Vortices and vortex structures in mesoscopic and nano-superconductors

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Vortices and Vortex Structures
in Mesoscopic and Nano-superconductors

by

Wai Man Wu

A Doctorial Thesis
Submitted in Partial Fulfillment of the Requirements
for the Award of the degree
Doctor of Philosophy
of
Loughborough University

Supervisor: Dr. Binoy Sobnack
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Abstract

The study is an investigation of the nucleation of quantised vortices in mesoscopic superconducting discs and superconducting nanowires. Vortices nucleate in these systems when an applied magnetic field penetrates into the systems. A quantised vortex always carries a discrete quantum of flux. The vortex lattices in bulk samples are known to be triangular. However, in a small confined superconductor, the pattern of the vortices will be different. This is due to the fact that the effect of the boundary effect cannot be ignored in the small sample.

It is interesting to understand how the presence of a boundary influences the pattern of vortices in a mesoscopic superconducting disc. To start with, we shall use London’s equations. To study the systems at finite temperatures, one needs to include the entropy associated with the configuration of vortices. We also study the systems using Ginzburg-Landau equations.

Recent experimental studies on Pb (lead) superconducting nanowires has found that at low temperatures far from the superconducting transition temperature, the response of the wires to a transverse applied magnetic field shows hysteresis, namely Type II response: the magnetisation curves are different under magnetic heating and cooling. Lead is a Type I superconductor and the experimental results are puzzling. The research involves a detailed numerical study of the response of Pb nanowires in applied magnetic fields at different temperatures using Ginzburg-Landau equations.
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1 Introduction

1.1 Superconductivity - Overview

Helium was liquefied in 1911 and at the same time, it was found that the resistivity of mercury (Hg) suddenly dropped to zero at $T_c \approx 4.2K$. The critical temperature $T_c$ separates the two phases of mercury: below 4.2K, mercury is a superconductor and above a normal metal. Further, it was found that there was super-current remaining in the mercury sample for a long period without dissipation. At that time, it was common understanding that the properties of superconductor were the same as the perfect conductor.

A few decades later, a series of experiments showed that there should be some fundamental differences between the superconductor and the perfect conductor. For a superconductor, the local magnetic field inside the sample is zero, $B_{\text{local}} = 0$. The superconductor always excludes the external magnetic field and the field only penetrates into the surface of the sample.

Take a superconductor and put it in the magnetic field at $T > T_c$. As the temperature is decreased down to $T < T_c$, the sample changes to the superconducting phase and excludes all the external field. This is the so-called 'Meissner-Ochsenfeld Effect'. See Figure 1.

For a perfect conductor, it is not always that the sample expels the external magnetic field at $T < T_c$. It depends on the history. For example, if the external field already existed when $T > T_c$ and penetrated into the sample, magnetic field can be found inside the sample even we cool it down to $T < T_c$ and take out the external field. The current state relates to the previous state. It differentiates the superconductor from the perfect conductor. However, there are some restrictions on superconductors. If the current is so large that it exceeds some critical density current $j_c$, the superconductivity is destroyed and the system becomes normal. Similarly, superconductivity disappears if the external field is higher than some critical limit $H_c$. 


Figure 1: For $T > T_c$ (left fig.), the external field penetrates into the sphere which is in the normal state. For $T < T_c$ (right fig.), the external field is expelled from the sphere (superconducting state) and total field inside the sphere is zero - this is called the Meissner-Ochsenfeld Effect.

1.2 Types of Superconductors

In bulk systems, the transition from normal state to the superconducting state, as the temperature is lowered, takes place at the superconducting temperature $T_c$. In the presence of a magnetic field, superconductivity is destroyed at the thermodynamic critical field $H_c(T)$, related to the free energy difference between the normal and superconducting states, the so-called condensation energy of the superconducting state. When the transition at $T_c$ takes place in the absence of a magnetic field, it is of second order.

We define two characteristic length scales, the London penetration depth $\lambda$ and the Ginzburg-Landau coherence length $\xi$. The applied magnetic field penetrates into the surface of a sample and it decays exponentially inside the sample on the scale of $\lambda$. $\xi$ is the length scale over which the normalised superconducting density changes from $|\psi|^2 = 0$ (on surface) to $|\psi|^2 = 1$ inside the sample, where $\psi$ is the order parameter which describes the state of system and $|\psi|^2$ is the superconducting density. Both $\lambda(T)$ and $\xi(T)$ are functions of temperature and diverge at $T_c$. (See, for example, Tinkham [1])
The Ginzburg-Landau parameter $\kappa$

\[ \kappa(T) = \frac{\lambda(T)}{\xi(T)}, \quad (1.1) \]

also depends on the temperature.

There are two kinds of the superconductors, Type I and Type II. The critical value $\kappa = 1/\sqrt{2}$ separates Type I and Type II superconductors. Fig. 2 shows schematically the magnetisation vs applied magnetic field for Type I and Type II superconductors.

For $\kappa < 1/\sqrt{2}$, the superconductor is classified as Type I. The energy of a Type I superconductor without vortices is lower than one with vortices, so that it is not energetic favourable for vortices to nucleate in Type I (see Tinkham [1]). Type I (left, Fig. 2) superconductors in an ideal sense exclude applied magnetic field completely if the field is below the critical field $H_c$: the sample exhibits perfect diamagnetism and is in the Meissner state. At $H = H_c$, there is a discontinuous jump in the magnetization of the sample, and for $H > H_c$, the applied magnetic field penetrates the sample and the sample is in the normal state. The transition at $H_c$ arising as a result of a change in magnetic

Figure 2: Type I (left Fig.) expels all the external field below $H < H_c$. For Type II (right Fig.), flux passes through the sample under $H_{c1} < H < H_{c2}$. 
For $\kappa > 1/\sqrt{2}$, the superconductor is classified as Type II (right, Fig. 2). We define two critical fields, $H_{c1}$ ($H_{c1} < H_c$) and $H_{c2}$. For $H < H_{c1}$, the sample is in the Meissner state. For $H_{c1} < H < H_{c2}$, magnetic field can enter the system as quantised magnetic flux or fluxiods – this phase is the Abrikosov mixed state [2]. The energy of system with vortices is lower than the one without vortices. In this case, the normal region (core of vortex) and the superconducting region mix together and consume less energy than the pure superconducting state. At $H_{c2}$ the sample becomes normal. The transition from Meissner state to normal state is of second order.

$H_{c2}$ is the highest field at which superconductivity can nucleate in a decreasing magnetic field. Since Type I superconductors have $H_{c2} < H_c$, the system supercools and

![Figure 3: Schematics of the behaviour of the order parameter at $H_{c2}$ in an ideal bulk Type I (Fig. 3(a)) and in Type II (Fig. 3(b)) superconductors as a function of applied magnetic field $H$: typical hysteretic behaviour in Type I and reversible behaviour in Type II; see, for example, references [1, 2]; a mesoscopic superconductor with a surface parallel to the applied field (Fig. 3(c)) and the behaviour of the magnetisation $M$ of the sample as a function of $H$ (Fig. 3(d)).](image-url)
Figure 4: Schematic behaviour of the order parameter in Type I (Fig. 4(a)) and in Type II (Fig. 4(b)) superconductors as a function of applied magnetic field \( H \) in the presence of surface superconductivity: for Type I superconductors with \( \kappa \in (0.41, 0.707) \), there is no supercooling at \( H_{c1} \) in a decreasing magnetic field (Fig. 4(c)).

remains normal even at \( H_c \) (see Fig. 3(a)). At \( H_{c2} \) the superconducting density \( |\psi|^2 \) undergoes a discontinuous and irreversible jump. On cooling, the system exhibits hysteresis. Of course, sample defects limit the amount of supercooling to fields higher than the theoretical limit \( H_{c2} \). There is no such supercooling in Type II superconductors: expulsion of flux starts at \( H_{c2} \) and \( |\psi|^2 \) changes continuously (Fig. 3(b)).

In small samples, finite-size effects become important. For example, take a film of Type I superconductor of thickness \( d \) (see Fig. 3(c),(d)). It is known that if \( d \) is less than some critical thickness \( d_c \), the Landau domains (the intermediate state) become stable and the system reverts to the Abrikosov mixed state similar to that in Type II superconductors. Further, small samples have surfaces (as do real superconductors). Saint-James and De Gennes [3] showed that if there is a surface parallel to the applied magnetic field, superconductivity persists in a layer of the size of the coherence length.
up to fields $H_{c3} > H_c$. A Type I superconductor therefore is able to carry a supercurrent over the range $(H_c, H_{c3})$ at which there is no superconductivity in bulk. $H_{c3}$ is a strong function of the sample shape.

An interesting consequence of surface superconductivity is that it is $H_{c3}$, and not $H_c$, that should limit the range of supercooling of a Type I superconductor (Fig. 4(a)) since the surface layer of superconductivity serves to initiate the transformation of the interior. However, for Type I superconductors with $\kappa \in (1/(1.695\sqrt{2}), 1/\sqrt{2})$, $H_{c2} < H_c < H_{c3}$: the implication is that there is no supercooling at $H_c$ as $H$ is decreased from above $H_c$ despite the fact that the volume of the sample makes a first-order transition there (Fig. 4(c)). In Type II superconductor (Fig. 4(b)), $H_c < H_{c2} < H_{c3}$, nucleation starts from $H_{c3}$ and the system makes a second-order transition.

### 1.3 The Intermediate State

The intermediate state is a special case of Type I superconductor and it allows magnetic field to penetrate into the sample. When a magnetic field ($H < H_c$) is applied to the superconducting sample, the field near the surface of the sample would be distorted due to the shape and geometry of the sample (see Abrikosov [2]). The magnetic field varies and is not uniform in the vacuum. On the surface of sample, the magnetic strength can be higher than the original applied field. When the applied field is below $H_c$, the field near the surface can be above $H_c$ because the field is inhomogeneous. F. London [4] explained that the magnetic field near the surface has a higher field strength. Therefore, the superconducting density can be destroyed on the surface ($H > H_c$ on surface) even if the applied field is below $H_c$.

Fig. 5 is the Type I superconducting slab in the intermediate state. If the slab is under the applied field $H < H_c$, the field strength near the edge of slab can be above $H_c$ and therefore normal region is created. There are other domains of which the magnetic field is still below $H_c$ and maintain Messnier state, and hence, the alternative structures of superconducting and normal states are developed. However, the flux inside the in-
Figure 5: Type I superconducting slab under the applied magnetic field is shown. S represents the superconducting state and N represents the normal state. Flux entering into the slab is not in quanta $\phi_0$.

termediate state is not in quanta $\phi_0$. There is a significant difference from the Type II superconductor.
1.4 Two-Fluid Model

In 1930s, Kapitza [5] found that the viscosity of $^4$He tends to be zero when passing through a very narrow pipe at low temperatures. This means that the liquid can flow without any dissipation. Liquid helium undergoes a phase transition from gas to liquid at 4.2 K, and the liquid is called Helium-I. At 2.2 K, liquid helium undergoes another phase transition and changes to Helium-II or superfluid $^4$He.

Tisza [6, 7] developed the two-fluid model to describe $^4$He: it is assumed that below 2.2 K, liquid helium is made up of 2 coexisting liquids, the superfluid which moves without friction and has density $n_s$, and the normal fluid of density $n_n$, where $n = n_s + n_n$ is total density of fluid. As the temperature $T$ rises, the superfluid density $n_s$ decreases, while the normal density $n_n$ increases. We can approximate the density function as

$$\frac{n_s(T)}{n} \approx 1 - c \left( \frac{T}{T_c} \right)^4,$$

(1.2)

where $T_c$ is the critical temperature and $c$ is the constant. The basic idea is that the superfluid has more order than the normal fluid. The normal fluid has a larger entropy than the superfluid, and the superfluid plays the role of the transportation fluid. Analogous to a superfluid, an electric current in a superconductor can pass through the sample without resistance. (This is different from the case of a metal where the movement of the current-carrying electrons will be blocked and interacted on by the impurities or the vibration of the ions.) The main difference between superconductivity and superfluidity is that one has to consider the charge in superconductors, but not in the superfluid which is neutral.
1.5 Superconducting Electrodynamics - London’s Equations

In 1938, F. London published his results on the electrodynamics of superconductors in Nature [4]. The 1st London equation [8] relates the supercurrent $j_s$ and the electric field

$$E = \frac{m^*}{e^2 n_s} \frac{dj_s}{dt}, \quad (1.3)$$

where $e$ is the electron charge, $m^*$ is effective mass and $n_s$ is the superconducting density. Since $E = 0$ inside a superconductor, $j_s$ is constant and it will flow persistently. It is more convenient to define the supercurrent in terms of a magnetic vector potential $A$ ($B = \nabla \times A$). According to London approximation, they are related by

$$j_s \approx -\frac{e^2 n_s}{m^*} A, \quad (1.4)$$

showing that the superflow depends on the magnetic potential linearly.

From Maxwell’s equation, the local field $B$ satisfies $\nabla \times B = (4\pi/c) j_s$. The free energy is thus

$$F_s = F_n + \frac{1}{8\pi} \int \left[ B^2 + \lambda^2 (\nabla \times B)^2 \right] d^3 r, \quad (1.5)$$

the sum of magnetic potential and kinetic energies, where $F_n$ is the condensation energy at rest (an offset). Vary $B$, the 2nd London equation [8] is obtained as

$$B + \lambda^2 \nabla \times \nabla \times B = 0. \quad (1.6)$$

The important parameter $\lambda$ is called as London penetration depth and is defined by,

$$\lambda = \sqrt{\frac{mc^2}{4\pi n_se^2}}. \quad (1.7)$$

$\lambda$ determines how far the applied magnetic field penetrates the surface of the sample; and the magnetic field near the edge is $B(r) \approx B_0 \exp(-r/\lambda)$, where $B_0$ is the magnetic field outside the sample.
Figure 6: The magnitude of superflow of a single vortex, $j_v \propto (1/r)\hat{\theta}$, with cut-off value at $r = r_c$.

Schrieffer [9] showed that the London penetration depth depends on temperature.

$$\lambda(T) = \frac{\lambda(0)}{[1 - (T/T_c)^4]^{1/2}},$$

(1.8)

for $0 < T < T_c$, $\lambda(T)$ decreases as $T$ decreases.

$j_s$ is in fact a screening current which flows around the surface in a layer of thickness of order of $\lambda$. It generates a local opposing field against the applied external field. London equations inherently include the Meissner effect that the superconductor would expel any applied field.
1.5.1 London Vortex

We can apply the London equations to solve the problem of a vortex inside the superconductor or superfluid. Work in the cylindrical coordinates \((r, \theta, z)\) and let \(\mathbf{B} = (0, 0, B_v)\) be the local magnetic field of the vortex. Then Equation 1.6 reduces to

\[
\frac{d^2 B_v}{dr^2} + \frac{1}{r} \frac{dB_v}{dr} - \frac{B_v}{\lambda^2} = -\frac{\phi_0}{\lambda^2} \delta^2(r).
\]  

This is a Bessel’s equation, with solution \(B_v = (\phi/2\pi\lambda^2)K_0(r/\lambda)\). To a very good approximation, \(B_v \propto \ln(\lambda/r)\). The superflow around a vortex, \(j_v \propto (1/r)\hat{\theta}\), is shown graphically in Figure 6. There is a cutoff at \(r = r_c\), the vortex core radius. This will be discussed in detail later.

1.6 Ginzburg-Landau Equations

After Landau proposed his model to explain the properties of liquid helium, Ginzburg [10] worked together with Landau to develop the Ginzburg-Landau (GL) theory of phase transitions. The GL equations take superconducting density into account, and introduce the order parameter \(\psi(r)\). \(|\psi(r)|^2\) is the superconducting density varying in spatial domain. For \(T < T_c\), the superconducting region shows more order than the normal region. According to the GL model, the Gibbs free energy is

\[
G_s = \int [G_n + \alpha|\psi|^2 + \frac{\beta}{2}|\psi|^4 + \frac{1}{2m^*}((\frac{\hbar}{i}\nabla - \frac{2e}{c}\mathbf{A})\psi)^2 + \frac{B^2}{8\pi}] d^3r,
\]  

where \(\mathbf{B}\) is the local field and \(G_n\) is the free energy in normal phase. By varying with respect with \(\mathbf{A}\) and \(\psi\), we can derive the two GL equations. The first one is associated with the order parameter, and is essentially a non-linear Schrodinger equation,

\[
\alpha \psi + \frac{\beta}{2}|\psi|^2 \psi + \frac{1}{2m^*}((\frac{\hbar}{i}\nabla - \frac{2e}{c}\mathbf{A})^2 \psi = 0.
\]  

\[\]
The second equation is related to the supercurrent density,

\[ j_s = \frac{ihe}{m^*}(\psi^* \nabla \psi - \psi \nabla \psi^*) - \frac{(2e)^2}{mc} |\psi|^2 A. \] (1.12)

One can derive London’s equation and penetration depth, from GL equations, by choosing a suitable gauge (London gauge), \( \nabla \cdot A = 0 \). A new physical parameter, called the characteristics coherence length, \( \xi \sim \xi_0 / \sqrt{(1-T/T_c)} \), is introduced. It measures the distance over which the superconducting region returns to normal region. The ratio \( \kappa = \lambda / \xi \) distinguishes type I (\( \kappa < 1/\sqrt{2} \)) from type II (\( \kappa > 1/\sqrt{2} \)) superconductors, which exhibit respectively positive and negative energy between the superconducting and normal areas.

1.6.1 The Abrikosov Vortex Lattice

Abrikosov [11, 12] simplified the GL equations and solved the vortex lattice in the mixed state. He first considered the linear equation

\[ \frac{-\hbar^2}{2m^*}(\nabla + \frac{2ei}{\hbar} A)^2 \psi + \alpha \psi = 0. \] (1.13)

and worked with the Laudau gauge \( A = Hx \hat{y} \). The approximated ground state solution is therefore

\[ \psi = \sum_{n=-\infty}^{\infty} C_n \exp \left[ ik ny - \frac{\kappa^2}{2} \left( x - \frac{kn}{\kappa^2} \right)^2 \right]. \] (1.14)

Here it is assumed that the superconducting sample is sufficiently large to form the fluxoid pattern. The solution is periodic along the y axis. The optimal solution is a triangular lattice of vortices. The first experiment to observe the Abrikosov lattice was carried out by Essmann [13] at the Max-Planck Institute in 1967. Fig. 7 shows the vortex lattice image by Hess [14], which clearly shows the triangle pattern. More details of the GL model will be discussed later.
Figure 7: Scanning image of Abrikosov vortices with triangle pattern in $NbSe_2$ from Hess [14].
2 Superconductors in Confined Geometries

2.1 Mesoscopic Superconductors

Alan Dorsey [15] pointed out that the properties of superconductors are influenced by the size and the geometry of the samples, in particular at the small scale. For example, a thin film of Type I superconductor (aluminium) can show Type II behaviour. In a bulk sample, vortices would probably nucleate near the edge. If there is more than one vortex, vortices would repel each other in order to minimise the interaction energy. However, in a small superconductor, vortices do not necessarily nucleate near the edge. The effect of boundary becomes important and it would interact with the vortices (attractive or repulsive) depending on the shape of the sample.

The supercurrent always flows near the edge of the sample and would interact with the vortex. In a large sample, one can ignore this edge effect but not in the small one. De Gennes [3] predicted that surface superconductivity will increase the critical magnetic field, \( H_{c3} = 1.69H_{c2} \); and this surface superconductivity cannot be negligible if the sample size is small (see Tinkham [1]). Recent research groups [15] show that these properties, such as the current distribution of a vortex and the pattern of vortices, change with the size and shape of sample.

Recent studies have concentrated mostly on the magnetic properties of vortices in confined regions because such systems are the key to nano-superconducting devices. The idea is similar to that of logic gates in electronic components. In fact, the quantised fluxoid \( q\phi_0, q \in (-1, 0, 1) \), can be treated as the logic states in electronic devices. The main advantage is that superconducting devices have zero resistance and would not generate heat, so that it can provide more stable performance than traditional circuits.

2.2 Phase Transitions in different Sizes

In the Little-Parks experiment [16], a magnetic field is applied parallel to the axis of a small hollow superconducting cylinder, and fluxoid \( n\phi_0 \) is trapped inside the hollow
cylinder, where $n$ is an integer. This is due to the confinement of the mesoscopic sample. If the temperature is near $T_c$, the oscillating phase between superconducting state and normal state would appear in the sample. The critical temperature and resistance will also show a periodic oscillation when the applied field is increased. In fact, it is the quantum behaviour in the small size sample.

Geim and co-workers [17] studied Aluminum (Al) superconducting discs (Type I) at scales ranging from about the size of a cooper pair $\xi$ ($\sim 250$ nm) to 750 nm, to see if the system shows some special properties. The group developed a new technique, the ballistic Hall micro-magnetometry, to measure the field in the small sample below $T_c$ and analyse the characteristics of phase transitions in small superconducting discs. The coherence length of Al is about 250 nm and Geim and his group [17] worked on discs of different radii: $r = 250$ nm, $r = 500$ nm and $r = 750$ nm. They found that the magnetisation varies considerably in different sizes.

For $r = 250$ nm, the magnetisation curve shows a smooth change from superconducting state to normal state. It was also found that the magnetisation curves are the same under increasing and decreasing magnetic field, showing characteristic of second-order phase transition. It is interesting to note that the small thin disc exhibits Type II behaviour.

When the size of disc is doubled ($r = 500$ nm), the phase transition is of first-order. The sample jumps from normal (superconducting) state to superconducting (normal) state discontinuously, and no vortices are observed in the disc. Further there are metastable states which depend on the sweeping direction of the magnetic field. If the size is slightly larger ($r = 750$ nm), the transition is again a first-order transition and vortices were observed. However, it was found that the magnetization jump is not exactly one flux quantum and Geim and co-workers [17] explained that it is due to the boundary effects. They also mention the metastable solution has never been found when $T > 0.8$ K ($T_c = 1.3$ K). In brief, the magnetic properties (Al) undergoes radical change with the size of disc, from $r = \xi$ (second-order transition) to $r > 2\xi$ (first-order transition).
2.3 Paramagnetic Meissner Effect

It is a general characteristic that a superconductor expels magnetic field. However, recent studies have found that small superconductors exhibit paramagnetic (attractive) effect rather than the diamagnetic effect. The paramagnetic effect normally occurs in the high temperature superconductors but recent studies [18, 19] mention that it could happen in traditional superconductors, for example, Al and Nb. This effect is most likely observed during field cooling and flux is trapped inside the sample. Nielsen [18] and Moshchalkov [19] explain that it may be due to pinning effects, surface barrier or flux compression of the superconductors.

A.K. Geim [20] studied this effect in small superconducting discs and reported that the paramagnetic meissner effect is associated with surface superconductivity. In the experiment, the superconductors are studied in a constant applied field and the temperature is decreased. The experiment showed that flux may be captured on the sheath of the sample in high constant fields. It is important that the applied field is high enough but slightly smaller than $H_{c3}(T)$ (surface superconductivity). If the temperature decreases, then $H_{c3}(T)$ increases. More flux will be allowed to pass into the sample (compression flux) and hence paramagnetic effect appears. However, Geim [20] mentioned that the paramagnetic effect is bistable and one can recover the sample to the Meissner state by adding the external magnetic field. Further, it is found that only the traditional Meissner Effect will be observed in zero field cooling.

2.4 Non-Quantised Flux

Bardeen [21] first reported that the magnetic flux of a vortex can be smaller than one fluxoid, $\phi_0 = hc/2e$, in the thin-walled (hollow) cylinder. He discovered that the flux of a vortex relates to the size of the superconductor. Let the radius of cylinder be $R$ and the thickness of the thin wall be $d$. Bardeen [21] found that the relationship between the
size of sample and the flux \( \phi \) trapped is

\[
\phi = \frac{\phi_0}{1 + (2\lambda^2/Rd)},
\]

where \( \lambda \) is the penetration depth. Non-quantised flux is observed only when the wall of the cylinder is thin and the radius of the cylinder is small. On the other hand, the vortex fluxoid inside a bulk superconductor (> 100 \( \mu \)m) still remains quantised in units of \( \phi_0 \), since the effect mentioned by Bardeen [21] is very small (less than 1%).

Recent experiments by Geim [22] proved that the magnetic flux of a vortex in small superconductors can be smaller than one fluxoid - this effect is due to the distance of a vortex from the edge and the geometry of the surface. Each vortex generates a supercurrent around itself. If the vortex is close to the edge, the supercurrent around the vortex would be distorted. The applied magnetic field can penetrate the surface of the superconductor (normal state), and there is a supercurrent around the edge of the sample and it would interact with the supercurrent of the vortex.

Geim [22] also found that non-quantisation is due to the surface shape. He studied two discs of the same size but with different edge roughness. The disc with the smooth edge shows smooth change of magnetisation. This means that no obvious fluxoid jump is observed in the disc with smooth edge. However, he found a jump of about 0.5\( \phi_0 \) flux in the disc with rough edge. Geim [22] concluded that it is due to the different surface barriers that the two systems show different behaviour. The superheating causes the jump to be less than \( \phi_0 \).

2.5 Anti-Vortex in Confined Domains

Chibotaru et al. [23] and Mel’nikov [24] studied the possibility of anti-vortices penetrating a thin mesoscopic square sample. Chibotaru [23] studied the mesoscopic square superconductor and he measured the total flux in the superconducting sample. He proposed that the configuration of total flux 3\( \phi_0 \) is: four \( \phi_0 \) at the corners and one \(-\phi_0\)
at the center. He explained that an anti-vortex could be nucleated in order to preserve the total vorticity in the square. The occurrence of the anti-vortex inside the small scale superconductors seems to take place under some special geometries. In theory, the pattern of vortices depends on the size and geometries [20, 22]. Mel’nikov [24] also studied the superconducting square and made some defects on the sample. In his analysis, he found that the configuration with one anti-vortex and four vortices would be possible in the square sample. In addition, this configuration is very sensitive to the defect of the sample because the symmetry would be destroyed.

Misko et al. [25] analysed the stability of the anti-vortex. He reported that the anti-vortex can also happen in confined superfluids and Bosonic liquids. However, it has not been observed in experiments until now. He also asserted that the anti-vortex inside the confined square sample would be unstable and sensitive to the geometries of the sample. He studied vortices in Type I superconductor rather than Type II superconductor. Misko et al. [25] found that the interaction of the vortex-anti-vortex patterns are stable in Type I thin triangular sample but unstable in Type II sample. He proposed that it was due to a repulsive vortex-anti-vortex interaction in Type I superconductor and in confined geometries.

It is interesting to determine the possibility of a single anti-vortex together with vortices nucleating in the small superconducting sample, if it can exist separately. As the sample is small, the applied magnetic field would embrace the whole sample. Suppose there are vortices around an anti-vortex: they should be very close to each other and a detecting probe may not be able to differentiate between them easily. The anti-vortex has not yet been observed directly in experiments.

2.6 Giant Vortex

A giant vortex is a multi-fluxoid vortex (flux = $N\phi_0$, $N > 1$, $N \in \mathbb{Z}$). For a giant vortex, the self-generation energy is about $N^2 \ln(R/r_c) + E_c$, where $R$ is the size of the system, $r_c$ is the radius of the vortex core and $E_c$ is the energy associated with core; and
the self generation energy of \( N \) single quantum vortices is only \( N \ln(R/r_c) + E_c \). It is obvious that \( N^2 \ln(R/r_c) + E_c > N \ln(R/r_c) + NE_c \) if \( N > 1 \) (\( E_c \) is very small compared to \( \ln(R/r_c) \)). Hence it is energetically more favourable for \( N \) single fluxoid vortices to nucleate than a giant \( N \) fluxoid vortex. On the other hand, in a small confined sample, a giant vortex may be nucleated. This is because the sample size is not large enough to support \( N \) vortices. Instead of this, the applied magnetic field, which passes through the sample, is suppressed at the centre and hence the giant vortex forms.

Schweigert et al. [26] worked on the simulation on superconducting disc. They found that there is a state transition from \( N \) single vortices into a giant vortex. They also reported that a giant vortex will be nucleated when the disc thickness is large enough and under high magnetic field. Schweigert [26] also propose that the giant vortex depends on the disc radius. As the radius increases, the giant vortex will disappear and split into \( N \) single vortex. A.I. Buzdin [27, 28] also reported that a vortex may be trapped into the defects on the sample (pinning effect) and the vortex may carry more than a fluxoid.

On the other hand, Okayasu and co-workers [29] reported that the giant vortex could not be observed in their experiments on a thin circular superconductor and suggested that the multi-quanta vortex may not exist. They explained the reported existence of the giant vortex in the above experiment was due to the low resolution of the probe device. By enhancing the resolution of their scanning SQUID microscope, they showed that the 'giant' vortex is indeed composed of a few single vortices.

2.7 Configuration in Thin Disc

Vortices are nucleated when an external magnetic field is applied on mesoscopic superconducting disc, and the vortex configuration would be different from the one in bulk sample. While most recent theoretical studies (see Buzdin [27, 28] and Baelus [30, 31]) can indeed explain the creation of different vortex states and their stabilities in the disc very well, the theories fail to explain some of the experimental observations. In a series of experiments, Grigorieva and co-workers [32] studied vortex configurations in
mesoscopic superconducting discs as a function of applied magnetic field and found that for a broad range of vorticities \( L \), the vortices form concentric rings or shells – rather like shell filling in atoms and nuclei. They found that the \( L \) values (the so-called magic numbers), corresponding to the appearance of new shells, are robust in that they are reproducible in many experiments for different applied fields \( H \) and radii \( R \) of their discs. There is up to now no theory which explains the mechanism for vortex shell filling. Theories \([30, 31]\) also predict certain stable configurations which are different from those observed experimentally \([32]\). It is appropriate to remark here that while experiments are performed at finite \( T \neq 0 \) K temperature, most theoretical studies are strictly only valid at \( T = 0 \) K.

Buzdin \([27, 28]\) and Sobnack \([33]\) used London’s equations \([4, 34]\) and wrote down the free energy of the disc with an arbitrary configuration of vortices. The energy is minimised to obtain the stable configuration of vortices as a function of the applied field and temperature.

### 2.8 Energy of a Single Vortex

Consider a vortex is at position \( r \) in a disc. The London equation \([8]\) is

\[
\mathbf{B} + \lambda^2 \nabla \times \nabla \times \mathbf{B} = \hat{z} \phi_0 \delta^{(2)}(r),
\]

where \( \delta^{(2)} \) is a 2-D delta function. We work in cylindrical coordinates \((r, \theta, z)\). The magnetic field \( \mathbf{B} \) is chosen to be along the \( z \) axis, \( \mathbf{B} = (0, 0, B_z) \). The London equation then becomes

\[
\frac{d^2 B_z}{dr^2} + \frac{1}{r} \frac{dB_z}{dr} - \frac{B_z}{\lambda^2} = -\frac{\phi_0}{\lambda^2} \delta^{(2)}(r),
\]

as we discussed before. An approximate solution is

\[
B_z(r) \approx \frac{\phi_0}{2\pi \lambda^2} \ln(\lambda/r),
\]
for \( r_c < r < \lambda \). The self-generation energy of a vortex includes the magnetic field energy and the kinetic energy and is given by

\[
E_1 = \frac{1}{8\pi} \int_{r>r_c} (B^2 + \lambda^2(\nabla \times B)^2) dS. \tag{2.4}
\]

Using the vector identity

\[
\nabla \times B \cdot \nabla \times B = B \cdot \nabla \times \nabla \times B + \nabla \cdot (B \times \nabla \times B) \tag{2.5}
\]

gives

\[
E_1 = \frac{1}{8\pi} \int_{r>r_c} (B^2 + \lambda^2(\nabla \times B)) dS + \frac{\lambda^2}{8\pi} \int_{r>r_c} \nabla \cdot (B \times \nabla \times B) dS
\]
\[
= \frac{1}{8\pi} \int_{r>r_c} (|B|\phi_0|B^2|) dS + \frac{\lambda^2}{8\pi} \oint_C (B \times \nabla \times B) \cdot d\ell
\]
\[
= \frac{\lambda^2}{8\pi} \left[ \frac{\phi_0}{2\pi \lambda^2} \ln(\lambda/r_c) \right]_{r_c} \phi_0 \frac{\phi_0}{2\pi \lambda^2} \ln(\lambda/r_c)
\]
\[
= \left( \frac{\phi_0}{4\pi \lambda} \right)^2 \ln(\lambda/r_c). \tag{2.6}
\]

One should also include a constant term \( E_c \) which is the chemical potential energy of a vortex, the energy associated with the vortex core. That is, \( E_1 = \left( \frac{\phi_0}{4\pi \lambda} \right)^2 \ln(\lambda/r_c) + E_c \).

In a small thin film (thickness \( d \ll \lambda \)), the effective penetration depth will be increased, \( \lambda_{\text{eff}} = \lambda^2/d \gg \lambda \). If the sample size is \( R \), \( \lambda_{\text{eff}} \sim R \), then the energy per unit length is about \( E_1 \approx k^2 \ln(R/r_c) + E_c \), where \( k = \phi_0/4\pi \lambda \).
2.9 Mechanism of Vortex Interaction

The creation of two single vortices, located at \( r_1 \) and \( r_2 \) respectively, requires an amount of energy

\[
E_{1+2} \approx 2k^2 \left[ \ln \frac{R}{r_c} + E_c + \ln \frac{R}{|r_1 - r_2|} \right],
\]

where the last term is the repulsive interaction between two vortices and \( |r_1 - r_2| \) is the vortex-vortex separation (see Tinkham [1] and De Gennes [3]).

Next consider the energy required to create a vortex and anti-vortex pair in a thin film. This is (see Kosterlitz [35]),

\[
E_{\text{pair}} \approx 2k^2 \left[ \ln \frac{R}{r_c} + E_c - \ln \frac{R}{|r_1 - r_2|} \right],
\]

where the last term is the attractive interaction. This result comes from the early result by Berizinski [36], who showed that the interaction energy of a vortex-anti-vortex pair depends logarithmically on the distance \( |r_1 - r_2| \) between vortex and the anti-vortex. Since \( E_{1+2} > E_{\text{pair}} \), it is energetically more favourable to create a vortex-anti-vortex pair than two single-vortex, if \( R \) is sufficiently large and the boundary conditions can be ignored.

However, this may not be the case if the system is small enough. For a small system, the boundary effect cannot be ignored. \( E_{1+2B} + E_{1+2} < E_{\text{pairB}} + E_{\text{pair}} \) may occur, where \( E_{1+2B} \) and \( E_{\text{pairB}} \) are the energies between vortices and sample boundary. It means that it may be more energetically favourable for a single vortex to nucleate rather than a vortex-anti-vortex pair in a small superconducting system. The detail of the boundary conditions in small disc will be discussed in the next chapter.
3 London Model in Superconducting Disc

3.1 Introduction

In small scale, the physical properties of a superconductor can be remarkably different from those of bulk samples. This is because the boundary effects become important and cannot be ignored. In this chapter, we study how vortices nucleate in the thin mesoscopic superconducting disc. We apply London’s equations to formulate the mathematical model and follow the preliminary works of Buzdin [27, 28] and Sobnack [33]. The free energy of superconducting disc is constructed as a function of disc size, applied magnetic field and the number of vortices. One can obtain the optimal vortex configurations by minimizing the free energy.

3.2 Free Energies and Thermodynamics Variables

Consider the internal energy $U$ of a superconductor: it consists of the kinetic energy, the potential energy and the interaction energy between the particles, and can be written as

$$U = \sum_i \left( \frac{1}{2}m\mathbf{v}_{si}^2 + V_i \right) + \sum_{i>j} V_{ij}, \quad (3.1)$$

where $\mathbf{v}_{si}$ is the supercurrent velocity of $i^{th}$ particle, $V_i$ is the potential energy of $i^{th}$ particle and $V_{ij}$ is the interaction energy between the $i^{th}$ and $j^{th}$ particles (See for example, De Gennes [3]).

The Helmholtz and Gibbs free energies are commonly used to formulate the total energy. The Helmholtz free energy consists of the internal energy and the energy of order-disorder. The expression is

$$F = U - TS, \quad (3.2)$$

where $U$, $T$ and $S$ are the internal energy, temperature and entropy respectively. The
Helmholtz free energy assumes that the local magnetic field $B$ is constant and does not take into account the energy associated with the applied magnetic field $H$. For this one needs to consider the Gibbs free energy (see for example, Anett [37])

$$G(T, H) = U - TS - \int M \cdot H \, d^3r$$
$$= G(T, 0) - \int M \cdot H \, d^3r,$$  \hspace{1cm} (3.3)

where $M$ is the magnetisation of the sample under the applied magnetic field $H$, and $G(T, 0)$ is the Gibbs free energy in the absence of magnetic field. At fixed $T$, the Gibbs free energy can be rewritten as

$$G(T, H) - G(T, 0) = \int \int dG \, dV = \int \int_0^H -M \cdot dH \, d^3r,$$ \hspace{1cm} (3.4)

where $dG = -SdT - M \cdot dH$. For $dT = 0$, hence $dG = -M \cdot dH$.

The relationship between the local magnetic field $B$, magnetisation $M$ and external magnetic field $H$ is

$$B(H) = 4\pi M + H$$
$$M = \frac{B(H) - H}{4\pi}.$$ \hspace{1cm} (3.5)

For the Type I samples, the superconductor shows complete diamagnetism (Meissner effect) for $H \lesssim H_c$, where $H_c = H_c(T)$ is the temperature-dependent thermodynamic critical field. $B = 0 \Rightarrow M = -\frac{1}{4\pi}H$. Hence for $H \lesssim H_c$,

$$G(T, H) - G(T, 0) = \int \int_0^H \frac{H}{4\pi} \, dH \, dV = \int \frac{H^2}{8\pi} \, d^3r.$$ \hspace{1cm} (3.6)

Let $G_s$ and $G_n$ be the Gibbs free energy of the superconducting state and the normal state respectively. In thermal equilibrium, the superconducting and normal states can
coexist [1] and

\[ G_s(T, H_c) = G_n(T, H_c) \approx G_n(T, 0). \]  \hfill (3.7)

The energy difference between superconducting state and normal state is

\[ G_s(T, 0) - G_n(T, 0) \approx G_s(T, 0) - G_s(T, H_c) = -\frac{1}{8\pi} \int_V H_c^2 \, d^3r, \]  \hfill (3.8)

which is defined as the condensation energy. It refers to the work required to oppose the external magnetic field.

For Type II superconductors, we define two critical fields \( H_{c1} \) and \( H_{c2} \). For \( H_{c1} \lesssim H < H_{c2}, B \neq 0 \), and the Gibbs free energy is

\[
G_s(T, H) - G_n(T, H) = (U_s - TS_s - \int_B M \cdot dH \, d^3r) - (U_n - TS_n)
\]

\[
= \frac{1}{8\pi} \int_V (H - B)^2 \, d^3r + (U_s - U_n) - T(S_s - S_n), \]  \hfill (3.9)

where \( M \approx 0 \) in normal state, \( U_s \) and \( U_n \) are the internal energies in the superconducting and normal states, \( S_s \) and \( S_n \) are the entropies in the superconducting and normal states. In our studies, \( S \) is the entropy of vortices and \( S_n = 0 \) because no vortex nucleates in the normal state.

The internal energy \( U \) of the system consists of the kinetic energy (super-current) and the interaction energy. Since the kinetic energy is much larger than the interaction molecular energy, it is reasonable to assume that \( U_n \approx 0 \) since no current flows under constant field in normal metal and

\[
U_s \approx \int_V \frac{1}{2} m v_s^2 n_s \, d^3r. \]  \hfill (3.10)

The current density \( j_s \) and the velocity \( v_s \) are related by \( j_s = n_s e v_s \), and it follows from
Maxwell’s equation
\[ \nabla \times \mathbf{B} = \frac{4\pi}{c} \mathbf{J}_s, \]  
(3.11)
that
\[ \int_V \frac{1}{2} m v_s^2 n_s d^3r = \int_V \lambda^2 (\nabla \times \mathbf{B})^2 d^3r, \]  
(3.12)
where \( \lambda = \sqrt{mc^2/4\pi n_s e^2} \) is the London penetration depth. It then follows that in the presence of the applied magnetic field \( \mathbf{H} \), the Gibbs free energy difference between the superconducting and normal phases in terms of the temperature \( T \) and the applied magnetic field \( \mathbf{H} \) is
\[ G = G_s(T, \mathbf{H}) - G_n(T, 0) = \frac{1}{8\pi} \int_V [(\mathbf{H} - \mathbf{B})^2 + \lambda^2 (\nabla \times \mathbf{B})^2] d^3r - TS_s, \]  
(3.13)
where \( G_n(T, \mathbf{H}) \approx G_n(T, 0) \) is a constant in the normal state, and we use the symbol \( G \) as the energy difference between the superconducting and normal states in our remaining parts.
3.3 The 2D superconducting Disc at $T = 0 \text{K}$

Consider a small superconducting disc of radius $R$ and thickness $d$ in an applied magnetic field

$$\mathbf{H} = H\hat{k} = \nabla \times \mathbf{A}_{\text{app}} \quad (3.14)$$

normal to the plane of the disc. The local magnetic field is $\mathbf{B} = \nabla \times \mathbf{A}$. In a thin sample with thickness $d \ll R$, it is well known that the actual penetration depth in the film is larger than expected by London’s theory since the applied field penetrates the thin sample more easily. The penetration depth is called the effective London penetration depth (see Fetter [38]), $\lambda_{\text{eff}}(d) > \lambda$ and is a function of the thickness $d$.

Consider applied fields in the low field regime, i.e., $H$ is near the lower critical field $H_{c1}$. Assume that $d \lesssim r_c$, where $r_c$ is the size of the core of a vortex, so that the sample can be treated as a 2-D system. We use cylindrical coordinates $(r, \theta, z)$ in what follows. The Gibbs free energy of the disc at $T = 0 \text{K}$ is made up of the magnetic potential energy together with the kinetic energy of the superconducting currents and is given by

$$G = \frac{1}{8\pi} \int_V \left[ (\nabla \times (\mathbf{A} - \mathbf{A}_{\text{app}}))^2 + \lambda^2 (\nabla \times \mathbf{B})^2 \right] d^3r. \quad (3.15)$$

By using integration by parts and the vector identity $\mathbf{v} \cdot \nabla \times \mathbf{u} = \mathbf{u} \cdot \nabla \times \mathbf{v} + \nabla \cdot (\mathbf{u} \times \mathbf{v})$, with $\mathbf{v} = \nabla \times (\mathbf{A} - \mathbf{A}_{\text{app}})$ and $\mathbf{u} = \mathbf{A} - \mathbf{A}_{\text{app}}$, it follows that

$$G = \frac{1}{8\pi} \int_V \left[ (\mathbf{A} - \mathbf{A}_{\text{app}}) \cdot \nabla \times \nabla \times (\mathbf{A} - \mathbf{A}_{\text{app}}) \right. \left. + \lambda^2 (\nabla \times \nabla \times \mathbf{A}) \cdot (\nabla \times \nabla \times \mathbf{A}) \right] d^3r. \quad (3.16)$$

Since

$$\nabla \times \nabla \times \mathbf{A}_{\text{app}} = \nabla \times \mathbf{H} = 0, \quad (3.17)$$

noting that $\mathbf{H}$ is a constant applied field, we obtain
\[ G = \frac{1}{8\pi} \int_V \left[ (A - A_{\text{app}} + \lambda^2 \nabla \times \nabla \times A) \cdot (\nabla \times \nabla \times A) \right] d^3r. \] (3.18)

Using Maxwell’s equation \( \nabla \times \nabla \times A = 4\pi j_s/c \), one can write

\[ G = \frac{1}{8\pi} \int_V \left[ (A - A_{\text{app}} + \lambda^2 4\pi j_s/c) \cdot (4\pi j_s/c) \right] d^3r, \] (3.19)

where the free energy is now expressed in terms of supercurrent \( j_s \), the applied magnetic potential \( A_{\text{app}} \) and the local magnetic potential \( A \).
3.4 London Vortex on 2-D Plane

Next we need to calculate the supercurrent around a vortex. Up to this stage, we have assumed that the sample is a bulk sample for simplicity and ignored the boundary conditions. We will discuss the boundary effect in a later section.

For \( H < H_{c1} \), a Type II superconductor would expel the external magnetic field completely (Meissner effect) and no vortices penetrate the system. From London’s 2nd equation [4, 34], the superconducting current is given by

\[
\nabla \times j_s = -(c/4\pi\lambda^2)B = -(c/4\pi\lambda^2)\nabla \times A, \tag{3.20}
\]

where we have chosen the London gauge \( \nabla \cdot A = 0 \) and \( j_s = -(c/4\pi\lambda^2)A \).

3.4.1 Fluxoid Quantisation

On the other hand, for \( H_{c1} \lesssim H < H_{c2} \), magnetic field will penetrate the bulk of the sample as fluxoid (quantised magnetic flux). We can model the local field \( b_v(r) \) of vortex by London equation in the 2-D plane. Physically, the applied magnetic field passes through the core of vortex which is normal metal. One can think that the core is a hole inside the superconductor. The core is a multiply-connected region which is a singular point in the area. The field \( b_v \) satisfies the London equation [8, 39]

\[
b_v(r) + \lambda^2 \nabla \times \nabla \times b_v(r) = \hat{z}k\delta^{(2)}(r), \tag{3.21}
\]

where \( k \) is a constant related to the circulation flow.

According to Maxwell’s equations, the supercurrent around a vortex is

\[
j_v = \frac{c}{4\pi} \nabla \times b_v(r). \tag{3.22}
\]
By integrating the London Eq. 3.21, the total magnetic flux associated with the vortex is

\[
\int \int_S \hat{z} k \delta^{(2)}(r) \cdot dS = \int \int_S b_v(r) \cdot dS + \int \int_S \lambda^2 \nabla \times \nabla \times b_v(r) \cdot dS
\]

where \( b_v(r) = \nabla \times A \), \( j_v = n_s e^* v_s \) and \( \lambda^2 = m^* c^2 / 4\pi n_s e^* \) \((m^* \text{ is effective mass, } e^* \text{ is effective electron charge and } n_s \text{ is superconducting density})\).

Then, we can obtain the constant \( k \)

\[
k = \oint A \cdot d\ell + \frac{4\pi \lambda^2}{c} \oint j_v \cdot d\ell
\]

\[
= \oint A \cdot d\ell + \frac{m^* c}{e^*} \oint v_s \cdot d\ell,
\]

(3.23)

where \( j_v = n_s e^* v_s \) and \( \lambda^2 = m^* c^2 / 4\pi n_s e^* \) \((m^* \text{ is effective mass, } e^* \text{ is effective electron charge and } n_s \text{ is superconducting density})\).

Then, we can obtain the constant \( k \)

\[
k = \oint \left( A + \frac{m^* c}{e^*} v_s \right) \cdot d\ell
\]

\[
= \frac{c}{e^*} \oint \left( \frac{e^*}{c} A + m^* v_s \right) \cdot d\ell
\]

\[
= \frac{c}{e^*} \oint p \cdot d\ell
\]

\[
= \frac{q hc}{e^*} = q \phi_0 = \phi_i,
\]

(3.24)

where \( \oint p \cdot d\ell = q h \) (see Tinkham [1]) comes from the Bohr-Sommerfeld quantum condition and \( q \in Z \). Hence, the constant \( k \) is the total vortex flux which carries the quantised fluxoid \( \phi_i = q \phi_0 \), where

\[
\phi_0 = \frac{hc}{2e} = 2.07 \times 10^{-7} \text{ Gauss} \cdot \text{cm}^2 \text{ (cgs)}.
\]

(3.25)

3.4.2 Expression of London Vortex Field

If there are \( N \) vortices in the bulk sample, there will be \( N \) holes (normal cores) inside the sample and as shown by Tinkham [1], De Gennes [3] and Poole [40], the total field
$b_v$ of the $N$ vortices satisfies

$$b_v(r) + \lambda^2 \nabla \times \nabla \times b_v(r) = \sum_{i=1}^{N} \hat{z} \phi_i \delta^{(2)}(r - r_i), \quad (3.26)$$

with solution

$$b_v(r) = \sum_{i=1}^{N} \frac{\phi_i}{2\pi \lambda^2} K_0 \left( \frac{|r - r_i|}{\lambda} \right) \hat{z}, \quad (3.27)$$

where $K_0(r/\lambda)$ is the zeroth-order modified Bessel function (Hankel function with imaginary argument). For large $r$, $r \gg \lambda$,

$$K_0 \left( \frac{r}{\lambda} \right) \approx \left( \frac{\pi \lambda}{2r} \right)^2 e^{-r/\lambda}, \quad (3.28)$$

and for $\xi < r < \lambda$ ($\xi$ is of the same order as $r_c$),

$$K_0 \left( \frac{r}{\lambda} \right) \approx \ln \left( \frac{1.123 \lambda}{r} \right). \quad (3.29)$$

Hence the local magnetic field around a vortex is logarithmic. The circulating superconducting current around each vortex is

$$j_v = \frac{c}{4\pi} \nabla \times b_v(r) \approx \frac{c}{4\pi \lambda^2} \sum_{i=1}^{N} \left( \frac{\phi_i}{2\pi |r - r_i|} \hat{\theta} \right). \quad (3.30)$$

We write

$$j_v = \frac{c}{4\pi \lambda^2} \sum_{i=1}^{N} \Phi(r - r_i), \quad (3.31)$$

where $\Phi_i(r - r_i)$ is the magnetic vector potential due to the vortex at position $r_i$,

$$\Phi_i(r) = \Phi(r - r_i) = \frac{\phi_i}{2\pi |r - r_i|} \hat{\theta}. \quad (3.32)$$
3.4.3 Image Vortex and Boundary Conditions in 2-D Cylinder

For vortices in a confined superconductor, one has to take into account the boundary condition at the edge of the disc. Here the superconducting current should have a tangential component only - i.e. the normal component has to be zero. We impose this condition by using the method of images, in analogy with 2D electrostatics (see Thomason [41]). For each vortex of flux $q\phi_0$ at $r_i$ in the disc, we add an image anti-vortex of the flux at $-q\phi_0$ at $r'_i = (R^2/r_i^2)r_i$ beyond the disc.

The net potential due to a vortex and its image anti-vortex is

$$\Phi = \Phi_i(r) + \Phi'_i(r). \quad (3.33)$$

The boundary condition on the edge of the disc is

$$\mathbf{j}(\mathbf{R}) \cdot \mathbf{n}(\mathbf{R}) = 0, \quad (3.34)$$

where $\mathbf{n}$ is the normal to the edge.

From above, we can show that the total normal component of superconducting current at the boundary is zero. The total normal component of the current is

$$\mathbf{j}_n + \mathbf{j}'_n = \frac{\phi_i}{2\pi|\mathbf{R} - \mathbf{r}_i|} \sin \alpha + \frac{\phi'_i}{2\pi|\mathbf{R} - \mathbf{r}'_i|} \cos \beta,$$

where

$$\Phi_i(r) = \frac{q\phi_0}{2\pi|\mathbf{r} - \mathbf{r}_i|} \hat{\theta}, \quad (3.35)$$

and

$$\Phi'_i(r) = \frac{-q\phi_0}{2\pi|\mathbf{r} - \mathbf{r}'_i|} \hat{\theta}, \quad (3.36)$$

so that on the edge of the disc, $\Phi = 0$. By the equality of triangles (Fig. 8), one can show that

$$\frac{r_i}{\sin \alpha} = \frac{R}{\cos \beta}. \quad (3.37)$$
Figure 8: Schematic diagram of a vortex (V) in a disc together with its image anti-vortex (AV) beyond the disc. $\alpha$ is the angle that the current around the vortex makes with tangent at point P and $\beta$ is the corresponding angle for the current around the image anti-vortex.

Therefore,

\[
\frac{\phi_i'}{2\pi |\mathbf{R} - \mathbf{r}_i'|} = -\frac{r_i}{R} \frac{\phi_i}{2\pi |\mathbf{R} - \mathbf{r}_i|}
\] \hspace{1cm} (3.38)

and

\[
\mathbf{j}_n + \mathbf{j}_n' = \frac{\phi_i}{2\pi |\mathbf{R} - \mathbf{r}_i|} \sin \alpha - \frac{r_i}{R} \frac{\phi_i}{2\pi |\mathbf{R} - \mathbf{r}_i|} \cos \beta
\]

\[
= \frac{\phi_i}{2\pi |\mathbf{R} - \mathbf{r}_i|} \sin \alpha - \frac{\phi_i}{2\pi |\mathbf{R} - \mathbf{r}_i|} \sin \alpha = 0.
\] \hspace{1cm} (3.39)
3.5 Gibbs Free Energy of the disc at $T = 0$

We have to take into account the boundary condition at the edge of the disc. The supercurrent needs to include the current due to the image vortices and is given by

$$j_s = -(c/4\pi \lambda^2)(A - \Phi_v),$$

(3.40)

where

$$\Phi_v = \sum_{i=1}^{N} \left( \frac{\phi_i}{2\pi |r - r_i|} \hat{\theta} - \frac{\phi_i}{2\pi |r - r_i'|} \hat{\theta} \right),$$

(3.41)

is the total magnetic potential due to the vortices. We assume that all the vortices lie on a ring (of radius $r_i$) due to symmetry.

Substitute the above expression for $j_s$ into Eq.(3.19)

$$G = \frac{1}{8\pi} \int_V \left[ (A - A_{\text{app}} + \lambda^2 4\pi j_s/c) \cdot (4\pi j_s/c) \right] d^3r$$

to give

$$G = \frac{1}{8\pi \lambda^2} \int_V \left[ (\Phi_v - A_{\text{app}}) \cdot (\Phi_v - A) \right] d^3r. \quad (3.42)$$

By integrating over the thickness $d \ll R$ of the disc, we get

$$G = \frac{d}{8\pi \lambda^2} \int_S \left[ (\Phi_v - A_{\text{app}}) \cdot (\Phi_v - A) \right] d^2r, \quad (3.43)$$

where $S$ is the surface of the disc. Next we define a term

$$h = \nabla \times a = \nabla \times (A_{\text{app}} - A) = H - B,$$

(3.44)

which is the difference between the applied magnetic field $H$ and the local magnetic field $B$.

For the small disc, the screening current is weak, i.e., $a$ is very small and it is reason-
able to assume that
\[ A = A_{\text{app}} - a \approx A_{\text{app}} = \frac{1}{2} H \times r, \]
(3.45)
where the gauge has been chosen as \( A_{\text{app}} \) and \( H = \nabla \times A_{\text{app}} \) is along the \( \hat{z} \) direction. Under this condition, the Gibbs energy can be approximated to
\[ G \approx \frac{d}{8\pi \lambda^2} \int_D (\Phi_v - A_{\text{app}})^2 d^2r. \]
(3.46)
Physically, this approximation is essentially equivalent to saying that the magnetic potential energy \( (B - H)^2 \) is negligible compared to the kinetic energy, \( \lambda^2 (\nabla \times B)^2 \), i.e.
\[ \frac{(B - H)^2}{\lambda^2 (\nabla \times B)^2} \sim \delta, \]
where \( \delta \ll 1 \). The small value of \( R \) implies that the screening effects of the superconducting currents \( j_s \) are suppressed, so that the magnetic field \( H \) is approximately the same inside and outside the sample. Equivalently, one can write (3.46) as
\[ G = \frac{2\pi \lambda^2 d}{c^2} \int_D j_s \cdot j_s d^2r. \]
(3.47)
Following Budzin [28], we write the total supercurrent \( j_s \) as the curl of a source function \( f(r) = f(r)\hat{z} \), where \( f \) is to be determined.
\[ j_s = \nabla \times f = \nabla \times (f \hat{z}) = \frac{c}{4\pi \lambda^2} (\Phi_v - A_{\text{app}}). \]
(3.48)
Integrating the equation above, with the gauge \( A_{\text{app}} = 1/2(H \times r) \) and with \( H = H\hat{z} \),
gives

\[
\int_r^R \nabla \times (f \hat{z}) \, dr \int_0^{2\pi} \, d\theta = \frac{c}{4\pi \lambda^2} \int_r^R (\Phi_v - A_{\text{app}}) \, dr \int_0^{2\pi} \, d\theta
\]

\[
\int_r^R \frac{\partial f(r)}{\partial r} \, dr = \frac{c}{4\pi \lambda^2} \left[ \sum_{i=1}^N \phi_i \int_r^R \left( \frac{1}{|r - r_i|} - \frac{1}{|r - r'_i|} \right) \, dr - \frac{H}{4} (R^2 - r^2) \right].
\]

(3.49)

and the function \( f \) follows,

\[
f(r) = \frac{c}{4\pi \lambda^2} \left[ \sum_{i=1}^N \phi_i \left( \ln \frac{|R - r_i|}{|r - r_i|} - \ln \frac{|R - r'_i|}{|r - r'_i|} \right) - \frac{H}{4} (R^2 - r^2) \right],
\]

(3.50)

where \( f(R) = 0 \), and with \( N \) off-centre vortices in the disc.

With \( j_s = \nabla \times (f \hat{z}) \), one can write Eq. (3.47) for the Gibb’s free energy

\[
G = \frac{2\pi \lambda^2 d}{c^2} \int_D \mathbf{j}_s \cdot \mathbf{j}_s \, d^2 r
\]

as

\[
G = \frac{2\pi \lambda^2 d}{c^2} \int_D \mathbf{j}_s \cdot \nabla \times (f \hat{z}) \, d^2 r
\]

(3.51)

Integrate by parts,

\[
G = \frac{2\pi \lambda^2 d}{c^2} \int_D (f \hat{z}) \cdot \nabla \times \mathbf{j}_s \, d^2 r
\]

\[
= \frac{2\pi \lambda^2 d}{c^2} \int_D (f \hat{z}) \cdot \nabla \times (c/4\pi \lambda^2 (\Phi_v - A_{\text{app}})) \, d^2 r
\]

\[
= \frac{d}{2c} \int_D (f \hat{z}) \cdot [\nabla \times \Phi_v - H \hat{z}] \, d^2 r
\]

\[
= \frac{d}{2c} \int_D [(f \hat{z}) \cdot \nabla \times \Phi_v - H f(r)] \, d^2 r.
\]

(3.52)

\( \Phi_v \) satisfies,

\[
\nabla \times \Phi_v = \sum_{i=1}^N \phi_i \delta^{(2)}(r - r_i) \hat{z}.
\]

(3.53)
Hence,

\[
G = \frac{d}{2c} \int_D \left[ \phi_i \sum_{i=1}^{N} \delta^{(2)}(r - r_i)f(r) - H f(r) \right] d^2r \\
= \frac{d}{2c} \left[ \phi_i \sum_{i=1}^{N} f(r_i) - H \int_{S} f(r)d^2r \right]. \tag{3.54}
\]

Let us introduce dimensionless parameters here. The dimensionless Gibbs free energy is

\[
g = \frac{G16\pi^2\lambda^2}{d\phi_0^2}; \tag{3.55}
\]

the dimensionless applied magnetic field, which is total magnetic flux per unit fluxoid, is

\[
h = \frac{\pi R^2 H}{\phi_0}, \tag{3.56}
\]

and the normalised position is \(z_i = r_i/R\).

Recall that

\[
f(r) = \frac{c}{4\pi \lambda^2} \left[ \sum_{i=1}^{N} \frac{\phi_i}{2\pi} \left( \ln \frac{|R - r_i|}{|r - r_i|} - \ln \frac{|R - r'_i|}{|r - r'_i|} \right) - \frac{H}{4} (R^2 - r^2) \right].
\]

With the above definition and using the results (see Baelus [31])

\[
\int_{S} \ln \frac{|r - r_i|}{r_c} d^2r = \int_{0}^{R} \int_{0}^{2\pi} \ln \sqrt{r^2 + r_i^2 - 2rr_i \cos \alpha} \, d\alpha \, dr - \pi R^2 \ln r_c \\
= 2\pi \left( \int_{r_i}^{R} \ln r \, r \, dr + \int_{0}^{r_i} \ln r_i \, r \, dr \right) - \pi R^2 \ln r_c \\
= \pi R^2 \ln \frac{R}{r_c} - \frac{\pi}{2} (R^2 - r_i^2). \tag{3.57}
\]

and

\[
\int_{S} \ln \frac{|r - r'_i|}{r_c} d^2r = \pi R^2 \ln \frac{R^2}{r_c r_i}. \tag{3.58}
\]
one arrives at

\[
g = \frac{16\pi^2\lambda^2}{d\phi_0^2} G = q^2 \sum_{i=1}^{N} \sum_{j=1}^{N} \left( \ln \frac{|\mathbf{R} - \mathbf{r}_i|}{|\mathbf{r}_j - \mathbf{r}_i|} - \ln \frac{|\mathbf{R} - \mathbf{r}_i'|}{|\mathbf{r}_j - \mathbf{r}_i'|} \right) - qh \sum_{i=1}^{N} (1 - z_i^2) + h^2/4. \tag{3.59}
\]

At \( r_i \) approaches \( r_j \), we take the integration over \( r \) in the interval \([r_c, R] \) since \( r_c \) is the threshold limit, that is

\[
\lim_{r_i \to r_j} |r_i - r_j| = r_c. \tag{3.60}
\]

Using the relationship \( \mathbf{r}'_i = (R/r_i)^2 \mathbf{r}_i \), gives

\[
g = q^2 \sum_{i=1}^{N} \sum_{j \neq i} \left( \ln \frac{|\mathbf{r}_j - \mathbf{r}'_i|}{|\mathbf{r}_j - \mathbf{r}_i|} \right) + q^2 \sum_{i=1}^{N} \ln(1 - z_i^2) + q^2 N \ln(R/r_c) - qh \sum_{i=1}^{N} (1 - z_i^2) + h^2/4. \tag{3.61}
\]

For vortices on a circle of radius \( r \), we have \( |\mathbf{r}_i| = |\mathbf{r}_j| = r \) and \( z_i = r_i/R = r/R \). The distance \( |\mathbf{r}_j - \mathbf{r}_i| \) bewteen two vortices \( i \) and \( j \) is,

\[
|r_j - r_i| = 2r \left| \sin \frac{\pi n}{N} \right| \tag{3.62}
\]

\( \forall i, j = 1, 2, \ldots N(i \neq j) \). The distance of \( z_i \) and \( z_j \) are the same, so that \( z_i = z_j = z \). The distance between the vortex at position \( \mathbf{r}_j \) and the image anti-vortex at \( \mathbf{r}'_i \) is

\[
|r_j - \mathbf{r}'_i| = \sqrt{|r_i'^2| + |r_j|^2 - 2|r_i'||r_j| \cos(2\pi n/N)}
\]

\[
= \frac{R^2}{r} \sqrt{1 + z^4 - 2z^2 \cos(2\pi n/N)}. \tag{3.63}
\]

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Hence

\[
g = \frac{1}{4} h^2 + N q^2 \ln \frac{R}{r_c} - N(N - 1) q^2 \ln z + N q^2 \ln(1 - z^2) - N q h(1 - z^2)
\]

\[
+ \frac{1}{2} N q^2 \sum_{n=1}^{N-1} \ln \frac{1 - 2z^2 \cos(2\pi n/N) + z^4}{4 \sin^2(\pi n/N)}.
\]

(3.64)

The above is the free energy of the disc with \(N\) off centre vortices (each of flux \(\phi_i = q\phi_0\)).

To make the expression more general, we add a vortex with flux \(\phi = L\phi_0\) at the centre \((L > 0\) for a vortex and \(L < 0\) for an anti-vortex) and the free energy becomes

\[
g(N, L) = g(N, 0) + \frac{1}{4} h^2 + L^2 \ln \frac{R}{r_c} - 2LNq \ln z - Lh,
\]

(3.65)

where \(g(N, 0)\) is the energy of the \(N\) off-centre vortices,

\[
g(N, 0) = N q^2 \ln \frac{R}{r_c} - N(N - 1) q^2 \ln z + N q^2 \ln(1 - z^2) - N q h(1 - z^2)
\]

\[
+ \frac{1}{2} N q^2 \sum_{n=1}^{N-1} \ln \frac{1 - 2z^2 \cos(2\pi n/N) + z^4}{4 \sin^2(\pi n/N)}.
\]

(3.66)

and includes the self creation energy of the vortices, the interaction energy between the vortices and the magnetic energy.

The term \(h^2/4\) in Eq. (3.65) is the magnetic energy of the applied field, \(L^2 \ln(R/r_c)\) is the self-creation energy of the central vortex. \(-2LNq \ln z\) is the interaction energy between the central vortex and the off-centre vortices, and the last term \(-Lh\) is the interaction energy of the central vortex and the applied magnetic field.
3.6 Magnetisation and Optimal Solutions

The magnetisation (of the disc) is the change of Gibbs free energy $G$ with respect to $H$

$$M = -\frac{\partial G}{\partial H}. \quad (3.67)$$

The dimensionless magnetisation $m$ of the disc follows as

$$m(N, L) = -\frac{\partial g(N, L)}{\partial h} = -\left(\frac{1}{2} h - L + 2zNqh\right). \quad (3.68)$$

In order to estimate the position of vortices $z(N, L, h)$, we need to know implicit expression of $h$ in terms of $L$ and $N$. By differentiating $g$ with respect to $z$,

$$\frac{\partial g(N, L)}{\partial z} = 2Nqz\left(h - \frac{L}{z^2} - \frac{(N-1)q}{2z^2} - \frac{q}{1 - z^2}\right) + (2Nqz)\sum_{n=1}^{N-1} \frac{z^2 - \cos(2\pi n/N)}{1 + z^4 - 2z^2 \cos(2\pi n/N)} = 0, \quad (3.69)$$

we can obtain $h$ in equilibrium state

$$h(N, L) = \frac{L}{z^2} + \frac{(N-1)q}{2z^2} + \frac{q}{1 - z^2} - q\sum_{n=1}^{N-1} \frac{z^2 - \cos(2\pi n/N)}{1 + z^4 - 2z^2 \cos(2\pi n/N)}, \quad (3.70)$$

and substitute $h$ back into $\partial g(N, L)/\partial z = 0$. Therefore, the optimal position $z(N, L)$ can be found. Substituting the optimal $z$ into $g$, the minimum gibbs free energy can be obtained and hence the magnetisation.

3.7 Extension to Multiple Rings at $T = 0$ K

We have developed the formulation for the one shell (ring) vortex configuration in the superconducting mesoscopic disc at $T = 0$. The formulation will only be valid if the applied magnetic field is not very high. For stronger fields, more vortices will nucleate in
the disc. Then, a single ring (shell) will no longer be able to accommodate all the vortices if \( N \) is large and the system will be unstable. It is appropriate under these circumstances to extend the model to more than one shell.

### 3.7.1 Two Rings Configuration

First, we will extend the formulation of Gibbs free energy from one ring to two rings: this model has a central vortex, \( N_1 \) vortices at \(|r_i| = r_1\) on the 1st ring and \( N_2 \) vortices at \(|r_j| = r_2\) on the 2nd ring. Again, we assume that the central vortex carries flux \( \phi = L\phi_0 \) \((L > 0 \text{ for a vortex and } L < 0 \text{ for an anti-vortex})\). Similarly, we also assume that each off-centre vortex carries flux \( \phi = q\phi_0 \) \((q \in \mathbb{Z})\). The Gibbs free energy can be written as

\[
g(L, N_1, N_2) = \frac{1}{4} h^2 + L^2 \ln \frac{R}{r_c} - 2LN_1q \ln z_1 - 2LN_2q \ln z_2 - Lh + g(N_1, 0) + g(N_2, 0) + g_{12}(N_1, N_2),
\]

where \( g(N_i, 0) \) is the energy of the \( i^{\text{th}} \) ring with \( N_i \) off-centre vortices \((i = 1, 2)\). From Eq. (3.66), \( g(N_i, 0) \) is given by

\[
g(N_i, 0) = N_i q^2 \ln \frac{R}{r_c} - N_i(N_i - 1)q^2 \ln z_i + N_i q^2 \ln (1 - z_i^2) - N_i q h (1 - z_i^2) + \frac{1}{2} N_i q^2 \sum_{n=1}^{N_i-1} \ln \frac{1 - 2z_i^2 \cos(2\pi n/N_i) + z_i^4}{4 \sin^2(\pi n/N_i)}
\]

for \((i = 1, 2)\) and where \( r_c \) is a cutoff threshold.

\( g_{12}(N_1, N_2) \) is the interaction energy between vortices on the two rings and is given by

\[
g_{12}(N_1, N_2) = 2q^2 \sum_{n=1}^{N_1} \sum_{m=1}^{N_2} \left( \ln \frac{|R - r_m|}{|r_n - r_m|} - \ln \frac{|R - r'_m|}{|r_n - r'_m|} \right),
\]
where the first term is the interaction energy between the vortices on the first ring and those on the second ring, and the second term is the interaction energy with the boundary.

This expression can be simplified to

$$g_{12}(N_1, N_2) = q^2 \sum_{n=1}^{N_1} \sum_{m=1}^{N_2} \ln \left[ 1 + \frac{z_1^2 z_2^2 - 2z_1 z_2 \cos[\alpha_{jk} + 2\pi(n/N_1 - m/N_2)]}{z_1^2 + z_2^2 - 2z_1 z_2 \cos[\alpha_{jk} + 2\pi(n/N_1 - m/N_2)]} \right], \quad (3.74)$$

where $$\alpha$$ is the misalignment angle between vortices on the first ring and those on the second ring.

As discussed before, $$-2LN_i q \ln z_i$$ is the interaction energy between the central vortex and the vortices on the $$i^{th}$$ ring ($$i = 1, 2$$).

### 3.7.2 Extension to Multiple Rings

The two-ring model can be extended to one with $$m$$ rings, with $$N_i$$ vortices on the $$i^{th}$$ ring ($$i = 1, 2, ..., m$$). The Gibbs free energy of the disc is

$$g(L, N_1, N_2, ..., N_m) = \frac{1}{4} h^2 + L^2 \ln \frac{R}{r_c} - Lh - \sum_{i=1}^{m} 2LN_i q \ln z_i + \sum_{i=1}^{m} g(N_i, 0) + \sum_{j,k,j \neq k} g_{jk}(N_j, N_k), \quad (3.75)$$

where

$$g(N_i, 0) = N_i q^2 \ln \frac{R}{r_c} - N_i(N_i - 1)q^2 \ln z_i + N_i q^2 \ln(1 - z_i^2) - N_iqh(1 - z_i^2) + \frac{1}{2} N_i q^2 \sum_{n=1}^{N_i-1} \ln \frac{1 - 2z_i^2 \cos(2\pi n/N_i) + z_i^4}{4 \sin^2(\pi n/N_i)} \quad (3.76)$$

for ($$i = 1, 2, ..., m$$) and

$$g_{jk}(N_j, N_k) = q^2 \sum_{j=1}^{N_j} \sum_{k=1}^{N_k} \ln \left[ 1 + \frac{z_j^2 z_k^2 - 2z_j z_k \cos[\alpha_{jk} + 2\pi(n/N_j - m/N_k)]}{z_j^2 + z_k^2 - 2z_j z_k \cos[\alpha_{jk} + 2\pi(n/N_j - m/N_k)]} \right], \quad (3.77)$$
where $\alpha_{jk}$ is the misalignment angle between vortices on the $j^{th}$ ring and $k^{th}$ ring.
4 Numerical London Model

4.1 Simulation at $T = 0$ K

We model the small superconducting disc in an applied magnetic field using London equations and compare the simulation results with the experiments of Grigorieva et al. [32]. We first do the simulation at $T = 0$ and in the second part, we extend the London model to finite temperatures by including the entropy of the vortex states.

4.1.1 Model and Experimental Parameters

In our model, the Gibbs free energy is determined by several parameters. These are the flux $L\phi_0$ of the central vortex, the $N_i$ off-centre vortices in the $i^{th}$ ring, the flux $q\phi_0$ of the off-centre vortices, the applied magnetic field $H$, the radius of the disc $R$ and its thickness $d$. As mentioned before, we can take the values of $L$ to be $(-1, 0, 1)$ corresponding to the state of an anti-vortex, no vortex and a vortex respectively. We also take $q = 1$ for simplicity (less energy). The number of off-centre vortices $N_i$ is obtained by minimising free energy.

Grigorieva and her group [32] studied vortex configurations in mesoscopic superconducting discs as a function of applied magnetic fields. They found that for a broad range of vorticities $Z = N + L$, the vortices form concentric rings or shells, rather like shell filling in atoms and nuclei. They also found that the so-called magic numbers $Z$ corresponding to the appearance of new atomic shells are robust, i.e., they are reproducible in many experiments for different applied fields and discs. There is up to now no general theory to explain the mechanism for vortex shell filling. Grigorieva et al. [32] used small Niobium (Nb) superconducting discs of radius $R = 1.7 \mu m$ and thinkness $d = 150 \text{nm}$. Nb is a Type II superconductor. The critical temperature of Nb is $T_c = 9.1$ K, with coherent length $\xi_0 \approx 15 \text{ nm}$ and penetration depth $\lambda_0 \approx 90 \text{ nm}$. In the 2-D model, we assume that the thickness of the disc is very small and it is about $d \approx 0.1 \xi = 1.5 \text{nm}$. This approximation is valid in the 2-D model and we follow the same approximation from
Figure 9: Experimental data from Grigorieva [32]. The white dots correspond to fluxoid at \( T = 1.8 \text{K} \) under an applied magnetic field \( \sim 55 \text{Oe} \).

Baelus [30]. The sample was studied under the applied magnetic fields varying in the range \( 0 < H < 60 \text{(Oe)} \) and at a temperature of \( 1.8K \). Fig. 9 shows the vortices inside the disc in the experiment [32] with white dots representing vortices.

4.1.2 Numerical Simulation and Results

Table 1 shows the stable vortex configurations of the disc corresponding to the different ranges of the magnetic field. In the following discussions, brackets with only two entries \((L, N)\) refer to vortex states with a vortex of flux \( L\phi_0 \) at the centre of the disc and \( N \) off-centre vortices, each of flux \( \phi_0 \) (\( i.e., q = 1 \)), on a single ring, whereas those with three entries \((L, N_1, N_2)\) are configurations with 2 rings, with \( N_1 \) off-centre vortices on the first ring, \( N_2 \) off-centre vortices on the second, again each of flux \( \phi_0 \), and a vortex of flux \( L\phi_0 \) at the centre.

Fig. 10 and Fig. 11 are the free energy and vortex positions as a function of \( h \).
Table 1: Simulation results of the different vortex states with respect to critical fields.

<table>
<thead>
<tr>
<th>Critical fields</th>
<th>Vortex States (0K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$h_1 = 5.40$</td>
<td>$(L, N) = (1, 0)$</td>
</tr>
<tr>
<td>$h_2 = 7.75$</td>
<td>$(L, N) = (0, 2)$</td>
</tr>
<tr>
<td>$h_3 = 9.25$</td>
<td>$(L, N) = (0, 3)$</td>
</tr>
<tr>
<td>$h_4 = 10.88$</td>
<td>$(L, N) = (0, 4)$</td>
</tr>
<tr>
<td>$h_5 = 12.50$</td>
<td>$(L, N) = (0, 5)$</td>
</tr>
<tr>
<td>$h_6 = 14.07$</td>
<td>$(L, N) = (1, 5)$</td>
</tr>
<tr>
<td>$h_7 = 15.19$</td>
<td>$(L, N) = (1, 6)$</td>
</tr>
<tr>
<td>$h_8 = 16.75$</td>
<td>$(L, N) = (1, 7)$</td>
</tr>
<tr>
<td>$h_9 = 18.32$</td>
<td>$(L, N) = (1, 8)$</td>
</tr>
<tr>
<td>$h_{10} = 19.64$</td>
<td>$(L, N_1, N_2) = (0, 2, 8)$</td>
</tr>
</tbody>
</table>

Figure 10: The Gibbs free energy $g_{Lon}$ as a function of the applied magnetic field $h$ for different vortex states at $t = 0$. The stable configurations are successsively $(0, 0) \rightarrow (1, 0) \rightarrow (0, 2) \rightarrow (0, 3) \rightarrow (0, 4) \rightarrow (0, 5) \rightarrow (1, 5) \rightarrow (1, 6) \rightarrow (1, 7) \rightarrow (1, 8) \rightarrow (0, 2, 8)$. The states $(L, N) = (1, 5), (1, 6), (1, 7), (1, 8)$ and $(0, 2, 8)$ (corresponding to total flux $6\phi_0, 7\phi_0, 8\phi_0, 9\phi_0$ and $10\phi_0$ respectively) are more stable than $(N, L) = (0, 6), (0, 7), (0, 8), (0, 9)$ and $(0, 10)$ or $(1, 9)$.
As $h$ increases from zero (Fig. 10), the free energy of the screening currents increases quadratically with $h$ as expected until the first critical field $h_1 \sim 5.4$ is reached when a single vortex $(L, N) = (1, 0)$ penetrates the disc at the centre. This state persists until the second critical field $h_2 \sim 7.75$ is reached at which the single centre-vortex is replaced by two off-centre vortices $(0, 2)$. As $h$ is further increased, more off-centre vortices nucleate on the first ring, forming successively a triangle, a square and a pentagon, until the sixth critical field $h_6 \sim 14.07$ is reached. Then it is energetically more favorable for the next vortex to nucleate at the centre of the disc $(1, 5)$ than to form a hexagon of six off-centre vortices with a vortex at each vertex. This result agrees with those of other studies [17, 26, 28, 30] and is also analogous to the result of the study by Yarmchuk et al. [42] on the nucleation of vortices in superfluid $^4$He, which showed that a central vortex would appear in the system. As $h$ increases further, further off-centre vortices enter the disc and nucleate on the first ring, the stable vortex states going through transitions $(1, 5) \rightarrow (1, 6) \rightarrow (1, 7) \rightarrow (1, 8)$, until the tenth critical field $\sim 19.64$ is
Figure 12: Magnetisation $m$ of the disc as a function of the applied field $h$. The jumps in $m$ at $h_1 = 5.40$, $h_2 = 7.75$, $h_3 = 9.25$, $h_4 = 10.88$, $h_5 = 12.50$, $h_6 = 14.07$, $h_7 = 15.19$, $h_8 = 16.75$, $h_9 = 18.32$, $h_{10} = 19.64$ correspond to the entrance of extra vortices in the disc.

reached when, instead of the tenth vortex nucleating to form state $(1, 9)$, the vortices rearrange themselves to form the state $(L, N_1, N_2) = (0, 2, 8)$, with no vortex at the centre of the disc, two vortices on the first ring and eight on the second. The entry of each additional vortex at successive critical fields is accompanied by a jump in the magnetization $m$ of the disc (Fig. 12).

Fig. 11 gives the optimal position $z = r/R$ of the vortices as a function of $h$. The entrance of a new vortex in the disc is accompanied by a jump in $z$. The vortices tend to move away from each other as a result of the repulsive interaction between them. On the other hand, given a state of $N$ vortices, $z$ decreases monotonically as $h$ increases.

Since the size of the disc is very small $R \approx 1.7 \mu m$, it is not possible to have too many off-centre vortices into the disc. According to the experiments, the maximum flux can allow on the disc is about $16\phi_0$. 

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Table 2: The table shows the vortex states in the disc, from $\phi_0$ to $10\phi_0$ as $h$ is increased. The left column is the experimental data from Grigorieva [32], and the right hand column is the results of this study.

<table>
<thead>
<tr>
<th>Experiments</th>
<th>Simulation Results</th>
</tr>
</thead>
<tbody>
<tr>
<td>$(L, N) = (1, 0)$</td>
<td>$(L, N) = (1, 0)$</td>
</tr>
<tr>
<td>$(L, N) = (0, 2)$</td>
<td>$(L, N) = (0, 2)$</td>
</tr>
<tr>
<td>$(L, N) = (0, 3)$</td>
<td>$(L, N) = (0, 3)$</td>
</tr>
<tr>
<td>$(L, N) = (0, 4)$</td>
<td>$(L, N) = (0, 4)$</td>
</tr>
<tr>
<td>$(L, N) = (0, 5)$</td>
<td>$(L, N) = (0, 5)$</td>
</tr>
<tr>
<td>$(L, N) = (1, 5)$</td>
<td>$(L, N) = (1, 5)$</td>
</tr>
<tr>
<td>$(L, N) = (1, 6)$</td>
<td>$(L, N) = (1, 6)$</td>
</tr>
<tr>
<td>$(L, N) = (1, 7)$</td>
<td>$(L, N) = (1, 7)$</td>
</tr>
<tr>
<td>$(L, N_1, N_2) = (0, 2, 7)$</td>
<td>$(L, N) = (1, 8)$</td>
</tr>
<tr>
<td>$(L, N_1, N_2) = (0, 2, 8)$</td>
<td>$(L, N_1, N_2) = (0, 2, 8)$</td>
</tr>
</tbody>
</table>

Fig. 12 gives the magnetization $m$ as a function of with $h$. As expected, $m$ consists of a series of discontinuous jumps at the critical values of $h$ corresponding to the entrance of an additional fluxoid in the disc.

The left hand column of Table 2 gives the vortex states of the disc observed in the experiments. The right hand column is the results of the current study - our calculations predict/produce all the vortex states observed in the experiments, except for the state $(0, 2, 7)$. Our calculations show that the most stable vortex state with total flux $9\phi_0$ is the state $(1, 8)$ with one central vortex and eight off centre vortices arranged on a circle. It is worth noting here that while the experiments were performed at $T = 1.8\, \text{K}$, the calculations are only strictly valid at $T = 0\, \text{K}$. In the next section, we extend to model to finite temperatures ($T \neq 0\, \text{K}$).
4.2 Entropy and Simulation at $T \neq 0 \text{K}$

4.2.1 Entropy with One Ring Configuration

We now extend the model to finite temperatures ($T > 0 \text{K}$) by taking into account the entropy associated with the arrangement of vortices on the concentric rings. It is simpler first to consider a single ring of the radius $r$ with $N$ vortices. These vortices are equally spaced on the ring and are at positions $r_i$, $i = 1, ..., N$ with $|r_i| = r$. The diameter of a vortex core is $2r_c$ and it is reasonable to approximate that a vortex occupies $2r_c$ on the ring. Hence, the number of possible arrangements of $N$ vortices on the ring is

$$W = \frac{2\pi r}{2r_c N}.$$  (4.1)

We assume that all off-centre vortices are identical. The entropy associated with this is

$$S = k_B \ln W,$$  (4.2)

and the Gibb’s free energy at $T \neq 0 \text{K}$ follows from $G = U - \mathbf{M} \cdot \mathbf{H}V/4\pi - TS$. As the temperature increases, the entropy term $-TS$ will decrease and the free energy will decrease as a result.

In terms of dimensionless parameters, one can write the free energy as before,

$$g(N, L, t) = g(N, L) - t(\ln \pi - \ln N + \ln z + \ln (R/r_c)),$$  (4.3)

where $g = 16\pi^2 \lambda^2 G/d\phi_0^2$ is the normalised Gibbs free energy and $t = Tk_B(16\pi^2 \lambda^2/d\phi_0^2)$ is the dimensionless temperature. The corresponding dimensionless magnetisation can be obtained by the derivative $m = -\partial g/\partial h$, where $h = H\pi R^2/\phi_0$ is the normalised magnetic field.
4.2.2 Multiple Ring Model with Entropy

The entropy associated with $N_1$ vortices arranged on a ring of the radius $r_1$ and $N_2$ vortices on a ring of radius $r_2$ is

\[
S = S_1 + S_2 \\
= k_B \ln W_1 + k_B \ln W_2 \\
= k_B \ln \frac{2\pi r_1}{2N_1 r_c} + k_B \frac{2\pi r_2}{2N_2 r_c},
\]

(4.4)

where $S_i = k_B \ln(2\pi r_i/2N_i r_c), \forall i = 1, 2$. This gives the dimensionless Gibbs free energy as

\[
g(L, N_1, N_2, t) = g(N_1, N_2, L) - t(\ln W_1 + \ln W_2) \\
= g(N_1, N_2, L) - t \sum_{i=1}^{2} \ln W_i.
\]

(4.5)

This can be easily extended to $m$ rings of radius $r_i (i = 1, \ldots, m)$ with $N_i$ vortices on the $i^{th}$ ring to give

\[
g(L, N_1, N_2, \ldots, N_m, t) = g(L, N_1, N_2, \ldots, N_m) - t \sum_{i=1}^{m} \ln W_i \\
= g(L, N_1, N_2, \ldots, N_m) - t \sum_{i=1}^{m} \ln(\pi r_i/N_i r_c).
\]

(4.6)

Again, the magnetization $m$ of the disc follows from $m = -\partial g/\partial h$. 
Table 3: The table shows the experimental data of vortex states in disc, from total flux $\phi_0$ to $10\phi_0$. The first column gives the numerical critical field for each vortex state. The second column is the vortex state from our model at $t = 0.14$.

<table>
<thead>
<tr>
<th>Simulation (critical fields)</th>
<th>Simulation (states)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$h_1 = 5.40$</td>
<td>$(L, N) = (1, 0)$</td>
</tr>
<tr>
<td>$h_2 = 7.00$</td>
<td>$(L, N) = (0, 2)$</td>
</tr>
<tr>
<td>$h_3 = 9.26$</td>
<td>$(L, N) = (0, 3)$</td>
</tr>
<tr>
<td>$h_4 = 10.90$</td>
<td>$(L, N) = (0, 4)$</td>
</tr>
<tr>
<td>$h_5 = 12.52$</td>
<td>$(L, N) = (0, 5)$</td>
</tr>
<tr>
<td>$h_6 = 14.03$</td>
<td>$(L, N) = (1, 5)$</td>
</tr>
<tr>
<td>$h_7 = 15.22$</td>
<td>$(L, N) = (1, 6)$</td>
</tr>
<tr>
<td>$h_8 = 16.77$</td>
<td>$(L, N) = (1, 7)$</td>
</tr>
<tr>
<td>$h_9 = 17.50$</td>
<td>$(L, N_1, N_2) = (0, 2, 7)$</td>
</tr>
<tr>
<td>$h_{10} = 19.41$</td>
<td>$(L, N_1, N_2) = (0, 2, 8)$</td>
</tr>
</tbody>
</table>

4.2.3 Results and Analysis

In the experiments of Grigorieva and her group [32], vortices nucleate on two concentric rings on their discs and we restrict our calculation to the two-ring model. For a given temperature $t$, we minimize $g(L, N_1, N_2, t)$ with respect to $z_1$ and $z_2$ for a range of applied magnetic fields $h$, with different $L$, $N_1$ and $N_2$. The parameters $d$, $R$, $\lambda$ are chosen to correspond to those of the experiments by Grigorieva et al. [32], as we did in the last section. The details of superconducting disc are [Niobium, radius $R \approx 1.7 \mu m$, $\xi \approx 15 \text{nm}$, $\lambda \sim R, d \approx 0.1 \xi$, experiment temperature $T = 1.8 \text{K}$ and critical temperature $T_c = 9.1 \text{K}$]. In our dimensionless units, the critical temperature is $t_c = 0.7$, and $t = 0.14$ corresponds to the temperature $T = 1.8 \text{K}$ at which the experiments were performed.

Fig. 13 gives the Gibbs free energy as a function of $h$ at $t = 0.14$. Fig. 14 and Fig. 15 give the position of vortices and magnetisation respectively. Table 3 lists the different critical fields and the stable vortex states up to each critical field. As $h$ increases gradually from zero, the Meissner state persists until the applied magnetic field reaches the first critical field $h_1 \sim 5.4$. Then, a single vortex $(L, N) = (1, 0)$ nucleates at the centre of the disc. At the second critical field $h_2 \sim 7.0$, the energetically favorable configuration (with total flux $2\phi_0$) is the state with two off-centre single vortices $(L, N) = (0, 2)$.
Figure 13: The Gibbs free energy $g_{\text{Lon}}$ as a function of $h$ at $t = 0.14$ ($T = 1.8$ K). The stable vortex states and transitions are $(L, N) = (0, 0) \rightarrow (L, N) = (1, 0) \rightarrow (L, N) = (0, 2) \rightarrow (L, N) = (0, 3) \rightarrow (L, N) = (0, 4) \rightarrow (L, N) = (0, 5) \rightarrow (L, N) = (1, 5) \rightarrow (L, N) = (1, 6) \rightarrow (L, N) = (1, 7) \rightarrow (L, N_1, N_2) = (0, 2, 7) \rightarrow (L, N_1, N_2) = (0, 2, 8)$ as $h$ increases (for the range of $h$ shown).

As $h$ increases further, more vortices penetrate the disc, with the vortex state going successively through the transitions $(L, N) = (0, 3)$ at $h_3 = 9.26$, $(L, N) = (0, 4)$ at $h_4 = 10.90$, $(L, N) = (0, 5)$ at $h_5 = 12.52$, $(L, N) = (1, 5)$ at $h_6 = 14.03$, $(L, N) = (1, 6)$ at $h_7 = 15.22$ and $(L, N) = (1, 7)$ at $h_8 = 16.77$. This result is similar to that obtained from the model at $t = 0$.

As $h$ is increased from $h_9 = 17.50$, an extra vortex enters the disc and the stable vortex state with total flux $\phi_0$ is $(L, N_1, N_2) = (0, 2, 7)$, with no vortex at the centre of the disc, and the nine vortices arranged on two rings, with two vortices on the inner ring and seven on the outer. As $h$ is further increased, a further vortex penetrates the disc and nucleates on the outer ring, forming the state $(L, N_1, N_2) = (0, 2, 8)$. These results are in direct agreement with the experimental observations of Grigorieva et al. \[32\]. Fig. 15
Figure 14: It is the optimal position of vortices in the disc (distance from centre of the disc).

gives the calculated magnetisation as a function of \( h \) at \( t = 0.14 \).

Fig. 16 shows blown up parts of Gibbs free energy \( g \) (Fig. 13) as a function of \( h \) for which the total vortex flux in the disc is \( 9\phi_0 \) and Fig. 17 is the corresponding plot for total vortex flux \( 10\phi_0 \).

The stars (*) in Fig. 16 gives the free energy of the vortex state \((L, N_1, N_2) = (0, 2, 7)\). The curve represented by solid curve is the state \((L, N) = (1, 8)\). It is clear that for configurations with total flux \( 9\phi_0 \), while the most stable state at \( t = 0 \) (\( T = 0 \) K) is the state \((L, N) = (1, 8)\), with a central vortex and eight vortices on a ring. At \( t = 0.14 \) (\( T = 1.8 \) K), the most stable state is the state \((L, N_1, N_2) = (0, 2, 7)\). There is no vortex at the centre of the disc, with two vortices on the inner ring and seven on the outer ring.

This result is in excellent with the experiments of Grigorieva et al. [32], who also found that at \( T = 1.8 \) K, the state \((L, N) = (1, 8)\) was observed in only just a few cases, while the state \((L, N_1, N_2) = (0, 2, 7)\) was, by far, the most frequently observed state.
Figure 15: The magnization $m$ at $t = 0.14$ ($T = 1.8$ K). The stable vortex states and transitions are $(L, N) = (0, 0) \rightarrow (L, N) = (1, 0) \rightarrow (L, N) = (0, 2) \rightarrow (L, N) = (0, 3) \rightarrow (L, N) = (0, 4) \rightarrow (L, N) = (0, 5) \rightarrow (L, N) = (1, 5) \rightarrow (L, N) = (1, 6) \rightarrow (L, N) = (1, 7) \rightarrow (L, N_1, N_2) = (0, 2, 7) \rightarrow (L, N_1, N_2) = (0, 2, 8)$ as $h$ increases (for the range of $h$ shown).
Figure 16: Total flux = $9\phi_0$. The triangles, solid lines and $*$ represent the Gibbs free energy $g$ of the states $(L, N_1, N_2) = (0, 3, 6)$, $(L, N) = (1, 8)$ and $(L, N_1, N_2) = (0, 2, 7)$ respectively as a function of the applied magnetic field $h$. The figure on the left is for $t = 0$ ($T = 0$ K), while the one on the right is for $t = 0.14$ ($T = 1.8$ K).

In our simulation, the entropy for two shells $k_B(\ln W_1 + \ln W_2)$ is greater than the one $k_B \ln W_1$ in one shell, and hence the Gibbs free energy is smaller in the two shells model rather than in the one shell when $t \neq 0$ K. At $t = 0$, our model predicts only the state $(L, N) = (1, 8)$. (The studies of Baleus et al. [31] also found that the only stable state is $(L, N) = (1, 8)$ at $T = 1.8$ K.)

Fig. 17 shows the corresponding result for vortex states with total flux $10\phi_0$. The triangles show the dependence on $h$ of the free energy of the state $(L, N_1, N_2) = (0, 3, 7)$, the solid lines that of state $(L, N) = (1, 9)$ and the lines represented by stars ($*$) that of state $(L, N_1, N_2) = (0, 2, 8)$. At $t = 0$, the most stable vortex state is the state
Figure 17: Total flux = $10\phi_0$. The triangles, the solid lines and the stars (*) are the field dependence of the vortex states represented the states $(L, N_1, N_2) = (0, 3, 7)$, $(L, N) = (1, 9)$ and $(L, N_1, N_2) = (0, 2, 8)$ respectively. The figure on the left is for $t = 0$ ($T = 0\text{K}$), while the one on the right is for $t = 0.14$ ($T = 1.8\text{K}$).
\((L, N_1, N_2) = (0, 2, 8)\), with states \((L, N_1, N_2) = (0, 3, 7)\) and \((L, N) = (1, 9)\) having almost the same (slightly higher) energy. At \(t = 0.14\) \((T = 1.8\, \text{K})\), the state \((L, N_1, N_2) = (0, 2, 8)\) is again the most stable state, with the other two states having higher energies. This result is in very good agreement with the experimental studies of Grigorieva et al. [32] who reported that the state \((L, N_1, N_2) = (0, 2, 8)\) was the most frequently observed state and that the state \((L, N) = (1, 9)\) was never observed in their experiments. Baelus et al. [31], on the other hand, predicted only the state \((L, N) = (1, 9)\) for the state with total flux \(10\phi_0\).

When \(t > 0\) (Fig. 17, right diagram), the free energies in the vortex states \((0, 2, 8)\) and \((0, 3, 7)\) are lower than the free energy in the vortex state \((1, 9)\). It is because two shells model provides more freedom of disorder than the one shell when \(t > 0\). Finally, energy in the state \((L, N_1, N_2) = (0, 3, 7)\) is higher than \((L, N_1, N_2) = (0, 2, 8)\) because the later one shows more symmetry than the previous one. The energy differences between the vortex states \((0, 2, 8)\) and \((0, 3, 7)\) are small so that the temperature deviation may cause the change of priority.

4.2.4 Review of Two Rings’ Model

In conclusion, we have presented an extension of the early study of Sobnack and Kusmartsev [33] by including temperature into the formulation. Inclusion of the temperature term \(-TS\) (by taking into account the entropy \(S\) associated with the non-centre vortices) lowers the free energy of some of the vortex states and stabilises them. Our results are in very good agreement with those of the recent experiments of Grigorieva and co-workers [32] and in contrast with some of the earlier results of Baelus et al. [31]. Some of the states Baelus et al. theoretically predicted are either only rarely observed or not observed in the experiments [32]. A possible reason for the disagreement between the earlier studies of Baelus et al. [31] and the experiments of Grigorieva et al. [32] is that the experiments are performed at finite temperatures \(T \neq 0\, \text{K}\), whereas the previous studies of Baelus et al. [31] is only valid at \(T = 0\, \text{K}\). Misko et al. [45] (in the same research group
of Baelus) in his recent studies modified his model on the superconducting discs. He used
the London equations and took into account the molecular dynamics on the system. He
also added the temperature contribution in his formulation and finally found that his
simulation results agree with the experiments [32].
5 Anti-Vortex and Vortex Configuration

5.1 Possibility of Anti-Vortex

In this section, we investigate the possibility of anti-vortices nucleating in the disc. In our previous simulations, we did not obtain anti-vortices, neither at \( t = 0 \) nor at \( t > 0 \). Further, no anti-vortices were observed in the experiments of Grigorieva et al. [32]. However, it is still very interesting to determine whether an anti-vortex will appear in the superconducting disc under some special conditions.

Chibotaru et al. [23] studied the case of total fluxoids \( 3\phi_0 \) on their thin square sample and asserted that the optimal state in the square sample is the one with an anti-vortex at the centre and four vortices at the four corners in order to preserve the symmetry.

Geurts et al. [43] studied vortex and anti-vortex nucleation and claimed that an anti-vortex is difficult to observe in experiments. Because of the attractive interaction between vortices and anti-vortices, vortices and anti-vortices tend to be confined in a small region of size of the order of the coherence length. As a result, the minima in \( \psi \) lie near each other and this would make it difficult to experimentally resolve between the vortices and anti-vortices - the system essentially looks like a gain vortex. Further because the supercurrent in the region containing the vortices and anti-vortices is rather weak, it makes magnetic imaging difficult. Geurts et al. [43] also proposed that the anti-vortex would be easily destroyed by boundary defects.

In our study, we try out the possibility of the nucleation of anti-vortices. First, we increase the temperature in order to raise the entropy and hence decrease the free energy. Secondly, we adjust the size of the disc. Varying the parameter

\[
t = \frac{16\pi^2\lambda^2}{d\phi_0^2}k_B T,
\]

may change \( \lambda \). Since the penetration depth \( \lambda \) and the coherent length \( \xi \) characterise the type of superconductor, as well as the materials, it means that our model is no longer
restricted to Nb.

5.2 Simulations and Analysis, \( g(L, N, t = 0.05) \)

After many trials, it is possible to choose the dimensionless parameters \( t = 0.05 \), \( \ln(R/r_c) \sim 2.4 \) and \( h = H \pi R^2 / \phi_0^2 \), for which an anti-vortex nucleates in the simulation. For simplicity, we will only simulate the one-ring model, with an anti-vortex \((L < 0)\) at centre and with \( N \) off-centre vortices.

The simulation results at \( t = 0.05 \) are shown in Fig. 18 (Gibbs free energy), Fig. 19 (magnetisation) and Fig. 20 (optimal position of vortices). The Meissner state persists until the applied magnetic field reaches the first critical field \( h_1 \sim 2.3 \) when a single vortex \((L, N) = (1, 0)\) nucleates at the centre of the disc (see Fig. 18). At the second critical field \( h_2 \sim 4.0 \), the energetically favourable configuration (with total flux \( 2\phi_0 \)) is the state with three off-centre single vortices and a central single anti-vortex \((L, N) = (-1, 3)\) rather than the state \((L, N) = (0, 2)\) obtained at \( t = 0 \). In our simulation, we find that the state \((L, N) = (0, 2)\) is not as stable as \((L, N) = (-1, 3)\). In Fig. 20, the position \( z \) of the off-centre vortices is close to the centre and this is due to the attractive interaction between a vortex and an anti-vortex. As the magnetic field \( h \) increases further, the anti-vortex disappears and the next successive vortex states are \((0, 3)\), \((0, 4)\) and \((0, 5)\). From Fig. 20, we also find that the vortices move further away from the centre (when \( h \) increases). This is because \( N \) off-centre vortices, with the same spinning direction, repel each other. Therefore, the repulsive force makes the \( N \) vortices far away from centre. At \( h = 8.5 \), the system will slip to the state \((L, N) = (1, 5)\) rather than the state \((0, 6)\).

In our simulation, the vortex state \((-1, 3)\) is a special case and only occurs in the range \( 4.0 < h < 5.6 \); the anti-vortex is then destroyed as \( h \) is further increased. In brief, nucleation of an anti-vortex depends on three factors: the first is the attractive interaction between the vortices and the anti-vortex; the second is the repulsive force between the off-centre vortices and both factors would determine the distance between the vortices and anti-vortex; the third factor is the strength of the applied magnetic field.
Figure 18: The Gibbs free energy, \( g(L, N, 0.05) \) of the different vortices states as a function of \( h \). The transition configurations are from \((L, N) = (0, 0)\) to \((0, 1)\), \((-1, 3)\), \((0, 4)\), \((0, 5)\) and then \((1, 5)\) in the range of \( h \) investigated.

as the spinning direction of the anti-vortex is opposite to it.

In summary, we have extended the work of Buzdin [28] and Sobnack [33]. We write the free energy as a function of the temperature as well as the applied magnetic field. In this study, we also attempt to explain how vortices are nucleated in the mesoscopic scale. We conclude that the formation of vortices inside the disc is dominated by several factors: the interaction between the central vortex \( L \) and the \( N \) off-centre vortices; the repulsion between the \( N \) off-centre vortices and finally, the strength of the applied magnetic field \( h \) and temperature \( t \). At \( t = 0.05 \), we also investigate the stability of an anti-vortex at the centre and find that \((-1, 3)\) is the only stable vortex-anti-vortex state in the small superconducting disc.
Figure 19: It represents the reduced magnetization in the disc. It is found that the state $(0, 1)$ sweeps to $(-1, 3)$ (with total flux $2\phi_0$) rather than the state $(0, 2)$. 
Figure 20: Optimal position $z$ of vortices in the disc as a function of applied field $h$. In a vortex state $(-1, 3)$, the distance between the off-centre vortices and anti-vortex is very small compared to other vortex states.
6 Modified London Model (from Ginzburg-Landau Model)

We have already studied vortex configuration in the superconducting disc using London model. In this chapter, we set up the Gibbs free energy from Ginzburg-Landau equations, and then make approximations which compares with the London model. Our modified free energy is a function of the disc’s size $R$, applied magnetic field $H$ and temperature $T$, as well as the superconducting density $|\psi(r)|^2$. $|\psi(r)|^2$ is a function of position in the Ginzburg-Landau model, whereas the superconducting density is assumed to be constant in the London model. As vortices are generated, superconductivity is destroyed, the vortex core is normal metal and one cannot ignore this effect.

6.1 Formulation and Methodology

The parameters of the new model are similar to those in the previous chapters: Consider a thin disc under an applied field $H$ ($H = Hk = \nabla \times A_{\text{app}}$), with radius $R$ and thickness $d$. We restrict the scale to the case $R < \Lambda = \lambda^2/d$, $d \ll \Lambda$ - the system is essentially a 2D system. We work in cylindrical coordinates ($r, \theta, z$). The screening effects are suppressed: the whole disc can be thought of as soaking in the applied field $H$, so that the local magnetic field $B = \nabla \times A$ is approximately the same inside and outside the sample, $B \approx H$. We formulate the equation at a temperature $T < T_c$.

6.2 Ginzburg-Landau Equations

First, we have to formulate the Gibbs free energy in the small disc. The state of superconductors can be described by a wave function, $\Psi(r, \theta) = |\psi(r)| e^{i\theta}$ (see Fetter [38, 46, 47]) and it is a vector with planar orientation. We also assume that the spatial variation $|\psi(r)|$ is small. In absence of applied field, the free energy density (see Tinkham [1] and De Gennes [3]) of the system in superconducting state (in form of Talyor’s approximation)
is
\[ g_s \approx g_n + \alpha |\Psi|^2 + \frac{\beta}{2} |\Psi|^4, \quad (6.1) \]
where \( \alpha \) and \( \beta \) relate to the parameters of the superconducting material, \( g_n \) corresponds to the free energy density in normal state. Variation of \( g_s \) with respect to \( \Psi^* \), the minimum free energy is reached when \( |\Psi_0|^2 = |\alpha|/\beta \). In presence of magnetic field \( H \), two more terms have to be included.

The first one is the kinetic energy under the applied field (see De Gennes [3]) and is given by
\[ \frac{1}{2m} \left( p - \frac{q}{c} A \right) \Psi \cdot \left( p - \frac{q}{c} A \right) \Psi = \frac{1}{2m} \left| \left( \frac{\hbar}{i} \nabla - \frac{q}{c} A \right) \Psi \right|^2, \]
where \( q = 2e \) is the charge of the Cooper pair. \( A (B = \nabla \times A) \) represents the magnetic vector potential in which we can choose an arbitrary gauge.

The second term is the magnetic energy stored in the system, \( \frac{1}{8\pi} (B - H)^2 \), where \( B \) is the local field in the system itself. The total Gibbs free energy under applied magnetic field \( H \), is hence,
\[ G_s = G_n + \int \alpha |\Psi|^2 + \frac{\beta}{2} |\Psi|^4 + \frac{1}{2m} \left| \left( \frac{\hbar}{i} \nabla - \frac{q}{c} A \right) \Psi \right|^2 \]
\[ + \frac{1}{8\pi} (B - H)^2 \, d^3r. \quad (6.2) \]

For a small disc, the screening is weak and the last term is small comparable to the kinetic energy and can be neglected.

### 6.3 Vortices inside the Small Thin Disc

We introduce the order parameter \( \Psi(r) = |\Psi| e^{i f(\theta)} \), where \( f(\theta) \) is a function of \( \theta \). The gradient of \( \Psi(r) \) in cylindrical coordinates gives
\[ \nabla \Psi = \frac{\partial \Psi}{\partial r} \hat{r} + \frac{1}{r} \frac{\partial \Psi}{\partial \theta} \hat{\theta} + \frac{\partial \Psi}{\partial z} \hat{z}. \]
As discussed above, the system can be approximated to a 2-D system (so $\partial/\partial z = 0$). We assume that the amplitude of $|\Psi|$ is constant except at some singularities and the edge of the disc. Hence

$$\nabla \Psi \approx \frac{1}{r} \frac{\partial \Psi}{\partial \theta} = \frac{i}{r} \frac{\partial f(\theta)}{\partial \theta} \Psi \hat{\theta}. \tag{6.3}$$

With these approximations, the Gibbs free energy becomes:

$$G_s \approx G_n + \int \alpha |\Psi|^2 + \frac{\beta}{2} |\Psi|^4 + \frac{1}{2m} \left( \frac{\hbar}{r} \frac{\partial f(\theta)}{\partial \theta} - \frac{q}{c} A \right)^2 |\Psi|^2 \, d^3r,$$  \tag{6.4}

where $\partial f(\theta)/\partial \theta = k$ represents the change of phase angle and $k$ is an integer winding number.

The kinetic energy term becomes,

$$KE = \frac{1}{2m} \int \left| \frac{\hbar}{r} \frac{\partial f(\theta)}{\partial \theta} - \frac{q}{c} A \right|^2 |\Psi|^2 \, d^3r = \frac{\hbar^2}{2m} \int \left( \frac{k}{r} - \frac{2\pi}{\phi_0} A \right)^2 |\Psi|^2 \, d^3r = \frac{\hbar^2}{2m} \int \left( \frac{2\pi}{\phi_0} \right)^2 \left( \frac{\phi_0 k}{2\pi r} - A \right)^2 |\Psi|^2 \, d^3r, \tag{6.5}$$

where $A_v = (\phi_0 k/2\pi r) \hat{\theta}$ is the magnetic potential generated by the vortex. Now the Gibbs free energy expression is hence

$$G_{GL} = G_s - G_n = \int \left[ \alpha |\Psi|^2 + \frac{\beta}{2} |\Psi|^4 + \frac{\hbar^2}{2m} \left( \frac{2\pi}{\phi_0} \right)^2 (A_v - A)^2 |\Psi|^2 \right] \, d^3r, \tag{6.6}$$

where taking $G_{GL} = G_s - G_n$. The first two terms in above equation can be written as

$$\alpha |\Psi|^2 + \frac{\beta}{2} |\Psi|^4 = \frac{\hbar^2}{2m} \left( \frac{1}{\xi^2} |\Psi|^2 + \frac{\beta}{2\xi^2|\alpha|^2} |\Psi|^4 \right), \tag{6.7}$$

where $\xi^2 = \hbar^2/2m|\alpha|$ is the correlation length. Then we normalise the order parameter
to be $\tilde{\Psi} = \Psi/|\Psi_0|$, where $|\Psi_0|^2 = |\alpha|/\beta$. Therefore

$$
G_{\text{GL}} = \frac{\hbar^2 |\Psi_0|^2}{2m} \int \left[ -\frac{1}{\xi^2} |\tilde{\Psi}|^2 + \frac{1}{2\xi^2} |\tilde{\Psi}|^4 \right. \\
+ \left. \left( \frac{2\pi}{\phi_0} \right)^2 (A_v - A)^2 |\tilde{\Psi}|^2 \right] d^3r. \tag{6.8}
$$

Further, we can also approximate the applied magnetic potential $A_{\text{app}}$ to be very close to local magnetic potential $A$ [33, 27], $A_{\text{app}} \approx A$.

As discussed before, we use the notations $(L, N)$ and $(L, N_1, N_2)$ to represent the one shell model and the two shells model respectively. If there are no vortices ($L = 0, N = 0$), $|\tilde{\Psi}|^2$ is a constant, except near the boundary. However, $|\tilde{\Psi}|^2$ is no longer a constant when there are vortices. In this case, we need to consider the cores of the vortices which are in normal state: the value of superconducting density $|\tilde{\Psi}|^2$ is zero at the cores. Outside the region of the core, $|\tilde{\Psi}|^2$ remains constant. It is reasonable to assume that the volume of a core on the disc can be approximated as $\pi \xi_{\text{eff}}^2 d$, where $\xi_{\text{eff}}$ is the effective radius of a vortex and the $d$ is the thickness of disc. If there is a vortex inside the disc, the expectation value of superconducting density can be approximated as

$$
\langle |\tilde{\Psi}|^2 \rangle = \frac{1}{|\Psi_0|^2} \\
= \frac{\pi R^2 d - \pi \xi_{\text{eff}}^2 d}{\pi R^2 d} \\
= 1 - \left( \frac{\xi_{\text{eff}}}{R} \right)^2. \tag{6.9}
$$

If there are $M$ total vortices on the disc, the total vorticity is $M = |N| + |L|$, superconducting density becomes

$$
\langle |\tilde{\Psi}|^2 \rangle = 1 - M \left( \frac{\xi_{\text{eff}}}{R} \right)^2. \tag{6.10}
$$

The Gibbs free energy from GL model hence depends on the superconducting density.
6.4 Vortex Shell Configurations on the Disc

The last term of Eq. (6.8) (kinetic energy term) can be simplified as

\[
\frac{\hbar^2 |\Psi_0|^2}{2m} \int \left( \frac{2\pi}{\phi_0} \right)^2 (A_v - A)^2 |\tilde{\Psi}|^2 d^3r
= \frac{\hbar^2 |\Psi_0|^2}{2m} \langle |\tilde{\Psi}|^2 \rangle \int \left( \frac{2\pi}{\phi_0} \right)^2 (A_v - A)^2 d^3r
= \frac{\hbar^2 |\Psi_0|^2}{2m} \langle |\tilde{\Psi}|^2 \rangle \int (A_v - A_{app})^2 d^3r,
\]

(6.11)

where we assume the super-density $|\Psi|^2$ varies slowly in $r$ and $A \simeq A_{app}$. We further assume that $B \simeq H = (0, 0, H)$, whereas the gauge of magnetic potential is chosen as $A_{app} = (-yH/2, xH/2, 0)$ (London gauge). More specifically,

\[
A_{app} = \frac{1}{2} \mathbf{H} \times \mathbf{r} = \frac{1}{2} \begin{vmatrix}
\hat{i} & \hat{j} & \hat{k} \\
0 & 0 & H \\
x & y & z
\end{vmatrix}.
\]

As we did in the London model, it leads to $A_v = \sum_i [\Phi_i(r - r_i) - \Phi_i(r - r_i')] \hat{\mathbf{\theta}}$, where for each vortex of flux $\phi_i$ at $r_i$ in the disc, an image anti-vortex of flux $-\phi_i$ at $r_i' = (R/r_i)^2 r_i$ beyond the disc and $\Phi_i(r) = (\phi_i / 2\pi r) \hat{\mathbf{\theta}}$. It can show that (as we did in chapter 3), at $T = 0$ K, the Gibbs free energy of a configuration of $N_1$ vortices at $r_i = r_1$ and $N_2$ vortices at $r_j = r_2$ and a central vortex of flux $\phi = L\phi_0$ ($L > 0$ for a vortex and $L < 0$ for an anti-vortex) as

\[
g_{GL}(L, N_1, N_2) = -\frac{1}{2\xi'^2} \langle |\tilde{\Psi}|^2 \rangle + \frac{1}{4\xi'^2} \langle |\tilde{\Psi}|^4 \rangle + g_{Lon}(L, N_1, N_2) \langle |\tilde{\Psi}|^2 \rangle,
\]

(6.12)

where $g_{GL} = G_{GL}m/(\hbar^2 |\Psi_0|^2 \pi d)$ is the dimensionless Gibbs free energy, $\xi' = \xi/R$, $h = H\pi R^2/\phi_0$ is the dimensionless applied field and $z_i = r_i/R$ ($i = 1, 2$) shows the optimal position. It is important to note that $g_{Lon}(L, N_1, N_2)$ is exactly the Gibbs free energy we
obtained from the London model,

\[ g_{\text{Lon}}(L, N_1, N_2) = \frac{1}{4} h^2 + L^2 \ln \frac{R}{r_c} - 2L N_1 q \ln z_1 - 2L N_2 q \ln z_2 - L h + g'(N_1, 0) \]

\[ + \ g'(N_2, 0) + g_{12}(N_1, N_2), \quad (6.13) \]

where \( g'(N_1, 0) \) and \( g'(N_2, 0) \) are the dimensionless free energies of \( N_1 \) and \( N_2 \) off-centre vortices respectively, with

\[ g'(N_i, 0) = N_i q^2 \ln \frac{R}{r_c} - N_i(N_i - 1)q^2 \ln z_i + N_i q^2 \ln (1 - z_i^2) - N_i q h (1 - z_i^2) \]

\[ + \ \frac{1}{2} N_i q^2 \sum_{n=1}^{N_i-1} \ln \frac{1 - 2 z_i^2 \cos(2 \pi n/N_i) + z_i^4}{4 \sin^2(\pi n/N_i)} \quad (6.14) \]

for \( i = 1, 2 \) and, as is usual, we have introduced the core radius \( r_c \) as a cutoff. The interaction energy \( g_{12}(N_1, N_2) \) of the \( N_1 \) vortices in the first shell (radius \( r_1 \)) and the \( N_2 \) vortices in the second shell (radius \( r_2 \)) is

\[ g_{12}(N_1, N_2) = q^2 \sum_{n,m} \ln \frac{1 + z_1^2 z_2^2 - 2 z_1 z_2 \cos[\alpha + 2\pi(n/N_1 - m/N_2)]}{z_1^2 + z_2^2 - 2 z_1 z_2 \cos[\alpha + 2\pi(n/N_1 - m/N_2)]}, \quad (6.15) \]

where \( n \in [1, N_1], m \in [1, N_2] \) and \( \alpha \) is the misalignment angle between vortices in the two shells. Furthermore, we will take \( q = 1 \) and \( L = -1, 0, 1 \) for the reason of minimisation of energy.
6.5 Entropy of Ordered Vortices associated with Temperature

As in the previous chapters, the dimensionless free energy with the entropy term gives

\[ g_{GL}(L, N_1, N_2, t) = g_{GL}(L, N_1, N_2) - k_B T (\ln W_1 + \ln W_2) \]
\[ = g_{GL}(L, N_1, N_2) - t [2 \ln \pi + 2 \ln R/r_c] \]
\[ - \ln N_1 - \ln N_2 + \ln z_1 + \ln z_2 \]
\[ = g_{GL}(L, N_1, N_2) - t [2 \ln \pi + 2 \ln R/r_c] \]
\[ - \ln N_1 - \ln N_2 + \ln z_1 + \ln z_2 \]

(6.16)

where \( k_B \ln(W_i) \) is the entropy in \( i \) ring. \( z_i = r_i/R \) \( (i = 1, 2) \) and the normalised temperature is \( t = mk_B T/(\hbar^2 n_s \pi d) \) from GL model. From London model, we obtain \( t = \lambda^2 k_B 16\pi^2 T/\phi_0^2 d \) whereas \( \phi_0 = hc/q \). On can find that \( mk_B T/(\hbar^2 n_s \pi d) = \lambda^2 k_B 16\pi^2 T/\phi_0^2 d \) (\( \lambda = \sqrt{mc^2/4\pi n_s q^2} \) and \( 1/\pi n_s = 4\lambda^2 q^2/mc^2 \)). In fact, \( n_s, \xi \) and \( \lambda \) are temperature dependent, \( n_s(T) \approx n(1-(T/T_c)^4) \), \( \xi(T) \approx \xi_0/\sqrt{1-T/T_c} \) and \( \lambda(T) \approx \lambda_0/\sqrt{1-(T/T_c)^4} \).
Table 4: The table shows the critical fields (first column) and vortex states (second column) at $t = 0$.

<table>
<thead>
<tr>
<th>Simulation (critical fields)</th>
<th>Simulation (states)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$h_1 = 5.34$</td>
<td>$(L, N) = (1, 0)$</td>
</tr>
<tr>
<td>$h_2 = 7.52$</td>
<td>$(L, N) = (0, 2)$</td>
</tr>
<tr>
<td>$h_3 = 8.89$</td>
<td>$(L, N) = (0, 3)$</td>
</tr>
<tr>
<td>$h_4 = 10.36$</td>
<td>$(L, N) = (0, 4)$</td>
</tr>
<tr>
<td>$h_5 = 11.80$</td>
<td>$(L, N) = (0, 5)$</td>
</tr>
<tr>
<td>$h_6 = 13.16$</td>
<td>$(L, N) = (1, 5)$</td>
</tr>
<tr>
<td>$h_7 = 14.08$</td>
<td>$(L, N) = (1, 6)$</td>
</tr>
<tr>
<td>$h_8 = 15.39$</td>
<td>$(L, N) = (1, 7)$</td>
</tr>
<tr>
<td>$h_9 = 16.69$</td>
<td>$(L, N) = (1, 8)$</td>
</tr>
<tr>
<td>$h_{10} = 17.72$</td>
<td>$(L, N_1, N_2) = (0, 2, 8)$</td>
</tr>
</tbody>
</table>

6.6 Simulation Results and Analysis

We simulate the GL model, $g_{GL}(L, N_1, N_2)$, in this part. For $t = 0$, we summarise the simulation results in Table 4. It shows the same results (vortex states) as those obtained with the London model. Fig. 21 gives the Gibbs free energy and Fig. 22 shows the magnetisation at $t = 0$. It is found that the free energy from the GL model is smaller than the free energy from London model. The GL model takes into account the fact that the nucleation of a vortex is associated with the destruction of superconducting density of the system and it leads to lower free energy. Fig. 23 shows the optimal position of the vortices as a function of $h$.

For $t = 0.14$, the transition vortex states and corresponding critical fields are shown in Table 5. Again, the stable vortex configurations agree with the experimental results and with the simulations using London model. Fig. 24 and Fig. 25 show the Gibbs free energy and magnetisation at $t = 0.14$, and Fig. 26 the optimal positions of the vortices.

Fig. 27 gives the Gibbs free energy for a configuration with total flux $9\phi_0$ as a function of $h$. The black triangles and red stars show the free energy of states $(L, N_1, N_2) = (0, 3, 6)$ and $(L, N_1, N_2) = (0, 2, 7)$ respectively. The blue line represents the state $(L, N) = (1, 8)$. The most stable state at $t = 0$ ($T = 0$ K) for the range of $h$ shown is the state $(L, N) =$
Figure 21: The free energy $g$ with respect to $h$ at $t = 0$ is shown. The stable configurations are successsively $(L, N) = (0, 0) \rightarrow (L, N) = (1, 0) \rightarrow (L, N) = (0, 2) \rightarrow (L, N) = (0, 3) \rightarrow (L, N) = (0, 4) \rightarrow (L, N) = (0, 5) \rightarrow (L, N) = (1, 5) \rightarrow (L, N) = (1, 6) \rightarrow (L, N) = (1, 7) \rightarrow (L, N) = (1, 8) \rightarrow (L, N) = (0, 2, 8)$.

Table 5: The critical fields at which there is a change of the vortex configuration of the disc at $t = 0.14$.

<table>
<thead>
<tr>
<th>Simulation (critical fields)</th>
<th>Simulation (states)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$h_1 = 5.4$</td>
<td>$(L, N) = (1, 0)$</td>
</tr>
<tr>
<td>$h_2 = 7.0$</td>
<td>$(L, N) = (0, 2)$</td>
</tr>
<tr>
<td>$h_3 = 9.3$</td>
<td>$(L, N) = (0, 3)$</td>
</tr>
<tr>
<td>$h_4 = 10.9$</td>
<td>$(L, N) = (0, 4)$</td>
</tr>
<tr>
<td>$h_5 = 12.5$</td>
<td>$(L, N) = (0, 5)$</td>
</tr>
<tr>
<td>$h_6 = 14.0$</td>
<td>$(L, N) = (1, 5)$</td>
</tr>
<tr>
<td>$h_7 = 15.2$</td>
<td>$(L, N) = (1, 6)$</td>
</tr>
<tr>
<td>$h_8 = 16.8$</td>
<td>$(L, N) = (1, 7)$</td>
</tr>
<tr>
<td>$h_9 = 17.5$</td>
<td>$(L, N_1, N_2) = (0, 2, 7)$</td>
</tr>
<tr>
<td>$h_{10} = 19.4$</td>
<td>$(L, N_1, N_2) = (0, 2, 8)$</td>
</tr>
</tbody>
</table>
Figure 22: Magnetization $m$ with respect to $h$ at $t = 0$. The stable configurations are successsively $(L, N) = (0, 0) \rightarrow (L, N) = (1, 0) \rightarrow (L, N) = (0, 2) \rightarrow (L, N) = (0, 3) \rightarrow (L, N) = (0, 4) \rightarrow (L, N) = (0, 5) \rightarrow (L, N) = (1, 5) \rightarrow (L, N) = (1, 6) \rightarrow (L, N) = (1, 7) \rightarrow (L, N) = (1, 8) \rightarrow (L, N) = (0, 2, 8)$. 

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(1, 8), with a central vortex and eight vortices on a ring.

At $t = 0.14$ ($T = 1.8$ K), the most stable state is the state $(L, N_1, N_2) = (0, 2, 7)$, with no vortex at the centre of the disc, two vortices on the inner ring and seven on the outer. This result is in very good agreement with the experiments of Grigorieva et al. [32] (who found that at $T = 1.8$ K, the state $(L, N) = (1, 8)$ was observed in only just a few cases, while the state $(L, N_1, N_2) = (0, 2, 7)$ was, by far, the most frequently observed state). Fig. 28, Fig. 29 and Fig. 30 show the superconducting density with states $(L, N) = (1, 8)$, $(L, N_1, N_2) = (0, 2, 7)$ and $(L, N_1, N_2) = (0, 3, 6)$ respectively.

Fig. 31 shows the corresponding result for vortex states with total flux $10\phi_0$. The blue curve shows the free energy as a function of $h$ for state $(L, N) = (1, 9)$, the black triangle gives the state of $(L, N_1, N_2) = (0, 3, 7)$ and the red star gives the state $(L, N_1, N_2) = (0, 2, 8)$. At $t = 0$ (Fig. 31, left), the most stable vortex state is the state $(L, N_1, N_2) = (0, 2, 8)$, with states $(L, N_1, N_2) = (0, 3, 7)$ and $(L, N) = (1, 9)$ having almost the same (slightly higher) energy.
Figure 24: The free energy $g$ as a function of $h$ at $t = 0.14$ ($T = 1.8$ K). The stable vortex states and transitions are $(0, 0) \rightarrow (1, 0) \rightarrow (0, 2) \rightarrow (0, 3) \rightarrow (0, 4) \rightarrow (0, 5) \rightarrow (1, 5) \rightarrow (1, 6) \rightarrow (1, 7) \rightarrow (0, 2, 7) \rightarrow (0, 2, 8)$ as $h$ increases.
Figure 25: Magnetization $m$ as a function of $h$ at $t = 0.14$ ($T = 1.8$ K). The stable configurations are $(0, 0) \rightarrow (1, 0) \rightarrow (0, 2) \rightarrow (0, 3) \rightarrow (0, 4) \rightarrow (0, 5) \rightarrow (1, 5) \rightarrow (1, 6) \rightarrow (1, 7) \rightarrow (0, 2, 7) \rightarrow (0, 2, 8)$.
At $t = 0.14$ ($T = 1.8\, \text{K}$) (Fig. 31, right), the state $(L, N_1, N_2) = (0, 2, 8)$ is again the most stable state, with the other two states having higher energies. This result is in very good agreement with the experimental studies of Grigorieva et al. [32] who reported that the state $(L, N_1, N_2) = (0, 2, 8)$ was the most frequently observed state and that the state $(L, N) = (1, 9)$ was never observed in their experiments.

### 6.6.1 Thermal Fluctuation of Quantized Vortices

Experimentally, Grigorieva et al. [32] found that the state $(L, N_1, N_2) = (0, 2, 7)$ with total flux $9\phi_0$ occurs 7 times more frequently than the state $(L, N) = (1, 8)$. Similarly, the state $(L, N_1, N_2) = (0, 2, 8)$ was observed about 3 times more frequently than $(L, N_1, N_2) = (0, 3, 7)$.

The probability of the vortex state is $p_i \propto \exp(-G_i/k_BT)$, where $G_i$ is the Gibbs free
Figure 27: Free energy for configuration with total magnetic flux $9\phi_0$. Triangle, stars and curves represent the states $(L, N_1, N_2) = (0, 3, 6)$, $(L, N_1, N_2) = (0, 2, 7)$ and $(L, N) = (1, 8)$ respectively. The diagram on the left gives the result at $t = 0$ and the one on the right at $t = 0.14$. 
Figure 28: Illustration of the superconducting density - State \((L, N) = (1, 8)\), with one central vortex and eight off-centre vortices, with total flux = \(9\phi_0\).

Figure 29: Illustration of the superconducting density - State \((L, N_1, N_2) = (0, 2, 7)\) with two off-centre vortices on the first ring and seven off-centre vortices on second ring, with total flux = \(9\phi_0\).
Figure 30: Illustration of the superconducting density - State \((L, N_1, N_2) = (0, 3, 6)\) with three off-centre vortices on the first ring and six off-centre vortices second ring, with total flux \(= 9\phi_0\).

energy of state \(i\) and \(k_B\) is the Boltzmann constant. It can also be written as

\[
p_i \propto \exp\left(-\frac{g_i}{t}\right),
\]

where \(g_i\) is the dimensionless free energy. Our approximation shows that the occurrence of state \((L, N_1, N_2) = (0, 2, 7)\) is around 8 times more than \((L, N) = (1, 8)\). We also predict that state \((L, N_1, N_2) = (0, 3, 6)\) will appear up to 2-3 times more than \((L, N) = (1, 8)\). Similarly, the appearance of state \((L, N_1, N_2) = (0, 2, 8)\) is around 2 times more frequently than \((L, N_1, N_2) = (0, 3, 7)\). Both cases are consistent in the experiment.

### 6.6.2 Gibbs Free Energy Compared with London Approximation

The simulation results obtained from the GL model and the London model are in good agreement with experiments. Fig. 35 shows comparison of the free energies from two models, with the free energy from London model in red line and the from GL model in blue line. The GL free energy is lower than that using the London model. The two free
Figure 31: Free energy with total magnetic flux $10\phi_0$. The black triangles, red stars and the blue line represent the states $(L, N_1, N_2) = (0, 3, 7)$, $(L, N_1, N_2) = (0, 2, 8)$ and $(L, N) = (1, 9)$ respectively, with the left figure showing the results at $t = 0$ and the right one at $t = 0.14$. 
Figure 32: Illustration of the superconducting density - State \((L, N) = (1, 9)\) with one central vortex and nine off-centre vortices, with total flux = \(10\phi_0\).

Figure 33: Illustration of the superconducting density - State \((L, N_1, N_2) = (0, 2, 8)\) with two off-centre vortices on the first ring and eight off-centre vortices on the second, with total flux = \(10\phi_0\).
energies differ due to the extra term $-\frac{R^2}{2\xi^2} |\tilde{\Psi}|^2 + \frac{R^2}{4\xi^2} |\tilde{\Psi}|^4$ in GL model. As the magnetic field increases, the superconducting density is destroyed and hence the free energy bends downward. However, in the London model, the superconducting density is assumed to be constant ($|\tilde{\Psi}|^2 = 1$).

In summary, we have formulated the Gibbs free energy using Ginzburg-Landau equations. Our results are in agreement with those of the recent experiments of Grigorieva and co-workers [32] as in our London model. We find that free energy using GL theory provides lower energy as it takes into account the decrease in superconductivity associated with the nucleation of a vortex in the disc. However both theories predict the same stable states.
Figure 35: Comparison of the dimensionless Gibbs free energy formulated by London theory (red line) and Ginzburg-Landau theory (blue curve) at $t = 0.14$. 
6.7 Differential GL Equations on Discs

This is a supplementary section on the exact 1st differential GL equation to solve for vortex structures in the disc.

\[ (-i \tilde{\nabla} - \tilde{a})^2 \tilde{\Psi} - \tilde{\Psi}(1 - |\tilde{\Psi}|^2) = 0, \quad (6.18) \]

where the dimensionless parameters \( r = R/\xi, \tilde{\nabla} = \xi \nabla = \xi(\partial_x, \partial_y, \partial_z), \tilde{\Psi} = \Psi/|\Psi_0| \) and \( \tilde{a} = A(2\pi \xi/\phi_0) \), together with the boundary condition that the normal component of supercurrent should vanish at the edge

\[ (-i \tilde{\nabla} - \tilde{a}) \tilde{\Psi} \cdot \hat{n} = 0. \quad (6.19) \]

We assume (as in London model) that the applied magnetic fields inside and outside the disc are the same, \( h = b \), where \( h = H/H_{c2} \) and \( b = B/H_{c2} \) are the normalised applied and local magnetic fields. The 1st GL equation is enough to model the disc system if \( \kappa \) is large. For Nb (Type II superconductor), \( \kappa \approx 6 > 1/\sqrt{2} \), so that we can approximate the system by only using the 1st GL equation. In our simulation, we assume that the disc to be a 2-D system with \( R/r_c = 50 \).

The vortex states evolve from \((0,0), (1,0), (0,2), (0,3), (0,4), (0,5), (1,5), (1,6), (1,7), (0,2,7)\) to \((0,2,8)\) as \( h \) is increased. There are exactly the same vortex configurations as those obtained by the London model and GL approximation model in the previous chapters. The vortex states of the disc are shown in Fig. 36 and Fig. 37.
Figure 36: Superconducting density on the disc, red represents high density and blue represents low density. It shows the vortex states from $(0, 1)$ to $(1, 5)$. 
Figure 37: It shows the vortex states from (1, 6) to (0, 2, 8).
7 Vortex States in Superconducting Nanowires

7.1 Background of Superconducting Nanowires

We have studied the thermodynamically stable vortex structures in Lead nanowires. We write down the Gibbs free energy functional for the systems and we minimise the free energy to obtain the optimal position of vortices for different applied fields $H$ and temperatures $T$. We also study the nucleation of vortices in, and their escape from, the nanostructural superconductors.

The critical temperature of bulk Pb superconductor is $T_c = 7.2K$, with a coherent length $\xi_0 \sim 90 \text{nm}$ and penetration depth $\lambda_0 \sim 40 \text{nm}$ at $T = 0K$ (see, for example, references [54, 55]). However, in small samples, as discussed before, $\xi_0$ is smaller and $\lambda_0$ is larger than expected in bulk sample. Recently there has been a lot of interest in Pb superconducting nanowires. Zhang and Dai [50] experimentally studied the magnetisation of a Pb (bulk Pb is a Type I superconductor) nanowire of diameter 45 nm and length 6 $\mu$m in an external magnetic field applied transversely to the nanowire. They found that the response of the nanowire depends on the temperature: below $T = 5.0^\circ K$, the magnetisation is irreversible and shows Type II character ($H_{c1}$ and $H_{c2}$ have been observed). They also found that the mean free path $l$ of the Cooper pair is shorter than expected, and hence the measured coherent length $\xi_{\text{measured}}$ is shorter ($1/\xi_{\text{measured}} = 1/\xi_0 + 1/l$). Michotte [51] studied Pb nanowires with diameters varying from 40 nm to 270 nm in external fields applied parallel to the axis of the nanowires. The samples showed Type II superconductor properties during field cooling (decreasing magnetic field). Zhang and Dai [50] also observed that $H_c$ was further increased in the nanowires. Stenuit et al. [52] reported that the magnetisation $v/s$ applied field results for their Pb nanowires show hysteresis and they observed Type II “mixed states.” Ishii et al. [53] also reported that their Pb nanowires (with diameter 80 nm-100 nm) showed a wide phase transition around the critical field and hence deduced that Pb nanowires exhibited Type II structure. They also found that the coherent length $\xi_0$ is smaller than that expected in the clean limit,
and attributed this to the fact that mean free path $l$ is much smaller than in the bulk sample.

In our current study, we investigate theoretically the magnetisation of Pb nanowires as a function of both increasing and decreasing applied magnetic field. We also investigate the stable vortex structures in the systems.

### 7.2 Theory and Methodology

We study the magnetisation of nanowires both in a transverse applied magnetic field $(\mathbf{H} = H\mathbf{z})$ (see Fig. 38) and in a longitudinal applied field $(\mathbf{H} = H\mathbf{y})$ (Fig. 39). The wire has length $L$ and radius $R$ and lies with its axis along the y-axis.

The dimensionless Gibbs free energy (as shown in previous chapters) of the nanowire is given by

$$g_s - g_n = \int \left[ -|\tilde{\Psi}|^2 + \frac{1}{2} |\tilde{\Psi}|^4 + \frac{1}{2} \left( -i \nabla - \mathbf{a} \right) |\tilde{\Psi}|^2 + \kappa^2 (\mathbf{h} - \mathbf{b})^2 \right] dV, \quad (7.1)$$
Figure 39: Longitude magnetic field $\mathbf{H} = H\hat{y}$ applied to the nanowire.

where $\tilde{\Psi} = \Psi/|\Psi_\infty|$ is the normalised order parameter, $\mathbf{a} = \mathbf{A}/(\hbar/e\xi)$ is the dimensionless vector potential (with $\nabla \times \mathbf{A} = \mathbf{B}$, the local magnetic field), $\mathbf{b} = \mathbf{B}/H_{c2}$ is the dimensionless local magnetic field, $\mathbf{h} = \mathbf{H}/H_{c2}$ is the dimensionless applied magnetic field and $\tilde{\nabla} = \xi\nabla = \xi(\partial_x, \partial_y, \partial_z)$ is the dimensionless gradient operator. Length scales are in units of $\xi$: $r = R/\xi$ and $\ell = L/\xi$. The dimensionless temperature is $t = T/T_c$.

Minimising the free energy functional (Eq. (7.1)) gives the Ginzburg-Landau pair of coupled equations

$$(-i\tilde{\nabla} - \mathbf{a})^2\tilde{\Psi} - \tilde{\Psi}(1 - |\tilde{\Psi}|^2) = 0$$ (7.2)

$$\kappa^2\tilde{\nabla} \times \tilde{\nabla} \times \mathbf{a} = \text{Im}(\tilde{\Psi}^* \tilde{\nabla} \tilde{\Psi}) - a|\tilde{\Psi}|^2 = j_s$$ (7.3)

($j_s$ is the normalised superconducting current density), together with the boundary condition that on the surface $\partial\Omega$ of the nanowire, the normal component of supercurrent
should vanish

\[ (-i\tilde{\nabla} - a)\tilde{\Psi} \cdot \tilde{n} = 0, \quad (7.4) \]

and that (dimensionless) applied magnetic field should satisfy

\[ h = \tilde{\nabla} \times a_{\text{ext}}. \quad (7.5) \]

Given the applied magnetic field \( h \), the two parameters \((a, \tilde{\Psi})\) can be obtained by solving the two Ginzburg-Landau equations (Eqs. (7.2) and (7.3)) self-consistently.

The dimensionless (microscopic) magnetisation \( \langle m \rangle \) follows from

\[ \langle m \rangle = \frac{1}{V} \int \frac{1}{2} \mathbf{r} \times \mathbf{j}_s \, dV, \quad (7.6) \]

where \( \mathbf{r} = (x/\xi, y/\xi, z/\xi) \).

The thermodynamic relationship between the magnetisation \( m \), the applied field \( h \) and the local field \( b \) is \( h + 4\pi \langle m \rangle = b \). The magnetisation can also be expressed as

\[ \langle m \rangle = \frac{1}{4\pi} (\tilde{\nabla} \times a - h), \quad (7.7) \]

where \( m = M/H_{c2} \) and \( b = \tilde{\nabla} \times a \). Both of the expressions of magnetisation are equivalent in theory.

There are several approximations for \( \lambda(T) \) and \( \xi(T) \). The most typical ones from the Landau-Ginsburg model are

\[ \xi(T) \approx 0.74 \frac{\xi_0}{(1 - t)^{1/2}}, \quad (7.8) \]

where \( t = T/T_c \) is the reduced temperature (see Tinkham [1]) and

\[ \lambda(T) \approx \frac{\lambda_0}{(1 - t)^{1/2}}. \quad (7.9) \]

This gives \( \kappa \approx 0.74(\xi_0/\lambda_0) = 0.74\kappa_0 \), independent of temperature.
The two-fluid model $\lambda(t)$, can be approximated as

$$\lambda(T) \approx \frac{\lambda_0}{(1 - t^4)^{1/2}}, \quad (7.10)$$

and there is no specific corresponding model for $\xi(T)$. However, $H_{c2}$ can be roughly approximated $H_{c2}(t) \approx H_{c20}(1 - t^2) \approx \phi_0(1 - t^2)/(2\pi\xi_0^2) = \phi_0/(2\pi\xi(t)^2)$ and hence

$$\xi(T) \approx \frac{\xi_0}{(1 - t^2)^{1/2}}. \quad (7.11)$$
Table 6: $H_c, H_{c3}, \xi$ and $\kappa$ estimated from the experimental data by Simon Bending and his group [56]. The average values of $\lambda_0$ and $\xi_0$ are about 52 nm and 67 nm respectively.

<table>
<thead>
<tr>
<th>$T$(K)</th>
<th>$H_c$(Oe)</th>
<th>$H_{c3}$(Oe)</th>
<th>$\lambda$(nm)</th>
<th>$\xi$(nm)</th>
<th>$\kappa$</th>
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<tr>
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<td>95</td>
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<td>730</td>
<td>55</td>
<td>81</td>
<td>0.68</td>
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</table>

7.3 Simulation and Parameters of Nanowires (Transverse Magnetic Field)

In order to solve Eqs. (7.2) and (7.3), it is necessary to input the coherent length $\xi$ and penetration depth $\lambda$. The relationship of these two parameters can be estimated from experimental data in the following way. For a given temperature $t = t_0$, the thermodynamic relation between $H_c$, $\lambda$ and $\xi$ is

$$\xi(t_0) = \frac{\phi_0}{2\pi \sqrt{2\lambda(t_0)H_C(t_0)}}$$

where $\phi_0 = \frac{hc}{e^*}$ is the flux quantum. $\xi(t_0)$ can be estimated once $H_c(t_0)$ and $\lambda(t_0)$ are known. Eq. (7.10) and Eq. (7.11) (two-fluid model) give the temperature dependence of $\lambda(t)$ and $\xi(t)$. We calculate $H_c(t_0)$ from the experimental data.

In this part, we study numerically the lead nanowires in the transverse geometry. Fig. 40 gives the experimental results of Simon Bending and his group [56]. They used a $L = 20 \mu m$ long nanowire with diameter $R = 195 nm$, and measured the average magnetisation at the central $1 \mu m$ of the wire at four temperatures: $T = 6.6 K, 6.0 K, 5.2 K$ and $4.2 K$. Stenuit et al. [52] found that the average value of $\lambda_0$ in lead nanowire ($R = 120 nm, L = 4 \mu m$) is about 52 nm; together with Eq. (7.10) and Eq. (7.11) and the data by Bending et al. [56], one can estimate the average value of $\xi_0$ to be about 67 nm (see Table 6). $\kappa(T)$ increases as the temperature decreases (Table 6).
Figure 40: Experimental results of length $L = 20 \mu m$ and diameter $R = 195 nm$ on magnetisation of a lead nanowire by the group of Simon Bending [56] at $T = 6.6 K$, 6.0 K, 5.2 K and 4.2 K.
Table 7: The above table shows the input values of $\lambda$ and $\xi$ in our simulation. $H_c$ and $H_{c3}$ are results from the simulation. The average value of $\lambda_0$ and $\xi_0$ are about 60 nm and 68.5 nm respectively.

<table>
<thead>
<tr>
<th>$T$(K)</th>
<th>$H_c$(Oe)</th>
<th>$H_{c3}$(Oe)</th>
<th>$\lambda$(nm)</th>
<th>$\xi$(nm)</th>
<th>$\kappa$</th>
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<tbody>
<tr>
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<tr>
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<td>530</td>
<td>720</td>
<td>64</td>
<td>80</td>
<td>0.80</td>
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</tbody>
</table>

7.3.1 Numerical Results

Table 7 shows the simulation parameters in the GL model. In our simulation, the average value of $\lambda_0$ and $\xi_0$ are about 60 nm and 68.5 nm respectively, and $\kappa(T)$ is a function of temperature (Eq. (7.10) and Eq. (7.11)).

$$\kappa(t) = \frac{\lambda(t)}{\xi(t)} = \frac{\kappa_0}{\sqrt{1 + t^2}}$$

shows that $\kappa$ decreases with temperature; $\kappa_0 = \lambda_0/\xi_0$. $\lambda_0$ in our model is slightly larger than the one measured by Stenuit et al. [52] ($\lambda_0 = 52$ nm). One of the possible reasons is that Stenuit et al. [52] studied the nanowires under the longitudinal applied field while Simon Bending et al. [56] studied the wires under the transverse applied field.
Figure 42: The calculated magnetisation $M$ as a function of applied magnetic field $H$ at $T = 6.6\,\text{K}$ ($\kappa = 0.63$): the red dots and curve give the magnetisation for magnetic heating (increasing $H$) and the blue triangles and curve for magnetic cooling (decreasing $H$). The vertical dashed line represents the position of the critical magnetic field $H_c = 155$ Oe.
Fig. 42 gives our calculated magnetisation as a function of the applied magnetic field $H$ at $T = 6.6\, \text{K}$. The curve and dots in red are the result in an increasing applied magnetic field (from 0 Oe to 210 Oe) and the blue curve and triangles that for magnetic cooling ($H$ decreasing from 210 Oe to 0 Oe), where the critical magnetic field $H_c$ is 155 Oe at $T = 6.6\, \text{K}$. From the Table 7, $\kappa(6.6\, \text{K}) = 0.63$ and the magnetisation $M$ and the magnetic field $H$ follow from the non-dimensional (normalised) values through

$$M = H_{c2}m \quad \text{and} \quad H = H_{c2}h$$

respectively, where $H_{c2} \approx \phi_0/(2\pi\xi^2)$ is the second critical field in Type II. The maximum $|M|$ in the experiment is about 2.5 Oe (Fig. 40), compared with 2.8 Oe in the simulation (Fig. 42). The magnetisation is reversible, with the dependence of $M$ on $H$ exactly the same for magnetic cooling and magnetic heating: the wire makes a transition from Meissner state to normal state during heating and no flux penetrates the system during the transition. During magnetic cooling from above $H_c$, the nanowire makes a transition from normal state to Meissner state with no flux trapped, and the magnetisation has exactly the same dependence on $H$ as for magnetic heating. In the experiment, the average magnetisation was measured over the central 1 $\mu\text{m}$ of the 20 $\mu\text{m}$ nanowire by the Hall probe and our simulations follow the same scheme.

Fig. 43 shows our calculated magnetisation at $T = 6.0\, \text{K}$. The maximum $|M|$ in the simulation is about 7 Oe compared with 7.5 Oe in the experiment. The $H_c$ is about 280 Oe in the experiment (Fig. 40) and is about 250 Oe in the simulation (Fig. 43). There is clear evidence of hysteresis, with the behaviour during increasing magnetic field different from that during decreasing magnetic field. While the magnetisation shows clearly Type I behaviour in increasing field (smooth transition to the normal state), the transition from normal state to Meissner state in a decreasing field has two distinct jumps in magnetisation at 285 Oe and 270 Oe. A jump in magnetisation curve is a signature of either expulsion of flux from the system (magnetic cooling) or penetration of flux.
Figure 43: Calculated magnetisation $M$ as a function of applied magnetic field $H$ at $T = 6.0 \text{K}$ ($H_c = 250 \text{ Oe}$, $\kappa = 0.65$) under increasing magnetic field (red dots and curve) and decreasing magnetic field (blue triangles and curve), showing hysteretic behaviour. There are two jumps in $M$ during cooling (285 Oe and 270 Oe), a signature that flux is being expelled from the nanowire. The green vertical dashed lines show the jumps of vortex states.
Figure 44: $T = 6.0\, \text{K}$, the figure gives the superconducting density profile along the nanowire at values of $H$ on either sides of the jumps, with red representing high $|\tilde{\psi}|^2$ (pure superconducting) and deep blue representing low $|\tilde{\psi}|^2$ (normal metal). The four different stable vortex states are shown. The central 1 $\mu\text{m}$ of wire is embraced by red square shown in the diagram.
The jumps separate the different stable vortex states of the system. The density plots in Fig. 44 are plots of the (normalised) superconducting density profile \(|\tilde{\Psi}|^2 = |\Psi|^2/|\Psi_\infty|^2|\) along the nanowire, with deep red representing \(|\tilde{\Psi}|^2 = 1\) and deep blue \(|\tilde{\Psi}|^2 = 0\), at four different values of the applied field: \(H > 310\) Oe (top profile), \(285 < H < 310\) Oe (2nd profile), \(270 < H < 285\) Oe (3rd profile) and \(H < 270\) Oe (bottom profile).

The vortex state of the wire at about \(H = 310\) Oe contains about 2 fluxiods within the probe (1 \(\mu\)m length). As \(H\) is decreased, at about 285 Oe, there is a jump in the magnetisation of the nanowire. The system changes to another vortex state and some vortices are expelled from the whole nanowire. However, there are still two fluxoids within the 1 \(\mu\)m probe. The state with two vortices then evolves with decreasing \(H\) along the magnetisation curve shown in Fig. 43 and Fig. 44, and at 270 Oe the two fluxoids are expelled. For \(H < 270\) Oe, the system evolves to the superconducting state. The hysteresis in the magnetisation curve shows that for each values of \(H \in (270, 310)\) Oe, the nanowire has at least two metastable vortex states (our calculations have identified the two shown) and different states are accessed during heating and during cooling.

At \(T = 5.2\) K (\(\kappa = 0.69\)), the response of the nanowire in both an increasing magnetic field (Fig.45 and Fig.46) and in a decreasing field (Fig.47, Fig.48 and Fig.49) shows typical Type II behaviour. The \(H_c\) is about 400 Oe in the experiment (Fig. 40) and about 380 Oe in the simulation. The maximum \(|M|\) is about 12.2 Oe in our result which is close to the experimental value.

As \(H\) is increased (red curve and dots), we identify one vortex state as the system evolves from the Meissner state to the normal state. The first jump in magnetisation is at \(H \approx 400\) Oe and corresponds to the nucleation of two fluxoids in the wire (see the density profile plot in Fig.46). For \(H > 400\) Oe, this state evolves along the red curve until \(H\) reaches \(H \approx 450\) Oe. As \(H\) is increased further, the wire makes a gradual transition to the normal state.

As \(H\) is decreased from the normal state, four vortices are found within the probe at...
Figure 45: $T = 5.2\,\text{K}$: magnetisation as a function of applied magnetic field ($H_c = 380\,\text{Oe}$, $\kappa = 0.69$). There are two jumps in $M$ during magnetic heating (red dots and curve). The vertical dashed lines show the jumps of vortex states.
Figure 46: $T = 5.2\, \text{K}$: as for Fig.45. The density profile plots: deep red is pure superconducting and deep blue normal metal. The $1^{\text{st}}$ jump is at $400\, \text{Oe}$ and the $2^{\text{nd}}$ one is at $450\, \text{Oe}$. 
Figure 47: $T = 5.2 \, \text{K}$ ($H_c = 380 \, \text{Oe}, \kappa = 0.69$): During magnetic cooling (blue triangles and curve), the magnetisation $M$ has four jumps (with the states of the nanowire on either sides of the jumps shown in Fig. 48 and Fig. 49). The vertical dashed lines show the jumps of vortex states.
Figure 48: $T = 5.2\, \text{K}$: Density profile: deep red is pure superconducting and deep blue normal metal ($355\, \text{Oe} < H < 485\, \text{Oe}$).
Figure 49: $T = 5.2\text{K}$: Density profile plots on the graph: deep red is pure superconducting and deep blue normal metal ($H < 355\text{ Oe}$).
Figure 50: Magnetisation $M$ as a function of $H$ at $T = 4.2 \, \text{K}$ ($H_c = 520 \, \text{Oe}$, $\kappa = 0.80$). There are two jumps in $M$ during magnetic heating (red dots and curve). The vertical dashed lines show the jumps of vortex states.

$H \approx 455 \, \text{Oe}$. There are four jumps in the magnetisation curve (blue curve and triangles in Fig. 47). These correspond to the expulsion of fluxoids at successive threshold magnetic fields: about half fluxoid at $H \approx 385 \, \text{Oe}$, half fluxoid at $H \approx 355 \, \text{Oe}$ and one fluxoid at $H \approx 335 \, \text{Oe}$ respectively, and the remaining two fluxoids at $H \approx 320 \, \text{Oe}$ (density profile in Fig. 48 and Fig. 49). The vortex jump is found in to be fractional because the magnetisation $M$ is measured within only the middle 1 $\mu$m of the whole nanowire: a number of fluxoid is expelled from the whole wire and the fractional vortex jump is the result of measuring over only a small section of the wire (see Fig. 48 and Fig. 49). After the last jump, the system evolves to the Meissner state.

Similarly at $T = 4.2 \, \text{K}$ ($\kappa = 0.80$), the magnetisation shows Type II response in both increasing (Fig.50 and Fig.51) and decreasing (Fig.52, Fig.53 and Fig.54) magnetic fields. The maximum $|M|$ is about 17.5 Oe which agrees with the experiment. $H_c$ is about 540 Oe.
Figure 51: At $T = 4.2$ K: Density profiles with two jumps at 530 Oe and 580 Oe during magnetic heating ($530 \text{ Oe} < H < 640 \text{ Oe}$).
Figure 52: $T = 4.2\, \text{K}$ ($H_c = 520\, \text{Oe}, \kappa = 0.80$): During magnetic cooling (blue triangles and curve), the magnetisation $M$ has five jumps. The vertical dashed lines show the jumps of vortex states.
Figure 53: $T = 4.2\,\text{K}$: Density profiles of the nanowire with three jumps at 640 Oe, 530 Oe and 470 Oe during magnetic cooling ($420\,\text{Oe} < H < 720\,\text{Oe}$).
Figure 54: $T = 4.2\, \text{K}$: Density profiles of the two jumps at 420 Oe and 385 Oe during magnetic cooling ($340\, \text{Oe} < H < 420\, \text{Oe}$).
in the experiment and is about 520 Oe in the simulation. Each jump in the simulation is a signature of flux either nucleating in the nanowire (increasing field) or expelled from it (decreasing field). The different vortex states on either sides of the jumps during heating and cooling are shown in the density profiles in Fig. 50 and Fig. 52 respectively.

When the applied field is increased, there are two jumps at \( H \approx 530 \text{ Oe} \) and \( H \approx 580 \text{ Oe} \), and the system goes to normal state at \( H \approx 640 \text{ Oe} \). There are three vortices (at \( H \approx 530 \text{ Oe} \)) and four vortices (at \( H \approx 580 \text{ Oe} \)) found within the probe respectively. As \( H \) is decreased from normal state, the stable vortex state at \( H \approx 640 \text{ Oe} \) is one with six fluxoids within the probe. There are five successive jumps in which flux is expelled in the nanowire: one fluxoid expulsion at \( H \approx 530 \text{ Oe} \), \( H \approx 470 \text{ Oe} \), \( H \approx 420 \text{ Oe} \), two at \( H \approx 385 \text{ Oe} \) and one at \( H \approx 340 \text{ Oe} \). In range of \( 385 < H < 340 \text{ Oe} \), the vortex state in the system is meta-stable. We studied this particular vortex state by varying the applied field \( H \) slightly and found that there are more than few stable configurations.
7.3.2 Concluding Remarks

We have presented the results of our calculations of the response of a 20 µm long Pb nanowire of radius 195 nm in a transverse applied magnetic field at four temperatures $T = 6.6\,\text{K}, T = 6.0\,\text{K}, T = 5.2\,\text{K}$ and $T = 4.2\,\text{K}$. Although Pb is a Type I superconductor (with superconducting transition temperature $T_c = 7.2\,\text{K}$), it is only the highest temperature investigated ($T = 6.6\,\text{K}$) that the magnetisation v/s applied magnetic curve shows characteristic Type I behaviour, with the response being completely reversible (i.e., symmetric under heating and cooling).

At the lower temperatures, the responses show Type II behaviour - fluxoids nucleate or are trapped in the wire (typical of the Abrikosov mixed state) and there are jumps in the magnetisation curves. These are signatures of quantised flux nucleating into (as $H$ is increased) or being expelled from (as $H$ is decreased) the nanowire. We have presented density profiles for the vortex states at values of $H$ on either side of the jumps. The magnetisation curves are not reversible - they all show hysteresis; this implies that at each values of $H > H_{c1}$ there are several (at least two) metastable vortex states and different states are accessed during magnetic heating and magnetic cooling. Further, at these three lower temperatures, there is evidence of surface superconductivity in a small layer near the “ends” of the wire, i.e., near the surfaces parallel to the applied magnetic field: superconductivity persists well beyond $H_c$ at which there is no superconductivity in the bulk of the wire. This is illustrated in Fig. 55, which gives the superconducting density profile at $T = 4.2\,\text{K}$ for an applied field $H_{c3} = 720\,\text{Oe}$.
Figure 56: Magnetisation measurements from the experiment by Stenuit et al. [52] at $T = 6.85\,\text{K}$, $5.5\,\text{K}$, and $2\,\text{K}$ for heating (black arrow) and cooling (red arrow).

### 7.4 Simulation of Nanowires (Longitudinal Magnetic Field)

The magnetic field is applied parallel to the axis of the nanowire. Stenuit et al. [52] studied Lead nanowires in this geometry. They used nanowires of length $4\,\mu\text{m}$, radius $120\,\text{nm}$, and measured the magnetisation at temperatures $T = 6.85\,\text{K}$, $5.5\,\text{K}$ and $2\,\text{K}$. The experimental results from Stenuit et al. [52] are shown in Fig. 56. Black and red arrows represent heating and cooling respectively. At $6.85\,\text{K}$ and $5.5\,\text{K}$, the figure shows that the magnetisation is reversible, but there is hysteresis at $2\,\text{K}$. The wire exhibits Type II behaviour at the lower temperature. Stenuit et al. [52] found that the average characteristic lengths are $(\lambda, \xi) = (125, 225)$ at $6.85\,\text{K}$ ($\kappa = 0.56$), $(\lambda, \xi) = (64, 115)$ at $5.5\,\text{K}$ ($\kappa = 0.56$) and $(\lambda, \xi) = (50, 70)$ at $2\,\text{K}$ ($\kappa = 0.71$).

Stenuit et al. [52] also studied the systems numerically. They assumed the wires to be infinitely long so that they could ignore the edge effects. They used the 2-D GL equations and also chose the radii $R = 150\,\text{nm}$ (at $5.5\,\text{K}$) and $R = 120\,\text{nm}$ (at $6.85\,\text{K}$ and $2\,\text{K}$). Their numerical results are shown in Fig. 57. From the results, they found that the magnetisation curves at $6.85\,\text{K}$ are reversible during magnetic cooling and heating.
Figure 57: Simulation results by Stenuit et al. [52] at $T = 6.85\text{ K}$, $5.5\text{ K}$, and $2\text{ K}$. The black curve follows the path of increasing field and the red one represents the decreasing field.

At $5.5\text{ K}$, one can find that there is a slight hysteresis, and at $2\text{ K}$ the magnetisation curves are irreversible.
Figure 58: Illustration of 3-D simulation model: 3-D density plot - red colour in the wire represents high superconducting density and blue represents low density; streamlines represent applied magnetic field along the axis of the cylindrical wire. The total fields around the edges are not straight since the edge effect is taken into account.

In our simulation, we use the 3-D Ginzburg-Landau model (Fig. 58), and take into account the edge effect in the small system. Fig. 59 shows the magnetisation v/s magnetic field at $T = 6.85\, \text{K}$. $H_c \approx 210\, \text{Oe}$, $\kappa = 0.56$ and the magnetisation is reversible. No vortex is found in the system during magnetic cooling and heating. The curve shows a second order phase transition in agreement with the experimental results [52].

Fig. 60 shows our calculated magnetisation v/s magnetic field $H$ at $T = 5.5\, \text{K}$, with $H_c \approx 530\, \text{Oe}$ and $\kappa = 0.56$. The magnetisation shows some hysteresis at about 610 Oe and the result is similar to the simulation obtained by Stennit et al. [52]. As at $T = 6.85\, \text{K}$, no vortex is found in the system.

Fig. 61 gives our calculated magnetisation curve at $T = 2\, \text{K}$. When $h$ increases, the magnetisation shows hysteresis ($\kappa = 0.71$). Upon heating, the system stays in the superconducting state until the magnetic field reaches 1250 Oe (Fig. 61) at which one
Figure 59: The calculated magnetisation at \( T = 6.85 \text{K} \) (red circle curve - heating, blue triangle curve - cooling) as a function of \( H \) (in Oe). The vertical dashed lines show the critical magnetic field (\( H_c = 205 \text{ Oe} \)).

Figure 60: As in Fig 59 but at \( T = 5.5 \text{K} \). The vertical dashed lines show the critical magnetic field (\( H_c = 520 \text{ Oe} \)).
Figure 61: The calculated magnetisation as a function of $H$ (in Oe) at 2K. Flux penetrates into the wire at 1250 Oe (pink vertical line) during heating and the system becomes normal at 1400 Oe. During cooling, flux is expelled when $H$ reaches 720 Oe (pale blue vertical line) and as $H$ is further decreased, the system evolves to the Meissner state.

Fluxion nucleates at the centre of the nanowire. The superconducting state is destroyed and the nanowire becomes normal metal above 1400 Oe. When the field is decreased from 1400 Oe, one fluxion is trapped into the system. The flux is expelled at 720 Oe and then evolves to the Meissner state (Fig. 61). Fig. 62 gives the density plot on heating (red - high density, blue - low density); the diagram on the left shows that the system stays in Meissner state ($0 < H < 1250$ Oe) and diagram on the right shows a fluxoid trapped into the system ($1250$ Oe $< H < 1400$ Oe). Fig. 63 gives the density plot during cooling, the diagram on the left shows a fluxoid trapped into the system for $720$ Oe $< H < 1400$ Oe and diagram at the right shows that the fluxoid is expelled as $H$ is further decreased.
Figure 62: Density plot during magnetic heating across the cross section of the wire. Red colour represents high superconducting density and blue represents low density (colour bar is shown here). The system stays in the Meissner state until $H$ reaches 1250 Oe (right diagram) at which one fluxoid (blue colour hole) enters the system (left diagram).
$T = 2K$  Superconducting Density

**One vortex inside**  **No vortex**

| 720$<H<1400$ Oe | H$<720$ Oe |

Figure 63: Plot of superconducting density for decreasing magnetic field. Flux is expelled at 720 Oe (left diagram).
8 References

8.1 Bibliography

References


