_{11}^a - \delta_{21}^a)
\]

\[
a_2 \to \frac{m}{ik_n} (\delta_{21}^a - \delta_{22}^a).
\]

Once again, the other terms appearing in the integral of equation (6.12) can be calculated in an analogous manner, and will not be shown.

All that now remains to be calculated in equation (6.12) is the momentum integral and the frequency sum, both of which can be performed numerically. To perform the remainder of the calculation, several parameters are required as input to the computer program. These are:

- The phase on either side of the region-II, \( \varphi_1 \) and \( \varphi_2 \).
- The reduced temperature, \( t \).
- The energy gap, which can be approximated by \( \Delta = \Delta_0 (1 - t)^{1/2} \), where the value of \( \Delta_0 \) can be taken from values sensible for HTcS.
- The applied magnetic field.
- The intergrain spacing, \( d \).

It is then possible to calculate the current for various values of temperature and magnetic field, and find its dependence on these parameters.

6.6 Calculation of the Current

Having derived the final terms involved in the current expression, it simply remains to obtain a solution. Unfortunately, when trying to obtain a numerical solution some numerical instability appears. At present this instability has not yet been overcome, and therefore a general set of solutions has so far not been obtained. It has been possible to generate values of current at selected temperatures under a small magnetic field, and these are shown in Figure 6.2. It can be seen from the figure that the temperature dependence of the critical current is consistent with known forms (Narlikar, 1994). However, until all of the stability problems are resolved, it is possible that the solution may be slightly more fortuitous than reliable.
That being said, it is possible to examine the form of the current close to the critical temperature. In this region a comparison of the temperature dependence can be made by fitting the solution to the form

$$J_c(T) \propto (T - T_c)\alpha.$$  

When this is performed, it is found that $\alpha \approx 1.4$, which is in reasonable agreement with the range of values known to exist for the various types of junctions (Narlikar, 1994).

6.7 Summary

A system of superconducting grains coupled via the Josephson effect has been examined. The property that was of interest was the critical Josephson current between the grains as a function of magnetic field. To calculate this current for small magnetic fields a linear response approximation has been made. Through such a method, it is possible to derive expressions for the current that depend only on the Green's functions in the absence of magnetic field, which are more straightforward to calculate.

Unfortunately, due to time limitations, this current work has not been completed. However, some preliminary solutions have been obtained, that show that
the calculated critical current agrees with previous work. While such results show promise, they should not be heavily relied upon until all the of the remaining problems with this method have been overcome. It is hoped that the numerical approach can be stabilised to allow a wider range of solutions to be obtained. In addition, it may also be possible to attempt to perform some of the remaining steps analytically, such as parts of the frequency sum for example. This will, however, need to be left for future work.
6. Critical Current in a Granular Superconductor
CHAPTER 7

Conclusion

This thesis has been concerned with a study of the behaviour of the flux lines inside a high temperature superconductor. Such knowledge is motivated by a need to understand the low values of critical current found in these materials, which greatly restricts their usefulness in real world applications.

It was shown that much interest has been devoted to studying the irreversible line. Many of the theoretical ideas that have been proposed to explain it were presented. It was argued that this line in fact represents a freezing transition between a flux liquid and a flux solid. Such a model was able to offer a relatively simple explanation for the drop in critical current after crossing the irreversible line, due to changes in the effectiveness of pinning centres. The freezing transition itself was studied in detail in Chapter 3, where a calculation based on density functional theory was presented. Such a calculation relies only on a knowledge of the density of the system under study, and in the HTcS materials this density is dependent on the value of applied magnetic field. In addition to the density, the interaction potential of the "particles" was also required. In this problem, the classical particles were identified with the pancake vortices present in the superconducting layers. Initially this potential was taken from the literature. It was then possible to use the theory developed to calculate the freezing temperature of the flux liquid for various values of magnetic field, enabling the calculated freezing line in the $H-T$ plane to be compared with experiment. Such a comparison showed that the results obtained were in good agreement with some HTcS materials but not with others. The explanation put forward for this discrepancy was that certain intrinsic properties of the materials, such as pinning centres etc., would effect the freezing of the flux lines, and that such properties were not included in the density functional theory formulation. It was argued that if such properties could be included in an improved theory, then better agreement ought to be obtained.

Because the theory is very much dependent on the form of the interaction potential, this was then studied in a little more detail. To do this, a simple model was constructed that consisted of just two superconducting layers coupled through a Josephson interaction. First, the form of the magnetic field surrounding the layers
due to the presence of vortices was calculated. This was then used to calculate the interaction of pancake vortices in the same layer. The intraplane interaction was more complicated to calculate, and the Lawrence-Doniach model was chosen as a starting point. From this, it was possible to construct the interaction between layers as a function of total vortex separation. After obtaining both these functions, a full 3D potential was constructed, and then used in an extended density functional calculation. The results obtained were in good agreement with those found earlier, however it was now possible to isolate the effects of material parameters on the freezing line. The results showed that as the layer spacing was increased, the interaction between layers decreased, as expected. It was also seen that the layers similarly decoupled with increasing field. In addition it was shown that the calculated transition showed a smooth crossover, from a 3D behaviour of the system to a 2D behaviour, as the applied magnetic field was increased. This was contrasted with renormalisation group calculations, which show a crossover occurring at a specific temperature.

Having obtained the freezing line, its low field-high temperature properties were examined. In this region the interparticle spacing is much larger than the interaction range, and so the system is better imagined as a vortex gas. The pair distribution function was calculated, and used to show that below a certain point correlations between individual flux lines vanish, signifying the gas phase. The approximate position of this transition was shown on the phase diagram. It was predicted that while such a phase was not directly observable, it should be measurable as a peak in the resistivity.

Finally, the critical current for a granular superconductor was examined. This was calculated by assuming weak-link connections between the grains, and then finding the Josephson current. The method of Green's functions was employed, and the current expression derived in the linear response approximation, valid for small fields. The final expressions were found to be quite involved, and due to time limitations only preliminary results have so far been obtained. These results show that the temperature dependence of the critical current in a magnetic field is consistent with earlier experimental results. It is hoped that if numerical difficulties can be overcome, then it should be possible to obtain a wider set of solutions.

In summary, the various transitions undergone by flux lines in HTcS materials has been examined. Such transitions have implications for the magnitude and form of the critical current. It was shown that the freezing transition was a reasonable model, and predicted a form for the irreversible line at low magnetic field that was in good agreement with experiment. The actual interaction of the flux lines was calculated to provide a more consistent 3D potential, and to help isolate the effect of the material parameters. An extension of the freezing idea for very low vortex density predicted the existence of the vortex gas phase, whose presence should be measurable through the Peak effect. Future work in this direction would involve...
calculating the melting line, and comparing this to the freezing line. This comparison would hopefully show the presence of magnetic hysteresis that is known to occur in these materials. Finally, the critical current in a granular superconductor under an applied field was examined. The form of the critical current as a function of temperature was found to be consistent with known results, although problems with the calculation remain to be resolved. It is hoped that if these problems are overcome in the future, more meaningful results can be obtained.
7. Conclusion
A.1 Properties of the Energy Functional

The derivation of density functional theory makes use of certain properties of the functional. These properties are straightforward to derive, and are presented here for completeness.

The first proof is that the equilibrium distribution function,

\[ f_0 = \frac{1}{\Xi} \exp[-\beta(H - \mu N)] , \]

is a true minimum of the Grand potential. To show this, first start by choosing some other function, \( f \), such that \( f \neq f_0 \). Substituting this function into the Grand potential gives,

\[ \Omega[f] = \text{tr}_{\text{Cl}} f \left( H - \mu N + \frac{1}{\beta} \ln f \right) \]
\[ = \text{tr}_{\text{Cl}} f \left( -\frac{1}{\beta} \ln f_0 - \frac{1}{\beta} \ln \Xi + \frac{1}{\beta} \ln f \right) \]
\[ = \Omega[f_0] + \frac{1}{\beta} (\text{tr}_{\text{Cl}} f \ln f - \text{tr}_{\text{Cl}} f \ln f_0) \]
\[ > \Omega[f_0] , \quad (A.1) \]

which verifies that \( f_0 \) is indeed a minimum of the potential.

The proof that \( f_0 \) is a unique functional of \( \rho_0 \), which is in turn determined uniquely by the external potential, \( V_{\text{ext}}(r) \), starts by assuming the contrary — that is that \( V_{\text{ext}}(r) \) and \( V'_{\text{ext}}(r) \) give rise to the same function \( \rho_0(r) \),

\[ \Omega' = \text{tr}_{\text{Cl}} f' \left( H - \mu N + \frac{1}{\beta} \ln f' \right) \]
\[ < \text{tr}_{\text{Cl}} f_0 \left( h' - \mu N + \frac{1}{\beta} \ln f_0 \right) \]
\[ = \Omega + \text{tr}_{\text{Cl}} f_0 (V'_{\text{ext}}(r) - V_{\text{ext}}(r)) \]
\[ = \Omega + \int dr \rho_0(r) (V'_{\text{ext}}(r) - V_{\text{ext}}(r)) , \quad (A.2) \]
exchanging the primed and unprimed functions leads to,

$$\Omega < \Omega' + \int dr \rho_0(r)(V_{\text{ext}}(r) - V'_{\text{ext}}(r)).$$ \hspace{2cm} (A.3)

The addition of equations (A.2) and (A.3) results in

$$\Omega + \Omega' < \Omega' + \Omega,$$

which is of course a contradiction, thereby proving that \( f_0 \) is indeed a unique functional of the density.

Finally, it is possible to show that \( \Omega_V \) is minimised at \( \rho = \rho_0 \). To this end, if it is assumed that \( f' \) corresponds to some other density \( \rho' \) then,

$$\Omega[f'] = \text{tr}_\text{cl} f' \left( H - \mu N + \frac{1}{\beta} \ln f' \right)$$

$$= \int dr \rho'(r)V_{\text{ext}}(r) + \mathcal{F}[\rho'] - \mu \int dr \rho'(r)$$

$$= \Omega_V[\rho'].$$

As was shown above, \( \Omega[f_0] < \Omega[f'] \) and therefore \( \Omega[\rho_0] < \Omega[\rho'] \) as required.


Bibliography


McQuarrie, D. A. 1976. *Statistical Mechanics*. New York: Harper & Row. The derivation of these equations is discussed in many advanced books on statistical mechanics. The equations can be derived from graphical expansions or functional analysis, as well as by plausible arguments.


