NUCLEATION AND DYNAMICS OF VORTICES IN TYPE-II SUPERCONDUCTORS

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TABLE OF CONTENTS

	Page
DEDICATION	iii
ACKNOWLEDGEMENTS	iv
ABSTRACT	v
CHAPTER 1. INTRODUCTION TO GINZBURG-LANDAU THEORY	1
CHAPTER 2. INTRODUCTION TO OUR APPROACH	16
CHAPTER 3. OUR WORK AT $\kappa=2.0$	27
CHAPTER 4. OUR WORK AT $\kappa=5.0$	76
CHAPTER 5. MODELING VORTEX NUCLEATION	92
CHAPTER 6. MODELING VORTEX DYNAMICS	103
CHAPTER 7. SUMMARY	117
BIBLIOGRAPHY	119

DEDICATION

This work is humbly dedicated to Sgt. James (Jimmy) Vincent Ballay. Born 5 January, 1949. Died 12 May, 1970. Fatally wounded by enemy gunfire while serving with the 101st Airborne Division (The Screaming Eagles) in Cambodia. Awarded the Bronze Star, the Combat Infantryman Badge, the Purple Heart, the Air Medal, the Army Commendation Medal, the Republic of Vietnam Campaign Ribbon, the Vietnam Service Medal, the National Defense Service Medal, the Good Conduct Medal, the Sharpshooter Badge with Automatic Rifle Bar and the Marksman Badge with Machine Gun and Rifle Bars.

In his Gettysburg Address Abraham Lincoln spoke words which are applicable here. "The world will little note nor long remember what we say here but it can never forget what they did here."

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Nucleation and dynamics of vortices
in type-II superconductors

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Under the supervision of John R. Clem
From the Department of Physics
Iowa State University

The one- and two-dimensional Ginzburg-Landau equations are numerically integrated in a slab geometry, which is appropriate for comparison to experimental work done on films. When two-dimensional variations become energetically favorable, a vortex is found to nucleate and move to the center of the film with the Gibbs free energy decreasing during the process. An important process by which the energy is lowered during this nucleation procedure is found to be the savings in condensation energy arising from the shrinking size of the vortex core as it moves to the center of the film.

The solutions of the Ginzburg-Landau equations are used to explain anomalies observed experimentally in the tunneling characteristics of thin films of PbIn. Excellent agreement between theory and experiment is found with the Ginzburg-Landau equations correctly predicting the field at which flux would first enter the films.

We then use the Clem model of an isolated vortex to model vortex nucleation and dynamics under the influence of a transport current. The entry fields predicted by the model are found to be off by almost a factor of two but have the advantage of requiring simple computer programs for their solution, while the Ginzburg-Landau solutions require substantially more numerical work.

CHAPTER 1. INTRODUCTION TO GINZBURG-LANDAU THEORY

A fundamental characteristic of superconductivity is the exclusion of magnetic flux from the bulk of a superconductor placed in an applied magnetic field. Although discovered jointly by Meissner and Ochsenfeld,¹ the exclusion of flux is usually called the Meissner Effect. When a magnetic field is applied to a superconductor, supercurrents arise spontaneously and flow in such a way as to screen the interior of the superconductor from the applied field. The behavior of the superconductor as the field is increased determines whether it is of the type known as type-I or type-II.

In a type-I superconductor the flux is excluded from the interior of the superconductor until some critical field H_c is reached, at which point bulk superconductivity is destroyed and flux enters the sample. H_c is known as the bulk thermodynamic critical field and is a function of temperature. Empirically it is found that its temperature dependence may be described approximately by $H_c(T) = H_c(0)[1 - (T/T_c)^2]$ where T_c is the transition temperature of the superconductor and $H_c(0)$ is the critical field at 0 K. If the applied field is denoted by H and the average flux density in the interior of a thick superconductor by B , the Meissner effect in a long superconducting cylinder with $\vec{H}$ parallel to the cylinder axis results in a B vs. H relation shown in Figure 1.

In a type-II superconductor the flux is completely excluded until the lower critical field H_{c1} is reached, at which point quantized bundles of flux known as vortices are admitted to the interior of the super-

Figure 1. B vs. H relation for a type-I superconductor.

conductor. The flux is concentrated around the core of these vortices with the superconductor being in a nearly normal state near the core. Increasing the field above H_{c1} pushes the vortices closer together until at H_{c2} the cores overlap and the superconductor goes into the normal state. The temperature dependence of both H_{c1} and H_{c2} may be described by relations similar to that describing H_c for the type-I superconductor. A B vs. H relation for a type-II superconductor is shown in Figure 2. This is the ideal B vs. H relation and is valid when the superconductor is a long cylinder with the field applied parallel to the axis. In other geometries demagnetization effects lead to a slightly different behavior. In this figure two additional fields, H_{sh} (the superheating field) and H_{sc} (the supercooling field) are included. The meaning of these fields will be discussed shortly.

The different behavior in the presence of an applied field results in differing magnetization curves. Figure 3 compares the magnetization curve for type-I and type-II superconductors. Superconductivity is destroyed in a type-I superconductor at H_c , which implies that an energy per unit volume of $H_c^2/8\pi$ is required to destroy superconductivity. This is the energy per unit volume given up when electrons go into the superconducting state, and it is seen to be the area under the magnetization curve divided by 4π . It is possible to define an H_c for a type-II superconductor by setting the area under its magnetization curve divided by 4π equal to $H_c^2/8\pi$. Although nothing physical happens in a type-II material at this field, one often works in reduced units when doing calculations and expresses magnetic fields in units of H_c or $\sqrt{2} H_c$.

Figure 2. B vs. H relation for a type-II superconductor.

Figure 3. Magnetization curves for type-I and type-II superconductors.

Before moving on to the Ginzburg-Landau theory, let us discuss the meaning of the superheating and supercooling fields which were pointed out in Figure 2. Suppose the superconductor were in the form of a slab and the field were applied parallel to the slab face. If the superconductor were type-II, it would be energetically favorable for the slab to go into the vortex state when the field reached H_{c1} . However, if the surfaces of the slab are very smooth, it sometimes occurs that flux does not enter until some higher field, the superheating field, is reached. The presence of a smooth surface can delay the entry of vortices to a field value higher than that at which it is first energetically favorable for the slab to go into the vortex state. If, once vortices are in the slab, the field is reduced, it is found that the smooth surface can trap vortices in the bulk of the slab to some field value which is less than H_{c1} , and which is known as the supercooling field. The condition of the sample surface is important in the interpretation of experimental results. Just how much effect a smooth surface can have will become apparent when we compare our theoretical results with experiment in Chapter 4.

In the Ginzburg-Landau theory of superconductivity²⁻⁶ one writes the Helmholtz free energy of the superconductor as the sum of three contributions. Electrons lower their energy by going from the normal state into the superconducting state and the energy given up is referred to as condensation energy. This condensation energy is written in terms of an order parameter $\psi = f e^{i\gamma}$ whose magnitude squared is related to the fraction of electrons in the superconducting state.

It can be shown that the condensation energy contribution to the free energy can be written as $\int d^3r \frac{H_c^2}{8\pi} (1 - f^2)^2$. When the order parameter has been suppressed to zero, this results in an energy per unit volume of $H_c^2/8\pi$, as expected from the earlier discussion.

The next contribution to the free energy is the kinetic energy associated with the screening supercurrents. It is evaluated quantum mechanically by calculating the expectation value of $\frac{1}{2}m^*v^2$. In a magnetic field the velocity operator is $\frac{1}{m^*}(\frac{\hbar}{i}\vec{\nabla} + \frac{e^*}{c}\vec{a})$ so that we must evaluate $\int d^3r \psi^* \frac{1}{2m^*} (\frac{\hbar}{i}\vec{\nabla} + \frac{e^*}{c}\vec{a})^2 \psi$. $m^* = 2m$ is the effective mass, $e^* = 2e$ the magnitude of the effective charge, c the speed of light, and $\vec{a}$ the vector potential, where m and $-e$ are the electronic mass and charge. An integration by parts is done and the resulting surface integral is set equal to zero, resulting in the boundary conditions of the problem, $\hat{n} \cdot (\frac{\hbar}{i}\vec{\nabla} + \frac{e^*}{c}\vec{a})\psi|_{\text{boundary}} = 0$, where $\hat{n}$ is the outwardly directed unit vector normal to the surface. At this point we depart slightly from the usual Ginzburg-Landau theory and introduce a quantity we call the gauge-invariant vector potential, $\vec{a}_s = \vec{a} + \frac{\phi_0}{2\pi}\vec{\nabla}\gamma$. $\phi_0 = \frac{hc}{2e} = 2.07 \times 10^{-7}$ G-cm² and is the quantum of flux in a vortex. Although both $\vec{a}$ and γ are gauge-dependent quantities, the combination $\vec{a}_s$ is gauge-invariant. Furthermore it is proportional to the superfluid velocity $\vec{a}_s = \frac{mc}{e}\vec{v}_s$.

Since the flux density is related to the vector potential by $\vec{b} = \vec{\nabla} \times \vec{a}$ and the curl of a gradient is zero, one would at first expect that $\vec{b} = \vec{\nabla} \times \vec{a}_s$. That this relation does not hold on the vortex axis becomes obvious when one considers the line integral

$$\oint_C d\vec{\ell} \cdot \vec{a}_s = \int d\vec{s} \cdot \vec{\nabla} \times \vec{a}_s \quad (1)$$

Suppose the path C contains a singly quantized vortex and recall that the gauge-invariant vector potential is proportional to the superfluid velocity. Far from the vortex axis the superfluid velocity will go exponentially to zero, so that, if the path C were to lie at a large radius from the core of the vortex, the value of the line integral would be zero. However, the flux through such a path should approach the quantum ϕ_0 as the radius of the path increases, indicating that something is not quite right. What has been overlooked is the fact that $\oint_C d\vec{\ell} \cdot \vec{\nabla} \gamma = \pm 2\pi$ when the path C contains a vortex. The $\pm$ sign depends upon the direction of the line integration and the direction of the magnetic field produced by the vortex. To account for this one must write $\vec{b} = \vec{\nabla} \times \vec{a}_s + \vec{\phi}_0 \delta(\vec{r} - \vec{r}_0)$ when the vortex is at $\vec{r}_0$. $\vec{\phi}_0$ is a vector of magnitude ϕ_0 parallel to the axis of the vortex and pointing in the direction of the magnetic field produced by the vortex.

The above relation between $\vec{b}$ and $\vec{a}_s$ is easily verified by calculating the flux through the path C containing a singly quantized vortex. We orient the path C in the right hand sense when referred to the direction of the magnetic field of the vortex and find the flux to be given by

$$\begin{aligned} \int d\vec{s} \cdot \vec{b} &= \oint_C d\vec{\ell} \cdot \vec{a}_s + \phi_0 \\ &= \oint_C d\vec{\ell} \cdot \vec{a} \quad (2) \end{aligned}$$

With this definition of $\vec{a}_s$ the boundary condition may be written as $\hat{n} \cdot \vec{\nabla} f|_{\text{surface}} = 0$ and $\hat{n} \cdot \vec{a}_s|_{\text{surface}} = 0$. The first boundary condition has no simple physical interpretation, but the second requires that no current flow through the surface of the sample.

In terms of the gauge-invariant vector potential the kinetic energy contribution to the free energy is given by

$$\int d^3r \left\{ \frac{H_c^2}{8\pi} \xi^2 (\vec{\nabla} f)^2 + f^2 a_s^2 / 8\pi \lambda^2 \right\}.$$

ξ and λ are lengths characteristic of the superconductor. f usually varies on a scale of ξ , while the flux density in the superconductor usually varies on a scale of λ . The ratio $\kappa = \lambda/\xi$ determines whether a superconductor will be of type-I or type-II. If κ is less than $1/\sqrt{2}$ the superconductor will be type-I while if the ratio is greater than $1/\sqrt{2}$ the superconductor will be type-II. Only two elements, Nb and V, are naturally type-II.

The final contribution to the free energy is the magnetic field energy, whose density is given by $b^2/8\pi$. Thus in the Ginzburg-Landau theory of superconductivity the Helmholtz free energy $\mathcal{F}$ is written as

$$\mathcal{F} = \int d^3r \left\{ \frac{H_c^2}{8\pi} (1-f^2)^2 + \frac{H_c^2}{4\pi} \xi^2 (\vec{\nabla} f)^2 + \frac{f^2 a_s^2}{8\pi \lambda^2} + \frac{b^2}{8\pi} \right\}. \quad (3)$$

The final two terms taken together are said to compose the electromagnetic contribution to the free energy. When vortices are widely separated, the main interaction is thought to be through this electromagnetic contribution.

When the applied field is held constant, the fundamental quantity that one should consider is the Gibbs free energy Q rather than the Helmholtz free energy $\mathcal{F}$. The superconductor will go into the state that minimizes the Gibbs free energy. Furthermore, if the field is held constant and the superconductor irreversibly changes from one configuration to another, the change in the Gibbs free energy is the amount of energy that will be dissipated as a result of the change. The Gibbs free energy is defined in Equation 4 and is seen to be closely related to the Helmholtz free energy.

$$Q = \mathcal{F} - \frac{1}{4\pi} \int d^3r \vec{H} \cdot \vec{b} \quad (4)$$

$\vec{H}$ is the applied field, which has no spatial dependence, while $\vec{b}$ is the local flux density, just as in the definition of the Helmholtz free energy.

To derive the Ginzburg-Landau equations one follows a procedure similar to the derivation of the Lagrange equations in classical mechanics. We take variations of the Gibbs free energy with respect to f and $\vec{a}_s$ and set the variations equal to zero. Since we have written the Gibbs free energy in terms of the gauge-invariant vector potential,

our Ginzburg-Landau equations will look a bit different from what one usually sees,⁴⁻⁶ but a simple substitution reveals that the two forms are equivalent. In our formalism the Ginzburg-Landau equations are given by

$$\xi^2 \nabla^2 f = -(1-f^2)f + a_s^2 f / (2H_c^2 \lambda^2) \quad (5)$$

$$\vec{\nabla} \times \vec{\nabla} \times \vec{a}_s = -f^2 \vec{a}_s / \lambda^2 \quad (6)$$

When doing calculations it is common to work in what is known as the system of Ginzburg-Landau reduced units. In this system lengths are measured in units of λ , magnetic fields in units of $\sqrt{2} H_c(T) = \frac{\phi_0}{2\pi\xi\lambda} = \frac{\kappa\phi_0}{2\pi\lambda^2}$, current densities in units of $\frac{c}{4\pi} \frac{\sqrt{2} H_c}{\lambda} = \frac{c\phi_0}{8\pi^2\xi\lambda^2} = \frac{\kappa\phi_0 c}{8\pi^2\lambda^3}$ and energy densities in units of $H_c^2/4\pi = \frac{\phi_0^2}{32\pi^3\xi^2\lambda^2} = \frac{\kappa^2\phi_0^2}{32\pi^3\lambda^4}$.

Letting a prime denote reduced quantities, we find that the Ginzburg-Landau equations are now given by

$$\frac{1}{\kappa^2} \nabla'^2 f = f(f^2 - 1) + a_s'^2 f \quad (7)$$

$$\vec{\nabla}' \times \vec{\nabla}' \times \vec{a}_s' = -f^2 \vec{a}_s' \quad (8)$$

Unless noted otherwise, all remaining work in the first four chapters will be done in these reduced units, and the primes will be deleted.

The geometry we would like to study is shown in Figure 4. The slab is considered to be infinite in the y and z directions. The slab width is denoted by W and the solutions will be assumed to be periodic in the y direction with a periodicity P . With these definitions the Helmholtz free energy per unit surface area is given by Equation 9 and the Gibbs free energy per unit surface area by Equation 10.

$$F = \frac{1}{P} \int_0^P dy \int_0^{W/2} dx \left\{ \frac{1}{2}(1-f^2)^2 + (\vec{\nabla}f/\kappa)^2 + a_s^2 f^2 + b^2 \right\} \quad (9)$$

$$G = F - \frac{2}{P} \int_0^P dy \int_0^{W/2} dx \vec{H} \cdot \vec{b} \quad (10)$$

In these units the gauge-invariant vector potential is equal to the superfluid velocity, and it is common in the literature to refer to only the superfluid velocity and denote it by the symbol $\vec{Q}$. That convention will be followed in the rest of this work. Allowing spatial variations only in directions perpendicular to the applied field the Ginzburg-Landau equations reduce to Equations 11, 12, and 13.

$$\frac{1}{\kappa^2} \left(\frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} \right) = f(f^2 + Q_x^2 + Q_y^2 - 1) \quad (11)$$

$$\frac{\partial^2 Q_y}{\partial x \partial y} - \frac{\partial^2 Q_x}{\partial y^2} = -f^2 Q_x \quad (12)$$

$$\frac{\partial^2 Q_x}{\partial y \partial x} - \frac{\partial^2 Q_y}{\partial x^2} = -f^2 Q_y \quad (13)$$

Figure 4. The geometry under study.

These equations have been numerically integrated by L. Kramer⁷ for a very thick slab with the boundary conditions shown in Figure 5. Since all the information is contained in the shaded region, it is necessary to integrate the equations only over this region. One wishes to keep the region over which the solutions are obtained as small as possible in order to conserve computer time. By letting W become very large, one finds the behavior of the solutions for a semi-infinite slab, or, in other words, the expected bulk behavior. Kramer's boundary conditions are seen to imply symmetric behavior about the middle of the slab, so that if a vortex nucleates at $(0,0)$, another vortex nucleates at $(W,0)$. As these vortices move into the bulk of the slab, vortex-vortex repulsion holds them apart and they do not go clear to the middle, as was noted by Kramer in Ref. 7. Since Kramer was interested in very thick slabs, it did not matter to him what was happening on the other side of the slab.

Figure 5. Kramer's boundary conditions.

CHAPTER 2. INTRODUCTION TO OUR APPROACH

We would like to calculate superheating fields and supercooling fields and to study the details of nucleation, all for a finite slab. To study supercooling fields in particular we must allow the vortices to penetrate to the center of the slab in the lowest energy configuration. A sensible way for vortices to nucleate is in what we have called a staggered configuration, where vortices nucleate on one side of the slab at y values of $0, \pm P, \pm 2P, \pm 3P, \dots$ and simultaneously on the other side of the slab at y values of $\pm P/2, \pm 3P/2, \pm 5P/2, \dots$. The appropriate boundary conditions are now shown in Figure 6. All boundary conditions have remained the same except along the middle of the slab. The boundary conditions there follow from the symmetry requirement $f(x,y) = f(W-x, P/2-y)$, $Q_x(x,y) = -Q_x(W-x, P/2-y)$, $Q_y(x,y) = -Q_y(W-x, P/2-y)$. We have integrated the Ginzburg-Landau equations for both sets of boundary conditions. Since it is found that the latter set has a substantially lower G , all further discussion will assume these boundary conditions. Again all information about the solutions is contained in the shaded region, and the solution for the entire slab can be constructed from the solutions in this region by the use of symmetry.

To solve the equations numerically,⁸ we replace the differential equations with difference equations and solve these difference equations above a grid of finite size. The smaller the grid spacing, the more accurate the solution, but the more computer time required to obtain the solution. For a kappa of two we choose a grid spacing of 0.2, which

Figure 6. Our boundary conditions.

is less than half a coherence length in these reduced units. An error analysis has been done for this grid size, and it gives an accuracy of about 0.01 in the values of f and Q . When the vortex is about a coherence length from the edge of the slab, this grid size is not small enough to handle the rapid spatial variations of the solutions. This particular case will be discussed in more detail later.

The difference relations used in the solution of the equations are given by Equations 14 and 15 in which h denotes the grid size.

$$\frac{\partial^2 f}{\partial x^2} = \frac{f(x+h,y) - 2f(x,y) + f(x-h,y)}{h^2} \quad (14)$$

$$\begin{aligned} \frac{\partial^2 f}{\partial x \partial y} = & \frac{f(x+h,y+h) - f(x-h,y+h) - f(x+h,y-h) + \dots}{(2h)^2} \quad (15) \\ & \dots + f(x-h,y-h) \end{aligned}$$

Then the Ginzburg-Landau equations are replaced by the following difference equations.

$$\frac{1}{h^2} \left[f(x+h,y) + f(x-h,y) + f(x,y+h) + f(x,y-h) - 4f(x,y) \right] = f(x,y) [f^2(x,y) + Q_x^2(x,y) + Q_y^2(x,y) - 1] \quad (16)$$

$$- 4f(x,y)] = f(x,y) [f^2(x,y) + Q_x^2(x,y) + Q_y^2(x,y) - 1]$$

$$\frac{1}{(2h)^2} [Q_y(x+h,y+h) - Q_y(x-h,y+h) - Q_y(x+h,y-h) + Q_y(x-h,y-h)] \quad (17)$$

$$- \frac{1}{h^2} [Q_x(x,y+h) - 2Q_x(x,y) + Q_x(x,y-h)] = - f^2(x,y) Q_x(x,y)$$

$$\begin{aligned} & \frac{1}{(2h)^2} [Q_x(x+h, y+h) - Q_x(x-h, y+h) - Q_x(x+h, y-h) + Q_x(x-h, y-h)] \\ & - \frac{1}{h^2} [Q_y(x+h, y) - 2Q_y(x, y) + Q_y(x-h, y)] = -f^2(x, y) Q_y(x, y) \quad (18) \end{aligned}$$

These difference equations are solved by a Newton-Relaxation method,⁸ where an initial guess is submitted for the solution, and this guess is then iterated until the difference equations are satisfied to the desired accuracy. In our work at a kappa of two we chose the grid size to be 0.2, as mentioned before, and then iterate until the left side of each equation equals the right side of the equation plus or minus 0.001. Since the grid size limits us to an accuracy of about 0.01, there is then no additional loss of accuracy due to the difference equations not being satisfied exactly. The amount by which the left side of the equation differs from the right side of the equation is said to be the residual of that difference equation, and when this residual is reduced to the desired accuracy, one is said to have relaxed the residual. The procedure by which the residuals are relaxed simultaneously is a three-dimensional Newton's method, which explains the name Newton-Relaxation Technique. The complicating feature is that the equations are coupled as well as nonlinear, and they must all three be integrated simultaneously.

The boundary conditions allow us to determine the solutions on the grid boundary as a function of the solution values in the interior. For example, the condition $\partial f / \partial y|_{y=0} = 0$ is applied as follows.

$$f(x,y) = f(x,0) + ay^2 \quad (19)$$

This is a Taylor's series expansion about the line $y=0$ for some fixed value of x . Evaluating at the interior grid points then gives

$$f(x,h) = f(x,0) + ah^2 \quad (20)$$

$$f(x,2h) = f(x,0) + 4ah^2 \quad (21)$$

Solving these equations gives Equation 22, the solution on the boundary as a function of the interior values.

$$f(x,0) = -\frac{1}{3}[f(x,2h) - 4f(x,h)] \quad (22)$$

All other boundary conditions are applied in a similar fashion. This then reduces the number of grid points at which we must iterate in order to obtain the solution. An exception to this procedure occurs when the vortex is sitting in the middle of the slab, a case that will be discussed later.

In one dimension we have $f=f(x)$ and $\vec{Q}=Q_y(x)\hat{y}$. The equations then simplify, and several authors have integrated them for a semi-infinite slab.^{7,9-11} In order to be sure our computer programs were operating properly, we first solved the one-dimensional equations for a slab of width 10.0 at various values of κ . The solutions can be specified by the applied field strength or by the value of the order parameter at

the surface of the slab. The most straightforward description turns out to be by specifying the value of the order parameter at the surface. If this procedure is followed, one fixes the value of the order parameter at the surface and allows the value of the applied field to float during the iteration process. The program then converges upon the functional values of f and Q and upon the applied field that is consistent with the assigned value of the order parameter at the surface. The order parameter at the surface can range from zero to one, and a plot of the order parameter at the surface versus the applied field then specifies the solutions for a given κ . In the literature the applied field in such a plot is often given in units of H/H_c rather than the Ginzburg-Landau reduced units of $H/(\sqrt{2} H_c)$, and that is the convention followed in Figure 7, where our results are displayed. The bulge in the graphs decreases as κ increases; the κ values displayed are 1.1, 2.0, 3.0, 10.0, and infinity. The infinite κ case can be solved analytically¹¹ to find

$$f(x=0) = (1 - H^2/H_c^2)^{1/4} \quad (23)$$

The results displayed in Figure 7 agree well with previously published results^{7,9} and lead to two conclusions: first that our programs are working correctly and second that a slab width of 10.0 is a good approximation for a semi-infinite slab. For a given value of κ , the solutions show that there is a maximum applied field at which Ginzburg-Landau solutions with only one-dimensional variations exist. This had

Figure 7. One-dimensional solutions for the reduced order parameter at the surface f_0 vs. the reduced magnetic field H/H_c . Curve a is for κ infinite, curve b for $\kappa=10.0$, curve c for $\kappa=3.0$, curve d for $\kappa=2.0$ and curve e for $\kappa=1.1$.

previously been interpreted as the superheating field. The work of Fink and Presson⁹ and of Kramer,⁷ however, showed that for a kappa greater than 1.1 two-dimensional fluctuations set in before this maximum field is reached and that this lower field is actually the superheating field.

As might be expected, it is easier to do an error analysis on the one-dimensional Ginzburg-Landau equations than on the two-dimensional equations. Let us now do such an analysis. In one dimension the equations reduce to

$$\frac{1}{\kappa^2} \frac{d^2 f}{dx^2} = f^3 + fQ^2 - 1, \quad (24)$$

$$\frac{d^2 Q}{dx^2} = f^2 Q. \quad (25)$$

It may be shown that using the difference relations instead of differential relations results in an error given by⁸

$$\frac{2h^2}{\kappa^2 4!} \frac{d^4 f}{dx^4}, \quad (26)$$

$$\frac{2h^2}{4!} \frac{d^4 Q}{dx^4}. \quad (27)$$

Equation 26 is the error introduced in Equation 24 while Equation 27 is the error introduced in Equation 25. By differentiating Equations 24 and 25 and using the fact that our solutions do satisfy Equations 24 and 25 we find the error in the numerical solution of Equations 24 and 25 to be given by

$$\frac{2h^2}{4!} [(3f_0^2 + Q_0^2 - 1)\kappa^2 f_0(f_0^2 + Q_0^2 - 1) + 2f_0^3 Q_0^2 + 2f_0 H^2], \quad (28)$$

$$\frac{2h^2}{4!} [2f_0 Q_0 \kappa^2 f_0(f_0^2 + Q_0^2 - 1) + f_0^4 Q_0]. \quad (29)$$

The expressions for the error have been evaluated at the surface of the slab, and f_0 denotes the value of the order parameter at the surface, Q_0 the value of the superfluid velocity at the surface, and H the value of the applied field in Ginzburg-Landau reduced units. In order to obtain very accurate results for comparison with the previously published material, the grid size chosen for the solutions displayed in Figure 7 was 0.078125. Inserting the appropriate values in Equations 28 and 29 for this grid size, we find that the kappa of 1.1 solutions are the most accurate with an error of about 0.001 and that the kappa of 10.0 solutions are the least accurate with an error of about 0.003. Since spatial variations of f occur on the scale of $1/\kappa$ it should be expected that for a given grid size the higher kappa solutions would be the least accurate.

Before moving on to the heart of this work and investigating two-dimensional fluctuations in finite slabs, let us look at the effect of a finite slab on the one-dimensional solutions. $\text{Pb}_{83}\text{In}_{17}$ has a kappa of about 4.0 and has been the subject of experimental work.^{12,13} Figure 8 shows the one-dimensional solutions for a kappa of 4.0 at slab

Figure 8. One-dimensional solutions for the reduced order parameter at the surface f_0 vs. the reduced magnetic field H/H_c with $\kappa=4.0$. Curve a is for $W=10.0$, curve b for $W=5.0$, curve c for $W=4.0$, curve d for $W=3.0$ and curve e for $W=2.0$.

widths of 2.0, 3.0, 4.0, 5.0, and 10.0. As the order parameter at the surface is depressed to zero, the solutions for a slab width of 10.0 go to an applied field of 1.0 in units of H_c . The thinner the slab, the more departure from this behavior. The thinner slabs require a much higher field to depress the order parameter a given amount, which is another way of saying that superconductivity is harder to destroy in a thin slab.

CHAPTER 3. OUR WORK AT $\kappa=2.0$

To begin, we would like to investigate two-dimensional solutions at a small value of κ , say 2.0, because the spatial variations of the solutions should be slower, allowing our programs to converge upon a solution more rapidly. Once we have a feel for how the solutions will change as various parameters are changed, we will move on to higher values of κ , where much of the experimental work has been done.

Consider a κ of 2.0 and a slab width of 4.0. With a grid size of 0.0625 the one-dimensional equations are integrated, giving the results recorded in Table 1. Equations 28 and 29 show that the accuracy of this data is about 0.001. In the table, H is given in Ginzburg-Landau reduced units, although, as mentioned before, it is not plotted in these units.

The next order of business is to integrate the two-dimensional equations for a κ of 2.0 and a slab width of 4.0. At low enough applied fields we expect the two-dimensional solutions to have only one-dimensional spatial variations. As the applied field is increased, two-dimensional fluctuations will occur, at which point a vortex will be found to form and move into the bulk of the slab. This is the picture suggested by Kramer⁷ and by Fink and Presson.⁹ The two-dimensional solutions are obtained by fixing the value of the order parameter at (0,0), allowing the order parameter to float in the bulk and elsewhere along the surface, and allowing the value of the applied field to float during the iteration process. This is the two-dimensional analogue of

Table 1. One-dimensional solutions.

$W=4.0$, f_0 is the order parameter at the surface, H is the applied field, F is the Helmholtz free energy per unit surface area and G the Gibbs free energy per unit surface area, all in Ginzburg-Landau reduced units.

f_0	H	F	G
0.1	1.050	2.615	-1.341
0.2	0.980	2.124	-1.093
0.3	0.953	1.832	-1.008
0.4	0.938	1.598	-0.963
0.5	0.923	1.380	-0.916
0.6	0.889	1.157	-0.845
0.7	0.836	0.916	-0.732
0.8	0.741	0.648	-0.562
0.9	0.569	0.345	-0.322

the procedure followed in one dimension. Our program then converges to the functional values of $f(x,y)$, $Q_x(x,y)$, and $Q_y(x,y)$ and to the applied field value that are all consistent with the chosen value of $f(0,0)$.

Experimentally one would simply apply a field to a slab, and this would determine f and $\vec{Q}$ everywhere in the slab including $f(0,0)$. We could follow this procedure numerically by fixing the applied field strength and allowing f and $\vec{Q}$ to float freely everywhere on the grid, but then we would never be able to generate the solutions which occur on the underside of the bulge in the plots of order parameter versus applied field.

We start with $f(0,0)=1.0$ and begin to depress it towards zero, assuming different periodicity lengths. At $f(0,0)=0.5$ we find a two-dimensional variation just starting to appear. All solutions with $f(0,0)$ greater than 0.5 converge to one-dimensional states. Recall that $f(0,0)$ is fixed and the value of the applied field is allowed to float during iteration. Thus the value of the applied field arrived at for the solution might be expected to depend upon the periodicity length chosen, and this is indeed found to be the case. As discussed by Kramer⁷ and by Fink and Presson⁹ the smallest applied field at which two-dimensional fluctuations appear is the point at which vortices would be expected to form and enter the slab. Fixing $f(0,0)=0.5$, we find that with a period of 4.0 the applied field is 0.937, with a period of 5.6 the field is 0.932, and at a period of 10.0 the field is 0.931. Since these differences in field strength are beyond the accuracy of this work, which

is of the order of 0.01 for this grid size, we cannot use these results to determine whether a given periodicity is preferred. Since we are dealing with very small two-dimensional fluctuations, it is not surprising that the periodicity has a small effect. As the order parameter at the origin is depressed further and the two-dimensional nature of the solutions becomes more pronounced, the periodicity would be expected to play a more important role. Moreover, when nucleated vortices penetrate into the bulk of the slab, we expect the periodicity to become even more important.

To study the onset of two-dimensionality, we numerically integrate the equations for a periodicity of both 5.6 and 10.0. Figure 9 shows the order parameter at the origin versus the applied field (in units of H_c) for the one-dimensional solutions and for the two-dimensional solutions at periods of 5.6 and 10.0. For $f(0,0)$ greater than 0.5 the two sets of two-dimensional solutions are identical, while for $f(0,0)$ less than or equal to 0.5 the periodicity of 10.0 solutions have a lower value of the applied field at a given value of $f(0,0)$ than the 5.6 periodicity solutions. For $f(0,0)$ greater than 0.5, where all solutions are of a one-dimensional nature, it is seen that the more accurate solutions obtained by integrating the one-dimensional equations on a smaller grid have lower field strengths at a given $f(0,0)$ than the corresponding solution obtained by integrating the two-dimensional equations. To allow a quantitative comparison in the region where only one-dimensional

Figure 9. Periodicity dependence of the solutions for $\kappa=2.0$ and $W=4.0$. Curve a has $P=10.0$, curve b $P=5.6$ and curve c shows the one-dimensional solutions.

fluctuations occur, we give in Table 2 the characteristics of the 5.6 periodicity solutions. Although these results are only accurate to about 0.01 we give three figures for comparison.

As mentioned above, the solution at $f_0=0.5$ is obtained by allowing the value of the applied field to float while $f(0,0)=0.5$ is fixed. The results in Table 2 show that there is another solution which has the same applied field strength of 0.932. This solution occurs on the underside of the bulge in the plot of order parameter versus applied field and was obtained by fixing the applied field strength and allowing $f(0,0)$ to float during the iteration process. That is, if one takes the solution at $f(0,0)=0.5$ with a periodicity of 5.6 for which the two-dimensional fluctuations just begin to appear and fixes the applied field at 0.932 while allowing $f(0,0)$ to float, it is found that the order parameter at the surface of the slab plummets to about 0.002 and that G , the Gibbs free energy per unit surface area, is minimized at the expense of F , the Helmholtz free energy per unit surface area. Thus, G has been lowered by the admission of additional flux to the interior of the slab. Later when we allow vortices to penetrate the slab, we shall calculate the various contributions to the free energy and see exactly how each one changes during the nucleation process.

Before moving on to the nucleation of a vortex, let us look at the solutions in the region where large two-dimensional fluctuations occur. Since the grid size is 0.2 for both periodicities, there will be a larger number of data points at the larger period and a more detailed

Table 2. Two-dimensional solutions.

 $W=4.0$, $\kappa=2.0$, $P=5.6$

f_0	H	F	G
0.0023	0.932	1.835	-1.000
0.025	0.874	1.496	-0.812
0.1	0.862	1.304	-0.786
0.2	0.875	1.263	-0.813
0.3	0.895	1.278	-0.858
0.4	0.912	1.306	-0.897
0.5	0.932	1.406	-0.947
0.6	0.904	1.197	-0.877
0.7	0.854	0.968	-0.766
0.8	0.761	0.694	-0.592
0.9	0.587	0.377	-0.342

plot may be constructed. We thus plot the solutions for a periodicity of 10.0 in Figures 10 through 15. These are three-dimensional computer-generated plots and to the right of some are shown contour plots of the function.

Figure 10 shows the magnitude of the order parameter. The view is from the front with one half of the slab width being shown over a distance of one period. To the right is a contour plot of the same data. Figure 11 is a three-dimensional plot of the local flux density and an accompanying contour plot. This is viewed from behind the slab with half of the slab width again being shown over a distance of one period. The flux density decays into the middle of the slab with a concentration in the region of low order parameter. Also apparent is the entry of flux at the edges of the plot associated with regions of low order parameter on the other side of the slab. Figure 12 shows the x component of the superfluid velocity. The view is from the back with half a slab width being shown. Figure 13 shows the negative of the y component of the superfluid velocity, Figure 14 the x component of the supercurrent density, and Figure 15 the y component of the supercurrent density, all viewed from the same orientation as Figure 12. We see that the y component of the superfluid velocity peaks very strongly in the region of low order parameter, and later we shall see that it actually diverges on the axis of a vortex. This is only a mathematical divergence, though, since the superfluid velocity is not a physical measurable quantity.

Figure 10. Magnitude of the reduced order parameter, f , for $W=4.0$, $\kappa=2.0$, $P=10.0$, and $f_0=0.05$, for which $H=0.812$. This is viewed from the front of the slab with one period and half the slab width shown. On the right are contours of f with increments of 0.1 .

Figure 11. Local flux density, b , for $W=4.0$, $\kappa=2.0$, $P=10.0$, and $f_0=0.05$, for which $H=0.812$. This is viewed from the back of the slab with one period and half the slab width shown. On the right are contours of b with increments of 0.1 .

Figure 12. X component of the superfluid velocity, Q_x , for $W=4.0$, $\kappa=2.0$, $P=10.0$, and $f_0=0.05$. This is viewed from the back of the slab with one period and half of the slab width shown.

Figure 13. Negative of y component of the superfluid velocity, $-Q_y$, for $W=4.0$, $\kappa=2.0$, $P=10.0$, and $f=0.05$. This is viewed from the back of the slab with one period and half the slab width shown.

Figure 14. X component of the supercurrent density, J_x , for $W=4.0$, $\kappa=2.0$, $P=10.0$, and $f=0.05$. This is viewed from the back of the slab with one period and half the slab width shown.

Figure 15. Y component of the supercurrent density, J_y , for $W=4.0$, $\kappa=2.0$, $P=10.0$, and $f_0=0.05$. This is viewed from the back of the slab with one period and half the slab width shown.

Since at the core of a vortex the order parameter rises linearly,¹⁴ one could not enforce the boundary condition $\frac{\partial f}{\partial x}|_{\text{surface}} = 0$ if the vortex core were at the surface of the slab. In order to simulate the situation, we have a program in which the applied field strength is fixed, the value $f(0,0)$ is fixed, and the slope of f at the origin floats during the iteration. The boundary condition on $f(x,y)$ at the surface of the slab is taken as

$$\frac{\partial f}{\partial x}|_{(0,0)} = \frac{\partial f}{\partial y}|_{(0,0)} \neq 0, \quad \frac{\partial f}{\partial x}|_{x=0, y \neq 0} = 0. \quad (30)$$

The usual boundary conditions on f at the surface are maintained everywhere except right at the vortex core. Holding $\frac{\partial f}{\partial x}|_{(0,0)} = \frac{\partial f}{\partial y}|_{(0,0)}$ is an attempt to allow for the circular symmetry that is expected at the core. If we attempt to set $f(0,0)=0.0$ and impose the usual boundary conditions all along the surface of the slab, we find that the whole slab is driven into the normal state. Allowing the slope to float at the origin gives solutions with $f(0,0)=0.0$ and a slope typically of the order of 0.01 or smaller, so that there is no large discontinuity in the slope of f along the surface of the slab.

If at a periodicity of 5.6 we hold the field at $H=0.932$ and depress $f(0,0)$ to zero, allowing the slope at the origin to float, we find a solution with $\frac{\partial f}{\partial x}|_{(0,0)} = \frac{\partial f}{\partial y}|_{(0,0)} = 0.0065$ and $Q_y(0,0)=-3.69$. At the core of a vortex the superfluid velocity actually diverges,¹⁴ and the only reason we are able to get a nondivergent value for $Q_y(0,0)$ is

that we are dealing with a finite grid size. As the grid size is reduced and the accuracy of the solutions increased, $\vec{Q}$ shows more of a divergence at the core. Nothing physical diverges, however, since at the core f and hence the density of electrons in the superconducting state go to zero, but the mathematical divergence of $\vec{Q}$ might be expected to hinder the convergence of the program when the vortex is in the slab. This problem is handled by expressing Q as the sum of two contributions, $\vec{Q} = \vec{Q}_0 + \vec{Q}_1$. $\vec{Q}_0$ contains the divergent contribution, which will be important near the vortex core, while $\vec{Q}_1$ is the deviation of the solution from this divergent contribution. We will assume an analytical form for $\vec{Q}_0$ and write a computer program which calculates the required $\vec{Q}_1$ so that the total $\vec{Q}$ is a solution of the Ginzburg-Landau equations.

As shown by Neuman and Tewordt¹⁴ and by Kramer,⁷ near the vortex core $\vec{Q}$ goes approximately as

$$\vec{Q}_0 = -\frac{\hat{\theta}}{\kappa r} \quad (31)$$

$\hat{\theta}$ is the usual unit vector in polar coordinates and the kappa is necessary for flux quantization. Before moving on let us take a look at why $\vec{Q}$ does diverge on the vortex axis and why the factor kappa appears in the divergent contribution to $\vec{Q}$.

Recall that in cgs units we defined $\vec{a}_s = \vec{a} + \frac{\phi_0}{2\pi} \vec{\nabla}\gamma$. Suppose there is an isolated vortex and consider the path C of radius R surrounding the vortex and lying in a plane perpendicular to the vortex axis. The

line integral of $\vec{a}_s$ around this path is $\oint_C \vec{a}_s \cdot d\vec{\ell} = \oint_C \vec{a} \cdot d\vec{\ell} + \frac{\phi_0}{2\pi} \oint_C \vec{\nabla} \gamma \cdot d\vec{\ell} = \oint_C \vec{a} \cdot d\vec{\ell} - \phi_0$ where we have used the fact that the phase changes by -2π when the path encircles the vortex in the right hand sense. That is, $\oint_C \vec{\nabla} \gamma \cdot d\vec{\ell} = \gamma(\theta=2\pi) - \gamma(\theta=0) = -2\pi$. The line integral $\oint_C d\vec{\ell} \cdot \vec{a}$ is the flux passing through the path C , and as the radius of the path, R , goes to zero this contribution to $\oint_C d\vec{\ell} \cdot \vec{a}_s$ will vanish, leaving us with $\oint_C d\vec{\ell} \cdot \vec{a}_s \Big|_{R \rightarrow 0} = -\phi_0$. Clearly $\vec{a}_s$ must diverge on the vortex axis. In order for the line integral to remain nonzero, $\vec{a}_s$ must vary as $-1/r$ near the vortex axis. To arrive at the dependence for $\vec{Q}_0$ quoted in Equation 31, we must go to Ginzburg-Landau reduced units. The reduced units for flux density are $\frac{\kappa \phi_0}{2\pi}$, and in reduced units the gauge-invariant vector potential is equal to the superfluid velocity, allowing us to write $\oint_C d\vec{\ell} \cdot \vec{Q}_0 \Big|_{R \rightarrow 0} = -\left(\frac{2\pi}{\kappa \phi_0}\right) \phi_0 = -2\pi/\kappa$. Since $\vec{Q}_0$ must go as $\frac{-A\hat{\theta}}{r}$ near the vortex this requires $A=1/\kappa$, which is the result given in Equation 31. As we mentioned before, this divergence of $\vec{Q}_0$ is only a mathematical divergence and no physical quantities diverge. This becomes apparent when we calculate the local flux density, which in reduced units is $\vec{b} = \vec{\nabla} \times \vec{Q} + \frac{2\pi}{\kappa} \delta(\vec{\rho} - \vec{\rho}_0) \hat{z} = \vec{\nabla} \times \vec{Q}_0 + \vec{\nabla} \times \vec{Q}_1 + \frac{2\pi}{\kappa} \delta(\vec{\rho} - \vec{\rho}_0) \hat{z} = \vec{\nabla} \times \vec{Q}_1$. This assumes that the vortex is at $\vec{\rho}_0$ and makes use of the fact that in reduced units $\vec{a}_s = \vec{Q}$, and that $\vec{\nabla} \times \vec{Q}_0 = -\frac{2\pi}{\kappa} \delta(\vec{\rho} - \vec{\rho}_0)$. Only the well-behaved contribution to $\vec{Q}$ contributes to the local flux density.

The boundary condition at the surface of the slab is that no supercurrent may flow through the surface of the slab. To construct a $\vec{Q}$ that not only diverges as in Equation 29 but also satisfies the surface

boundary condition, it is convenient to use the method of images, just as one does in electrostatics for the problem of a charge placed between parallel conducting planes. Kramer⁷ considered a semi-infinite slab and so had only a single image, but for a finite slab there will be an infinite number of both positive and negative images. The total $\vec{Q}$ will be a sum of the contributions from each of the positive and negative images and could be obtained by vector addition. There is, however, a more efficient approach which yields an analytic expression of remarkably simple form.

As pointed out above, the problem under consideration is closely related to that of a line charge placed between parallel conducting planes or to that of a vortex in a fluid between two parallel walls. To account for the images in these two problems, and in other analagous problems, Morse and Feshbach in Methods of Theoretical Physics¹⁵ have developed a complex variable approach. We want to describe the contribution of a single vortex by $Q_0 = -\hat{\theta}/\kappa r = \frac{y\hat{x} - x\hat{y}}{\kappa(x^2 + y^2)}$. Consider the complex valued function $\Lambda(z) = \frac{1}{\kappa} \ln z$ for which $-i(\Lambda'(z))^* = \frac{y-ix}{\kappa(x^2 + y^2)}$. We see $\text{Re}[-i(\Lambda'(z))^*] = \frac{y}{\kappa(x^2 + y^2)}$, $\text{Im}[-i(\Lambda'(z))^*] = \frac{-x}{\kappa(x^2 + y^2)}$. The real and imaginary parts of $-i(\Lambda'(z))^*$ are the components of the superfluid velocity. Morse and Feshbach consider the problem in detail on page 1231 but the essential feature is that the vortex and each of the images will have a contribution of the form of $\Lambda(z)$ and that the net $\Lambda_{\text{tot}}(z)$ will be the sum of these separate contributions. They then do the sum to find that if the divergent

contribution of the vortex and all images are considered the total

$\vec{Q}_0$ has the components

$$q_{0x} = \frac{\pi}{4\kappa W} \sinh\left(\frac{\pi y}{W}\right) \frac{1}{\sin^2 \frac{\pi}{2W}(x-x_0) \cosh^2 \left(\frac{\pi y}{2W}\right) + \cos^2 \frac{\pi}{2W}(x-x_0) \sinh^2 \left(\frac{\pi y}{2W}\right)} - \frac{1}{\sin^2 \frac{\pi}{2W}(x+x_0) \cosh^2 \left(\frac{\pi y}{2W}\right) + \cos^2 \frac{\pi}{2W}(x+x_0) \sinh^2 \left(\frac{\pi y}{2W}\right)}, \quad (30)$$

$$q_{0y} = \frac{\pi}{4\kappa W} \frac{\sin \frac{\pi}{W}(x+x_0)}{\sin^2 \frac{\pi}{2W}(x+x_0) \cosh^2 \left(\frac{\pi y}{2W}\right) + \cos^2 \frac{\pi}{2W}(x+x_0) \sinh^2 \left(\frac{\pi y}{2W}\right)} - \frac{\sin \frac{\pi}{W}(x-x_0)}{\sin^2 \frac{\pi}{2W}(x-x_0) \cosh^2 \left(\frac{\pi y}{2W}\right) + \cos^2 \frac{\pi}{2W}(x-x_0) \sinh^2 \left(\frac{\pi y}{2W}\right)}. \quad (31)$$

This is in Ginzburg-Landau reduced units. W is the slab width and the vortex in slab is located at $(x_0, 0)$. The reason we have used the lower case $\vec{q}_0$ will become apparent shortly.

This expression accounts for the vortex located at $(x_0, 0)$. Our assumption, however, is that if a vortex is found at $(x_0, 0)$ there will also be vortices at $(x_0, \pm P, \pm 2P, \dots)$ and at $(W-x_0, \pm P/2, \pm 3P/2, \dots)$. To allow for these additional vortices and their images one must superimpose the various contributions. Letting $q_{0x}(x, y)$, $q_{0y}(x, y)$ denote the contribution from the vortex at $(x_0, 0)$, the total $\vec{Q}_0$ is then

$$Q_{0x} = \sum_{n=-\infty}^{\infty} q_{0x}(x, y-nP) - \sum_{n=-\infty}^{\infty} q_{0x}(x-W, y-\frac{2n-1}{2}P), \quad (34)$$

$$Q_{0y} = \sum_{n=-\infty}^{\infty} q_{0y}(x, y-nP) - \sum_{n=-\infty}^{\infty} q_{0y}(x-W, y-\frac{2n-1}{2}P) . \quad (35)$$

By constructing $\vec{Q}_0$ in this fashion, we find that it satisfies all the symmetry conditions that $\vec{Q}$ must satisfy; that is, $\vec{Q}_0$ satisfies all the required boundary conditions along the lines $x=W/2$, $y=0.0$, and $y=P/2$. Along the surface of the slab it satisfies $Q_{0x}(x=0, y)=0$, $\frac{\partial Q_{0y}}{\partial x} \Big|_{\text{surface}} = 0$. This then requires that $\vec{Q}_1$ satisfy the symmetry conditions along the lines $x=W/2$, $y=0.0$, $y=P/2$, and $Q_{1x}(x=0, y)=0$, $\frac{\partial Q_{1y}}{\partial x} \Big|_{\text{surface}} = H$, where H is the applied field, since $\vec{Q}$ must satisfy all the symmetry conditions and $Q_x(x=0, y)=0$, $\frac{\partial Q_y}{\partial x} \Big|_{\text{surface}} = H$. We then write our computer programs to solve simultaneously for $f(x, y)$ and $\vec{Q}_1(x, y)$ subject to the required boundary conditions. We again use a Newton-Relaxation Technique, obtaining the solution by constructing an initial guess at what the solution will be and iterating on this guess until it satisfies the difference equations.

Previously we mentioned that it was never necessary to relax residuals at the grid points lying on the boundary. The value assumed by f and $\vec{Q}$ on the boundary was either fixed at zero (this was the case for $Q_x(x=0, y)$, for example) or else determined as a function of the values assumed at the interior grid points by use of the boundary conditions. An exception to this rule occurs when the vortex is at the middle of the slab. When the vortices are sitting in the middle of the slab, we found it necessary to relax residuals along the line $x=W/2$. It is possible to get a solution by using the boundary conditions to

determine f and $\vec{Q}$ along the line $x=W/2$, but if one determines the values of f and $\vec{Q}$ along this line by relaxing residuals, a slightly smoother solution with a slightly lower Gibbs free energy results. This exception occurs because if the zero of f is located on the line $x=W/2$ and we determine the functional values of f and $\vec{Q}$ along this line by the application of the boundary conditions, none of the difference equations at the interior grid points directly sample this zero of f . Since f is changing very rapidly near the vortex core, this results in a slightly rougher solution, which has a slightly higher Gibbs free energy. If we relax residuals along the line $x=W/2$, then the difference equations at $(W/2, h)$, where h is the grid spacing, directly sample this zero in f . As the grid size shrinks to zero, the difference in the two procedures will vanish, but on the finite grid sizes with which we are dealing there is a noticeable difference.

Now we are ready to watch a vortex nucleate and move into the slab. Recall that at a periodicity of 5.6 two-dimensional fluctuations set in when $f(0,0)=0.5$ with a corresponding applied field of $H=0.932$. Holding the field fixed and allowing the program to iterate, we find that the order parameter plummets to 0.002. We then hold $f(0,0)=0$ and $H=0.932$ and allow the slope of f at the origin to float to get a solution with $\frac{\partial f}{\partial x}|_{(0,0)} = \frac{\partial f}{\partial y}|_{(0,0)} = 0.0065$. Now we hold the field at $H=0.932$ and move the zero of f into the slab with all boundary conditions being satisfied except at the vortex core where $\frac{\partial f}{\partial y}|_{\text{core}} \neq 0$. This allows for the linear rise in f near the vortex core. As the vortex moves into the slab, it is

illuminating to watch what each of the contributions to the free energy does. We then define the following quantities.

$$F = \langle \frac{1}{2}(1-f^2)^2 \rangle + \langle (\vec{\nabla}f/\kappa)^2 \rangle + \langle Q^2 f^2 \rangle + \langle b^2 \rangle \quad (36)$$

$$\langle \frac{1}{2}(1-f^2)^2 \rangle = \frac{1}{P} \int_0^P dy \int_0^{W/2} dx \frac{1}{2}(1-f^2)^2 \quad (37)$$

$$\langle (\vec{\nabla}f/\kappa)^2 \rangle = \frac{1}{P} \int_0^P dy \int_0^{W/2} dx (\vec{\nabla}f/\kappa)^2 \quad (38)$$

$$\langle Q^2 f^2 \rangle = \frac{1}{P} \int_0^P dy \int_0^{W/2} dx Q^2 f^2 \quad (39)$$

$$\langle b^2 \rangle = \frac{1}{P} \int_0^P dy \int_0^{W/2} dx b^2 \quad (40)$$

Another quantity which is useful to those who do tunneling measurements is the average value of the order parameter along the surface of the slab.

$$\langle f \rangle = \frac{1}{P} \int_0^P dy f(x=0, y) . \quad (41)$$

We find that, once two-dimensional fluctuations become possible, the order parameter at the origin spontaneously plummets to zero, and this zero of f then moves into the bulk of the slab with G decreasing monotonically. The field at which these two-dimensional fluctuations first occur is called the superheating field. Figures 16 through 25 are three-dimensional plots of the magnitude of the order parameter and

of the flux density as the vortex forms and moves into the bulk. Especially apparent in the plots is the shrinking of the vortex core size as the vortex moves into the bulk. This lowers G by reducing the amount of lost condensation energy. Table 3 gives numerical values of F , G , and the various contributions to the free energy as the vortex is formed.

We should note that the solution with the vortex at 0.4 appears to be rather rough due to vortex-surface interaction. The accuracy of this solution is probably less than that of the other solutions. Although the roughness of the solution can be cured by reducing the grid size, the computer time required to get the smoother solution becomes prohibitive. On a grid of 0.2 a typical solution requires about 15 minutes or less on an IBM 360-65, while on a grid of 0.1 a single solution requires on the order of 4 hours.

As the applied field is increased on a slab with no vortices in the bulk, there will be some field value at which it is energetically favorable for a vortex to exist in the bulk of the slab. However, the surface barrier prevents the vortex from nucleating and moving into the bulk of the slab, so that some higher field must be reached before this barrier is overcome and the vortex is able to move into the bulk of the slab. This higher field is the superheating field and for a periodicity of 5.6 it is seen to be 0.932. The field at which it first becomes energetically favorable for a vortex to exist in a bulk sample is denoted by H_{C1} and has been evaluated by Harden and Arp.¹⁶ For

Figure 16. Magnitude of the reduced order parameter, f , for $W=4.0$, $\kappa=2.0$, $P=5.6$, and $f_0=0.5$, for which $H=0.932$. This is viewed from the front of the slab with one period and half the slab width shown. On the right are contours of f with increments of 0.1.

Figure 17. Local flux density, b , for $W=4.0$, $\kappa=2.0$, $P=5.6$, and $f_0=0.5$, for which $H=0.932$. This is viewed from the back of the slab with one period and half the slab width shown. On the right are contours of b with increments of 0.1.

Figure 18. Magnitude of the reduced order parameter, f , for $W=4.0$, $\kappa=2.0$, $P=5.6$, and $H=0.932$, for which $f_0=0.002$. This is viewed from the front of the slab with one period and half the slab width shown. On the right are contours of f with increments of 0.1.

Figure 19. Local flux density, b , for $W=4.0$, $\kappa=2.0$, $P=5.6$, and $H=0.932$, for which $f=0.002$. This is viewed from the back of the slab with one period and half the slab width shown. On the right are contours of b with increments of 0.1.

Figure 20. Magnitude of the reduced order parameter, f , for $W=4.0$, $\kappa=2.0$, $P=5.6$, $H=0.932$, and $f=0.0$. This is viewed from the front of the slab with one period and half the slab width shown. On the right are contours of f with increments of 0.1 .

Figure 21. Local flux density, b , for $W=4.0$, $\kappa=2.0$, $P=5.6$, $H=0.932$, and $f=0.0$. This is viewed from the back of the slab with one period and half the slab width shown. On the right are contours of b with increments of 0.1.

Figure 22. Magnitude of the reduced order parameter, f , for $W=4.0$, $\kappa=2.0$, $P=5.6$, and $H=0.932$, with the zero of f at one penetration depth from the surface. This is viewed from the front of the slab with one period and half the slab width shown. On the right are contours of f with increments of 0.1.

Figure 23. Local flux density, b , for $W=4.0$, $\kappa=2.0$, $P=5.6$, and $H=0.932$, with the zero of f at one penetration depth from the surface. This is viewed from the back of the slab with one period and half the slab width shown. On the right are contours of b with increments of 0.1 .

Figure 24. Magnitude of the reduced order parameter, f , for $W=4.0$, $\kappa=2.0$, $P=5.6$, and $H=0.932$ with the zero of f in the middle of the slab. This is viewed from the front of the slab with one period and half the slab width shown. On the right are contours of f with increments of 0.1.

Figure 25. Local flux density, b , for $W=4.0$, $\kappa=2.0$, $P=5.6$, and $H=0.932$ with the zero of f in the middle of the slab. This is viewed from the back of the slab with one period and half the slab width shown. On the right are contours of b with increments of 0.1 .

Table 3. Vortex nucleation results for

$$W=4.0, \kappa=2.0, P=5.6$$

f	H	F	G	$\langle \frac{1}{2}(1-f^2)^2 \rangle$	$\langle (\nabla f/\kappa)^2 \rangle$	$\langle Q^2 f^2 \rangle$	$\langle b^2 \rangle$
.5	.932	1.406	-.947	.193	.032	.329	.851
.002	.932	1.835	-1.000	.336	.093	.221	1.183
0.	.932	1.834	-1.000	.336	.093	.221	1.182

Vortex Position	H	F	G	$\langle \frac{1}{2}(1-f^2)^2 \rangle$	$\langle (\frac{\nabla f}{\kappa})^2 \rangle$	$\langle Q^2 f^2 \rangle$	$\langle b^2 \rangle$	$\langle f \rangle$
.4	.932	1.765	-1.017	.300	.090	.231	1.142	.573
.6	.932	1.569	-1.020	.216	.076	.271	1.004	.679
.8	.932	1.467	-1.045	.151	.072	.292	.951	.771
1.0	.932	1.448	-1.070	.127	.080	.288	.952	.807
1.2	.932	1.434	-1.101	.112	.072	.289	.960	.823
1.4	.932	1.433	-1.119	.105	.079	.280	.907	.832
1.6	.932	1.427	-1.138	.098	.070	.284	.974	.836
1.8	.932	1.429	-1.145	.099	.081	.271	.977	.838
2.0	.932	1.424	-1.151	.094	.069	.283	.978	.839

a kappa of two they find $H_{c1}/H_c = 0.54$ or $H_{c1} = 0.38$ in Ginzburg-Landau reduced units. In this finite slab geometry we would find the analogous field by plotting, as a function of the applied field, the Gibbs free energy G of the state with no vortex in the bulk and on the same graph the Gibbs free energy of the state with vortices in the bulk. At very low fields the no-vortex state should have the lower G , while at higher fields, which are still less than the superheating field, the state with vortices in the bulk should have the lower G . Integrating the Ginzburg-Landau equations for the two cases at various fields shows that the field at which the two cases have about the same G and hence the intersection on such a graph $H/H_c = 0.813$ or 0.575 in Ginzburg-Landau reduced units. At this field the vortex state has $G = -0.323$ and the no-vortex state has $G = -0.327$. This difference in energies is well down in the noise level, and we see that it is energetically favorable for the slab to be in the vortex state at a much lower field than 0.932 , which is the field at which it actually enters the vortex state due to the surface barrier. Let us denote the field at which it is energetically favorable for the slab to be in the vortex state as $H_{c1}(\kappa=2, W=4, P=5.6) = 0.575$. Note that as defined $H_{c1}(\kappa, W, P)$ will be a function of the periodicity P .

One of the first theoretical treatments of superheating was the well-known paper by Bean and Livingston¹⁷ in which only the electromagnetic interaction was considered. There it was shown that the inter-

action of a vortex with its image could lead to such a superheating effect. The image is required by the boundary conditions and exerts an attractive interaction on the vortex, holding it to the surface.

If once the vortices are in the slab the applied field is reduced, an analogous situation occurs in which it is favorable energetically for the slab to be in a state with no vortices in the bulk, but the vortices are unable to exit until the field is substantially reduced. This effect is known as supercooling and may be simulated here by fixing the applied field at some value and calculating G as a function of the vortex position. The force a vortex would experience is the negative of the gradient of G , and thus the values of G , which we are able to calculate, will tell us at what field the vortices will be expelled from the slab. We find that the field must be reduced to about 0.250 before the vortices actually exit once they are in the slab, even though it is energetically favorable for them to exit at a field of 0.575. The surface barrier not only delays vortex entry but also delays its exit.

Figure 26 is a plot of G versus the vortex position for different field strengths. The periodicity is held at 5.6 and the field strengths are, from top to bottom on the graph, 0.250, 0.300, 0.400, 0.500, 0.650, 0.750, 0.850, and 0.932.

Such superheating and supercooling lead to hysteric effects, which have been well documented experimentally.¹⁸⁻²⁹ Fink and Presson⁹ give

Figure 26. Gibbs free energy G vs. vortex position for $\kappa=2.0$, $W=4.0$, and $P=5.6$. Curve a has $H=0.250$, curve b $H=0.300$, curve c $H=0.400$, curve d $H=0.500$, curve e $H=0.650$, curve f $H=0.750$, curve g $H=0.850$, and curve h $H=0.932$.

an analytic expression which approximates the superheating field of a semi-infinite slab as a function of kappa.

$$H_{sh}/H_c = \frac{\sqrt{5}}{3} (1 + 1/\sqrt{2\kappa}) \quad (42)$$

For a kappa of two this predicts a superheating field of 1.118 in units of H_c . In these units our superheating field is 1.318, which is a bit higher as expected, since our slab is finite with a thickness of 4.0. Joseph, Tomasch, and Fink²⁹ measured the superheating field of a film with a kappa of two and a thickness of 20.5 and found it to be 1.35. A thickness of 20.5 should probably exhibit bulk behavior so the agreement between theory and experiment is only fair.

The preceding set of solutions showing the vortex nucleation sequence indicates that when the zero of f is near the surface there is a large near-normal core formed. As the vortex moves to the center of the slab this large core shrinks, lowering G as a result of the savings in condensation energy. If we hold the zero of f near the surface and increase the periodicity we find that the size of this near-normal core grows, eventually becoming what Kramer⁷ has called the giant zero.

We found earlier that for $W=4$, $\kappa=2$, and $P=10$, the superheating field was 0.931. If, in this case, we locate the zero of f in the range $0.0 \leq x < 0.8$, and allow the computer program to iterate, we are never able to converge upon a solution. As iteration proceeds the size of the near-normal core grows, with $\bar{Q}$ getting very large in the region of

depressed f . Kramer called such a state the giant zero state. If the zero of f is located in the range $0.8 \leq x < 2.0$, we are able to easily converge upon solutions showing the usual nucleation sequence with the Gibbs free energy decreasing as the vortex moves to the middle of the slab.

Figures 27 and 28 show the solutions obtained when $W=4$, $\kappa=2$, $P=10$, $H=0.931$, and the vortices have reached the middle of the slab. Now the order parameter is modulated along the surface due to the interaction of vortices in the bulk with the surface screening currents. These figures should be compared with Figures 24 and 25 which show f and b when $W=4$, $\kappa=2$, $P=5.6$, $H=0.932$, and the vortices are along the middle of the slab. Both sets of figures show the solutions at the respective superheating fields, and the increased periodicity is seen to result in more vortex-surface interaction. When the vortices reach the middle of the slab, the periodicity will be effectively cut in half but we will always characterize a state by its entry periodicity.

Walton^{12,13} has interpreted the results of microwave surface impedance measurements as inferring the type of modulation seen in Figure 27. He suggested that the regions of low order parameter are depressed with a further increase in applied field and will serve as the nucleation sites for the next row of vortices to enter the slab.

Walton also predicted that, if vortices are in the bulk and the field is reduced, such modulation of f occurs prior to the exit of a row of vortices. This would be the result of the soon-to-exit row of vortices approaching the surface as the magnetic pressure is reduced

Figure 27. Magnitude of the reduced order parameter, f , for $W=4.0$, $\kappa=2.0$, $P=10.0$, and $H=0.931$, with the zero of f in the middle of the slab. This is viewed from the front of the slab with one period and half the slab width shown. On the right are contours of f with increments of 0.1.

Figure 28. Local flux density, b , for $W=4.0$, $\kappa=2.0$, $P=10.0$, and $H=0.931$, with the zero of f in the middle of the slab. This is viewed from the back of the slab with one period and half the slab width shown. On the right are contours of b with increments of 0.1.

and interacting with the surface screening currents. He labeled this modulation of the order parameter a nascent vortex and experimentally watched it appear prior to the entry and exit of vortices.

Although our work supports the nascent vortex concept just prior to vortex nucleation, we do not see nascent vortices prior to vortex exit. That is, as the field is reduced to the supercooling field with a row of vortices sitting along the middle of the slab, we never see such a modulation of f along the surface of the slab. We do not interpret the lack of a nascent vortex state prior to vortex exit as contradicting Walton's conclusions but rather attribute it to the fact that we are dealing with a simpler case. Walton's slabs were thick, allowing multiple rows of vortices in the bulk, while our slab is thin enough that only a single row is found in the middle. If a vortex lattice were in the bulk of the slab, it is conceivable that a reduction in the applied field would allow the lattice to expand, pushing the outer row of vortices closer to the surface and resulting in a nascent vortex.

Next we consider the solutions obtained by increasing the applied field above the superheating field with a row of vortices along the center of the slab. We find that the modulation of the order parameter along the surface becomes more pronounced, until some higher field is reached, at which point solutions cease to exist. We interpret the field at which solutions cease to exist as the critical entry field for the next row of vortices. At $W=4$, $\kappa=2$, $P=5.6$, with vortices sitting in the middle of the slab, we are able to get a solution at $H=1.240$

and are unable to converge upon a solution at $H=1.250$. If the periodicity is increased to 10 we are able to find a solution at $H=0.99$ but unable to converge upon a solution at $H=1.0$. The grid size for the $P=5.6$ and $P=10.0$ solutions are the same so there will be a greater density of data points in the $P=10.0$ solution and it is shown in Figures 29 and 30.

In Figure 29 we see that the modulation of the order parameter along the surface has been increased relative to what was shown in Figure 27. The flux density, shown in Figure 30, does not show any modulation along the surface because it is constrained to be equal to the applied field H at the surface.

At a period of 10 the supercooling field is found to be about 0.250, as was the case for a periodicity of 5.6. Figures 31 and 32 show the order parameter and flux density at the supercooling field. As was noted previously, the vortex is sitting in the middle of the slab and there is essentially no modulation in the order parameter along the surface. The flux density plot is striking because here the flux density in the regions of the vortex cores exceeds the applied field. The increments in the contour plots are again 0.1 and it is seen that the order parameter quickly rises to 0.9 as the distance from the vortex center increases.

Just as we determined $H_{c1}(\kappa=2, W=4, P=5.6) = 0.575$, we can find $H_{c1}(\kappa=2, W=4, P=10.0) = 0.550$. Increasing the periodicity lowers the field at which it is first energetically favorable for the slab to exist in the mixed state.

Figure 29. Magnitude of the reduced order parameter, f , for $W=4.0$, $\kappa=2.0$, $P=10.0$, and $H=0.99$, with the zero of f in the middle of the slab. This is viewed from the front of the slab with one period and half the slab width shown. On the right are contours of f with increments of 0.1.

Figure 30. Local flux density, b , for $W=4.0$, $\kappa=2.0$, $P=10.0$, and $H=0.99$, with the zero of f in the middle of the slab. This is viewed from the back of the slab with one period and half the slab width shown. On the right are contours of b with increments of 0.1.

Figure 31. Magnitude of the reduced order parameter, f , for $W=4.0$, $\kappa=2.0$, $P=10.0$, and $H=0.250$, with the zero of f in the middle of the slab. This is viewed from the front of the slab with one period and half the slab width shown. On the right are contours of f with increments of 0.1.

Figure 32. Local flux density, b , for $W=4.0$, $\kappa=2.0$, $P=10.0$, and $H=0.250$, with the zero of f in the middle of the slab. This is viewed from the back of the slab with one period and half the slab width shown. On the right are contours of b with increments of 0.1.

In the previous work the vortices have entered with some periodicity P , which was held fixed as the field was increased above the superheating field or decreased toward the supercooling field. Once the vortices reached the middle of the slab we never allowed the periodicity to vary in such a way as to minimize the Gibbs free energy. If we hold the field at 0.931, which is the superheating field for $W=4.0$, $\kappa=2.0$, and $P=10.0$, allow vortices to enter the bulk from the ends of the slab and then vary the periodicity until the lowest G is reached, we find that $P=3.6$ has the lowest Gibbs free energy. If $P=3.6$ and vortices are sitting along the middle of the slab, the effective periodicity is $3.6/2.0 = 1.8$. Thus, at a field of 0.931, if vortices somehow could enter through the ends of the slab, the vortices would like to be separated by about two penetration depths when they are in a single row along the middle of the slab. The applied field will force them together until their magnetic fields begin to overlap at which point an equilibrium is reached.

At $P=3.6$ we find $H_{c1}(\kappa=2, W=4, P=3.6) = 0.660$, well above the values found at the longer periods. At a given W and κ , decreasing P raises $H_{c1}(\kappa, W, P)$.

With a single row of vortices sitting in the middle of the slab at $P=3.6$, we find we are able to increase the field to $H=2.10$ and still converge upon a solution. If H is increased to 2.150, however, we are unable to converge upon a solution. At $P=10.0$ we were able to find solutions with a single row of vortices in the middle up to a field of

$H=0.99$ and at $P=5.6$ we found solutions up to $H=1.240$. At $P=10.0$ we found no solution at $H=1.0$ and at $P=5.6$ we found no solution at $H=1.250$. Decreasing the periodicity of the vortices allows us to find solutions at higher field values.

Although the nucleation of a vortex is a time-dependent and highly dissipative process, we have used here only the time-independent Ginzburg-Landau equations to obtain sets of solutions at various stages of the nucleation process. We anticipate that if a proper time-dependent theory were used, various details of the resulting solutions would be altered, but that essentially all the qualitative behavior discussed above would remain unchanged. We would expect in particular that our solutions would be found to increase in accuracy as the vortices approach their equilibrium or metastable equilibrium positions and the normal currents decay away. On the other hand, the giant zero, which occurs under certain conditions in the middle of the nucleation process where deviations from time-independent theory are expected to be greatest, may simply be an artifact resulting from the use of a time-independent theory and may not occur in a proper time-dependent treatment. No experiments performed to date, however, have been able to reveal fine details of the dynamical aspects of the nucleation process. Only essentially static quantities, such as the magnetic field at which vortex nucleation occurs, have been measured, but such static quantities should be given accurately by a time-independent theory.

CHAPTER 4. OUR WORK AT KAPPA=5.0

Sutton¹⁹ and Monceau, Saint-James, and Waysand²⁸ have done experimental work which may be directly compared with the previously presented theory. The most detailed work is that done by Sutton, since the other group was primarily concerned with tilted vortices, while Sutton concentrated on thin films with the field applied parallel to the face.

Before attempting to match Sutton's work with the Ginzburg-Landau theory, let us recall three things that were learned from the kappa=2.0 work. First, the superheating field was found to have a very weak dependence on the periodicity of the solutions. In fact all variations of the superheating field as a function of periodicity were well down in the noise level for the longer periodicities. At the very short periods the superheating field began to increase over the long period values. Second, we found that $H_{c1}(\kappa, W, P)$ had a stronger periodicity dependence, and third, we found that the field at which the second row of vortices would like to enter the slab had a very strong dependence on the periodicity.

Sutton characterized the degree of surface superconductivity by a quantity he called $\Delta I(H)$ where $\Delta I(H) = I_n - I_s(H)$. I_n is the tunneling current of the film under study when the film is in the normal state and $I_s(H)$ is the tunneling current at an applied field H when the film is in the superconducting state. Sutton devised a method for directly reading $\Delta I(H)$ rather than separately measuring I_n and $I_s(H)$ and then forming the difference. He fixed the bias across a given junction and

Figure 33. Sutton's results at four different film thicknesses. The bias across the junctions is held fixed at about half the zero field energy gap.

measured $\Delta I(H)$ as a function of H to find the results displayed in Figure 33. As H is increased and superconductivity is destroyed $\Delta I(H)$ approaches zero. Sutton found that the essential features of the $(\Delta I(H), H)$ curves are insensitive to the bias chosen if it is of the order of half the zero field energy gap. The junctions are Pb-In (20%wt). Sutton interpreted the dips in $\Delta I(H)$ as being due to the entry of vortices. It is apparent that at a given temperature the entry field for the first vortex increases as the slab width is decreased. Sutton also considered a film of thickness $650 \text{ \AA}$ and was able to increase the field up to about 6.5 kG without seeing any dips in $\Delta I(H)$, at which point superconductivity was destroyed. Apparently the very thin film never admitted quantized vortices before being driven normal.

Sutton suspected that the surface barrier was not effective in preventing the entry of flux in his films and that flux entered the films whenever it was energetically favorable for the vortices to exist in the bulk of the samples. He argued, "the surfaces of the films used in these experiments were sufficiently rough to prevent the surface barrier being effective in delaying fluxon entry. This view is further supported by the fact that the Pb-In film over one of the junctions had been very badly scored by fingerprints and yet its $(\Delta I(H), H)$ characteristic was identical with that of an adjacent unscored junction." He further suggested that the hysteresis in the data is due to a surface barrier to fluxon escape, stating "when H is accurately parallel to the film, surface barriers delay exit of fluxons in decreasing fields and flux may remain trapped when H is reduced to zero. The effect becomes less

pronounced as film thickness is reduced." We shall therefore calculate both the superheating field and $H_{c1}(\kappa, W, P)$ for the various film thicknesses, and it should not surprise us if Sutton's data does indicate that flux entry occurs at $H_{c1}(\kappa, W, P)$ for some appropriate value of P .

The first thing to do in trying to fit Sutton's data is to find the thickness of his films in Ginzburg-Landau reduced units. Using resistivity measurements, Sutton obtained kappa values for the material ranging from 4.4 to 5.4, and he used a value of 5.0 for the calculations which accompanied his experimental work. He then calculated the penetration depth by means of Equation 43.

$$\lambda^2 = \frac{\phi_0 \ln \sqrt{2\kappa}}{4\pi H_{c1}} \quad (\text{cgs units}) \quad (43)$$

Sutton found H_{c1} to be 170 G at a temperature of 4.2 K and he notes that Livingston³⁰ had previously found it to be 160 G for bulk alloys of the same composition. Using Sutton's value in Equation 43 gives a penetration depth of 1376 Å, while using Livingston's value gives 1419 Å.

An alternate way to calculate the penetration depth is to use Equation 44. This equation is in cgs units except for the quantity denoted by the prime which is in Ginzburg-Landau reduced units.

$$H_{c1} = \sqrt{2} H_c H'_{c1} = \frac{\kappa \phi_0}{2\pi \lambda^2} H'_{c1} \quad (\text{cgs units}) \quad (44)$$

Neumann and Tewordt¹⁴ have evaluated H'_{c1} for integral values of kappa by integrating the Ginzburg-Landau equations, and at a kappa of 5.0

they found it to be given by 0.224. It is interesting to note that an analytic expression has been found by Clem³¹ which predicts 0.228.

Solving for λ in Equation 44, using Newmann and Tewordt's value for H'_{c1} , and taking H_{c1} to be 170 G as found by Sutton, we obtain a penetration depth of 1472 Å. If we use Livingston's value of $H_{c1} = 160$ G, we find a penetration depth of 1518 Å. A third and final way to evaluate the penetration depth is to use Equation 45 to determine the coherence length and Equation 46 to then determine the penetration depth.

$$H_{c2} = \frac{\phi_0}{2\pi\xi^2} \quad (\text{cgs units}) \quad (45)$$

$$\lambda = \kappa\xi \quad (\text{cgs units}) \quad (46)$$

Sutton states that at 4.2 K H_{c2} was found to be 3.7 kG for bulk material and H_{c2} of the films was found to vary from 3.4 kG to 3.9 kG. Sutton determined H_{c2} applying a field perpendicular to the films and increasing the field until the current profile ΔI was reduced to zero. He noted that there appeared to be no correlation between the film thickness and the variations in H_{c2} as determined by this method and he attributed the different values of H_{c2} to variations in the In content of the films. If H_{c2} is taken as 3.9 kG, we find a penetration depth of 1450 Å, an H_{c2} of 3.7 kG gives 1490 Å, and an H_{c2} of 3.4 kG gives 1555 Å.

The point we are trying to make is that, depending on how we calculate the penetration depth, we get different values. In addition to

this, Sutton estimated that the film thicknesses were known only to $\pm 150 \text{ \AA}$, having been determined by a Michelson-type interferometer.

We use the final method to determine the penetration depth and take it to be $1490 \text{ \AA}$. The three film thicknesses we will consider are $650 \text{ \AA}$, $1870 \text{ \AA}$, and $3045 \text{ \AA}$, which in reduced units are 0.436, 1.255, and 2.044. We want to measure the field strengths in Ginzburg-Landau units also, and this requires a knowledge of the value of H_c . Using Equation 47, we take H_{c2} to be 3.7 kG to find an H_c of 523 G. This value of H_{c2} is the one corresponding to the chosen value of the penetration depth.

$$H_{c2} = \sqrt{2} \kappa H_c \quad (\text{cgs units}) \quad (47)$$

We first integrate the one-dimensional Ginzburg-Landau equations on a very small grid to obtain very accurate solutions for the film of thickness 2.044 ($3045 \text{ \AA}$). At small fields the two-dimensional equations should reduce to the one-dimensional ones, and this will give us a check on the work. We then choose a grid of 0.1022 and integrate the two-dimensional equations. This grid size is determined by the slab width and the number of grid points we wish to have across the slab. The periodicities in the y direction are then integral multiples of this grid size. There is nothing fundamental about the odd periodicity lengths used; they are just convenient lengths for this grid size.

We then increase the field and depress the order parameter while solving the two-dimensional equations to find that two-dimensional

variations arise when the order parameter has been depressed to 0.50 in the film of thickness 2.044. Recall that at a kappa of 2.0 two-dimensional variations also arose when the order parameter had been depressed to 0.50. To find the superheating field, we hold the order parameter at the origin to 0.50 and vary the periodicity. At a period of 1.226 we find a field of 1.267, at a period of 2.861 a field of 1.240, and at a period of 3.883 a field of 1.250. It appears that a preferred periodicity of the order of 2.861 may exist, but the range of fields lies in the noise range, and on a grid of this size we cannot unambiguously determine whether a particular value is preferred by looking at these results. It is clear, however, that Sutton saw flux enter the film at a much lower field (0.654 in reduced units) than these superheating fields. If we move the zero of the order parameter into the bulk of the film and watch the behavior of the various contributions to the free energy as the vortex moves to the center of the film, we again see that the Gibbs free energy decreases continuously and that the contribution coming from the $\langle \frac{1}{2}(1-f^2)^2 \rangle$ term is reduced by over one half during the process. The shrinking of the vortex core size appears to play an important role in vortex nucleation regardless of the kappa value.

We next find $H_{c1}(\kappa=5, W=2.044, P=2.861)=0.70$ by exactly the same procedure that was followed in the $\kappa=2.0$ work. This value is somewhat higher than the reduced field of about 0.65, at which the first dip occurs in Sutton's data, shown in Figure 33. We know that increasing the periodicity will lower this value and so are led to consider a periodicity of 3.474. But while we are at a period of 2.861, we reduce

the field with a row of vortices in the middle to find the supercooling field. Since increasing the period will serve to lower the supercooling field, this value will be an upper limit to the supercooling field. We wish to work with as short a period as possible to reduce the number of grid points and conserve computer time. We find that vortices will stay in the bulk of the film until a reduced field of about 0.4 is reached. This is well below the field at which Sutton sees the vortices exiting from the film and we conclude that the surface barrier to vortex exit in his film is not reaching the theoretical limit of effectiveness. If his films had smooth surfaces they should show more hysteresis.

We next increase the periodicity to find $H_{c1}(\kappa=5, W=2.04, P=3.474)=0.650$ and $H_{c1}(\kappa=5, W=2.04, P=3.883)=0.650$. The G of the no-vortex state is -0.330 and that of the state with the vortex sitting in the middle of the film is -0.330 . We give two values of $H_{c1}(\kappa, W, P)$ to show that a range of periods may be used to match Sutton's first dip. The position of the first dip may exclude some of the shorter periodicities but it admits a whole range of the longer periodicities. At a field of 0.650 the no vortex state is one-dimensional in character with the order parameter at the surface assuming the value of 0.906. With a vortex admitted and the field held constant, the order parameter at the surface rises to an average value of 0.981 for a periodicity of 3.474. This is the origin of the dips observed by Sutton. Admission of flux allows the average value of the order parameter at the surface to rise substantially with a concurrent decrease in the tunnelling current and an increase in the current profile ΔI .

If at a periodicity of 3.883 the field is increased to 1.65, we find we get a solution which shows considerable modulation of the order parameter along the surface with the order parameter at the surface varying from 0.16 up to 0.74. This solution is displayed in Figure 34. Sutton observes a second dip at a reduced field of about 1.62. It is possible that a state with two rows of vortices in the film would have a lower G than one in which the order parameter along the surface has such severe modulation and there is only a single row of vortices in the film. At the field corresponding to this change of internal structure there would probably be a discontinuous change in the value of the order parameter along the surface similar to that which occurs when a vortex nucleates, and this would cause the second dip in Sutton's data. In this work we do not concern ourselves with the second and subsequent dips in the current profiles. Figure 34 is shown because it shows the type of solutions found when the field is increased above the superheating field with a row of vortices along the middle of the slab.

For the film of thickness 1.255 (1870 Å) we integrate the one-dimensional equations on a grid of size 0.0196 obtaining very accurate solutions and then integrate the two-dimensional equations on a grid of 0.0896. When the two-dimensional equations converge to one-dimensional solutions, it is found that the field values differ by as much as 0.05 from those of the more accurate one-dimensional solutions at the same value of the surface order parameter. This discrepancy is larger than is found at a thickness of 2.044, implying that the thinner films require a finer grid to maintain accuracy. We find that the solutions for this thinner film remain one-dimensional in character until

Figure 34. Magnitude of the reduced order parameter, f , for $W=2.044$, $\kappa=5.0$, $P=3.883$, and $H=1.65$, with the zero of f in the middle of the slab. This is viewed from the front of the slab with one period and half the slab width shown. On the right are contours of f with increments of 0.1.

the order parameter at the surface is depressed to at least 0.40. This occurs at a field greater than 2.0 in Ginzburg-Landau units. We did not investigate higher fields, since it was clear that this was well above the field at which Sutton saw vortex entry. Thus there was evidently no surface barrier effect in this thinner film either.

At a field of 1.447 we find the G of the no-vortex state in the film of thickness 1.255 (1870 Å) to be -1.184 and that of the one-row vortex state to be -1.199. Since in the vortex state the entry periodicity of the vortices was 3.585 and the vortices were sitting in the middle of the film, we have $H_{c1}(\kappa=5, W=1.255, P=3.585) \approx 1.447$. Keep in mind that when the vortices are sitting in the middle of the film the effective periodicity is one half the entry periodicity. As we mentioned in the preceeding work, we do not mean to imply that the vortices must have entered the film with just this periodicity, since a whole range of periodicities will give the same entry field to the accuracy of this work. On the other hand, we do mean to imply that the periodicity was of this order or larger, since increasing the periodicity above about 3.5 has little effect on the value of $H_{c1}(\kappa, W, P)$.

Now let us consider the film of reduced thickness 0.436 (650 Å). Sutton's data, not shown here, indicates that no vortices entered the film, even when the field was sufficiently high to destroy superconductivity. In these reduced units a coherence length is equal to $1/\kappa = .20$ so a vortex diameter is equal to .40 for these films. Thus one might expect that it would not be energetically favorable for such a film to go into the vortex state.

We begin by integrating the one-dimensional Ginzburg-Landau equations on a grid of size 0.0136 to obtain accurate solutions. We then integrate the two-dimensional equations on a grid of 0.0430. Upon integrating the two-dimensional equations, we observe several things. First two-dimensional variations never develop at fields up to 8.5, at which point the order parameter at the surface has been depressed to 0.10. Secondly we note that pulling the order parameter down at the surface by an applied field also pulls it down radically completely across the film. For example when the order parameter at the surface is equal to 0.90, it is only able to rise to 0.93 in the middle of the film. When the order parameter at the surface is equal to 0.10, it rises to 0.13 in the middle of the film. The reason for this is that the order parameter varies on a scale of the coherence length and for such a thin film there is simply not enough room for the order parameter to recover from being pulled down at the surface. It is common in theoretical calculations on thin films to assume that the order parameter is constant across the film, and this approximation is seen to be reasonable for a film as thick as two coherence lengths. We have the situation of the order parameter being not only constant along the y axis but also reasonably constant along the x axis.

It is also revealing to look at the various energy contributions as the field is applied. In these units the upper critical field for very thick films occurs at a field equal to κ which is 5.0 here. We then set the field at 4.95 and integrate the two-dimensional equations to find a one-dimensional state with the order parameter along

the surface equal to 0.775. We find $F=5.308$, $G=-5.273$, $\langle \frac{1}{2}(1-f^2)^2 \rangle = 0.013$, $\langle (\nabla f/\kappa)^2 \rangle = 0.0009$, $\langle Q^2 f^2 \rangle = 0.051$, and $\langle b^2 \rangle = 5.243$. Practically all the energy is contained in the magnetic field. This concentration of the free energy in the magnetic field was found to occur at all field strengths investigated. We should say a word about the accuracy of these two-dimensional solutions. Fixing the value of the order parameter at the surface and integrating the one-dimensional equations often led to a corresponding field value that differed by as much as 0.20 from the field value obtained by integrating the two-dimensional equations, even though the grid for the two-dimensional equations was 0.0436, about a fifth of a coherence length. Clearly very small grids are required to obtain good accuracy in these thin films. We didn't go to smaller grids because the point of considering the two-dimensional equations was to see if two-dimensional variations did ever develop and admit fluxoids to the interior. We then generated an accurate record of order parameter versus applied field by integrating the less time-consuming one-dimensional equations when it became apparent that two-dimensional variations never developed. Figure 35 shows the result of integrating the one-dimensional equations. The field has been converted to kG to allow a more meaningful comparison with Sutton's data. The striking feature of this plot of order parameter at the surface versus the applied field is the similar appearance of Sutton's plot of ΔI versus the applied field. The two appear to be almost proportional

Figure 35. Order parameter at the surface vs. the applied field. Only one-dimensional spatial variations arise in this thin film situation. $\kappa=5.0$ and $W=0.436$ (650 Å).

to each other, although the relation between the order parameter, the resulting density of states and the tunneling current is actually more complicated.

Although the thin film never spontaneously goes into the vortex state, it is possible to hold the order parameter to zero at isolated points in the middle of the film and integrate the Ginzburg-Landau equations to obtain a solution with vortices sitting in the middle of the film. At an applied field of 4.95 such a solution with an entry periodicity of 2.616 is found to have $F=5.383$ and $G=-5.256$. The vortex state has a higher G than the previously reported no-vortex state at the same field strength. Although the Ginzburg-Landau equations do admit vortex solutions in the thin film, they are not energetically favored and the film does not enter such states. The appearance of this vortex state differs greatly from that of the previously reported vortex states because the core of the vortex is found to encompass the surface of the film. If the entry periodicity is denoted by P , then the zeroes of the order parameter will occur at $x=W/2, y=0, P/2, 3P/2, \dots$. In the previously reported vortex solutions, which showed a modulation of the order parameter along the surface, the regions of high order parameter would be found at $x=0, y=0, P/2, P, 3P/2, \dots$ and the regions of low order parameter would be found at $x=0, y=P/4, 3P/4, 5P/4, \dots$ due to the interaction of the vortex supercurrent and the Meissner screening current. In the vortex state in this very thin film the exact opposite is observed with regions of high order parameter being found at $x=0, y=P/4, 3P/4, 5P/4, \dots$ and the regions of low order parameter at $x=0,$

$y=0, P/2, P, 3P/2, \dots$ This is because the film is too thin to completely contain the vortex, and the near-normal regions in the vicinity of the vortex core penetrate clear to the surface.

Finally we should report on the related work done by E. Guyon, F. Meunier, and R. S. Thompson.³² They measured tunnelling currents in films of InBi and associated anomalies in the tunnelling characteristics with the entry of vortices into the films. They went on to note that the field at which the first anomaly occurred could be "associated with the change in the solution of the linearized Ginzburg-Landau equation from a one-dimensional and symmetric one to a two-dimensional solution peaked near a boundary (or equivalently to the creation of vortices in the film)." This group further noted that quantized flux did not enter films which were less than about two coherence lengths thick.

CHAPTER 5. MODELING VORTEX NUCLEATION

The previous work has all been based upon an exact numerical integration of the two-dimensional Ginzburg-Landau equations done by replacing the differential equations with difference equations and then using a Newton-Relaxation technique to solve the difference equations. This is conceptually simple, but the necessary computer programs typically require on the order of 2,000 statements and a rather fast computer if they are to execute in a reasonable amount of time. The information presented in the previous chapters has required about 125 hours of computer time on an IBM 360-65 which is no trivial amount.

In this chapter we use the Clem model³¹ of an isolated vortex to model vortex nucleation. This is the analogue of the Bean-Livingston calculation¹⁷ which used the well-known London model³³ of an isolated vortex to estimate surface barrier effects in one of the first works done on superheating. The London model suffers from an unphysical divergence of the supercurrent on the vortex axis, while with the Clem model the supercurrent goes to zero on the vortex axis as it is known to do. This becomes important when a vortex is close to a surface, because the boundary conditions require the presence of an image across the surface from the vortex, and if the supercurrent diverges on the vortex axis this will predict that the force of attraction between vortex and image will become infinite as they approach each other. Thus the London model breaks down in the region of most interest in this calcula-

tion, while the Clem model remains well behaved. Far from the vortex axis the two models converge to the same limits.

The Clem model assumes that the spatial variation of the order parameter of an isolated vortex is given by Equation 48.

$$f(\rho) = \frac{\rho}{\sqrt{\rho^2 + \xi_v^2}} \quad (48)$$

ρ is the usual radial coordinate in polar coordinates and ξ_v is a variational parameter that is chosen to minimize the Helmholtz free energy of the isolated vortex.

If Equation 48 is inserted into the second Ginzburg-Landau equation and the resulting equation is solved, one obtains the following expression for the flux density,

$$b(\rho) = \frac{\phi_0}{2\pi\lambda\xi_v} \frac{K_0(R/\lambda)}{K_1(R/\lambda)} \quad (\text{cgs units}), \quad (49)$$

$$R = \sqrt{\rho^2 + \xi_v^2} \quad (\text{cgs units}). \quad (50)$$

$K_n(\rho)$ is the modified Bessel function of order n . Using Maxwell's equation, one obtains a supercurrent density given by

$$j(\rho) = \frac{c}{4\pi} |\vec{\nabla} \times \vec{b}| = \frac{c\phi_0}{8\pi\lambda^2\xi_v} \frac{\rho}{R} \frac{K_1(R/\lambda)}{K_1(\xi_v/\lambda)} \quad (\text{cgs units}). \quad (51)$$

Using these quantities to calculate the Helmholtz free energy per unit length of an isolated vortex and then minimizing this energy with respect to ξ_v , one obtains Equation 52 which gives ξ_v as a function of κ .

$$\kappa = \frac{\sqrt{2}}{\xi_v/\lambda} \left[1 - \frac{\kappa_0^2(\xi_v/\lambda)}{\kappa_1^2(\xi_v/\lambda)} \right]^{\frac{1}{2}} \quad (\text{cgs units}) \quad (52)$$

For a kappa of 2.0 this equation has the solution $\xi_v/\lambda = 0.573$ and if kappa is increased up to, say, 10.0 we find $\xi_v/\lambda = 0.135$.

As discussed previously, the last two terms in the Ginzburg-Landau free energy functional make up the electromagnetic interaction. It may be shown that these two terms together predict that the force per unit length on a vortex in a current distribution is given by³³

$$\vec{F} = \vec{j} \times \vec{\Phi}_0 / c \quad (\text{cgs units}). \quad (53)$$

$\vec{j}$ is the current density per unit length at the vortex core, $\vec{\Phi}_0$ is a vector along the vortex axis with magnitude equal to the flux quantum and c is the speed of light.

As we saw in the earlier Ginzburg-Landau work, it is necessary to consider rows of vortices moving into and out of the slab. To calculate the electromagnetic interaction between rows of vortices, we need to know the current density of the complete row as a function of position. We assume that the vortices have a spacing d along the y direction and that they extend to $\pm\infty$. This will be a two-dimensional calculation with

only x and y dependence, just as in the Ginzburg-Landau work. Since the vortex lattice in the bulk of a superconductor is known to be triangular,³⁴ we need to calculate the force only at the positions $y=md$ and $y=(2m+1)d/2$, where m is an integer, with x ranging from 0 to ∞ . Using straightforward vector addition to find the total current density per unit length and Equation 53 to then find the force per unit length, one finds that the force a vortex would experience due to an entire row of vortices is given by

$$F_x(x, md) = \frac{\phi_0^2}{8\pi^2 \lambda^2 \xi_V} \frac{1}{K_1(\xi_V/\lambda)} \left\{ \frac{x}{\sqrt{x^2 + \xi_V^2}} K_1\left(\frac{\sqrt{x^2 + \xi_V^2}}{\lambda}\right) + \sum_{n=1}^{\infty} \left(\frac{2x}{\sqrt{x^2 + (nd)^2}} \right) \frac{\sqrt{x^2 + (nd)^2}}{\sqrt{x^2 + (nd)^2 + \xi_V^2}} K_1\left(\frac{\sqrt{x^2 + (nd)^2 + \xi_V^2}}{\lambda}\right) \right\} \text{(cgs units)}, \quad (54)$$

$$F_x\left(x, \frac{2m+1}{2}d\right) = \frac{\phi_0^2}{8\pi^2 \lambda^2 \xi_V} \frac{1}{K_1(\xi_V/\lambda)} \sum_{n=0}^{\infty} \left\{ \left(\frac{2x}{\sqrt{\frac{(2n+1)^2 d^2}{4} + x^2}} \right) \frac{\sqrt{\frac{(2n+1)^2 d^2}{4} + x^2}}{\sqrt{\frac{(2n+1)^2 d^2}{4} + x^2 + \xi_V^2}} K_1\left(\frac{\sqrt{\frac{(2n+1)^2 d^2}{4} + x^2 + \xi_V^2}}{\lambda}\right) \right\} \text{(cgs units)}. \quad (55)$$

The force has only an x component denoted by the subscript x .

There is another more elegant way of calculating this same force using a Fourier series approach. Since the field of the row of vortices has the property $b(x, y) = b(x, y + md)$, a Fourier series expansion is appropriate, and we are led to write Equation 56.

$$\begin{aligned}
 \vec{b}(x, y) &= \frac{\phi_0}{2\pi\lambda\xi_V} \frac{1}{K_1(\xi_V/\lambda)} \sum_{n=-\infty}^{\infty} K_0 \left(\frac{\sqrt{x^2 + (y-nd)^2 + \xi_V^2}}{\lambda} \right) \\
 &= \sum_{k=-\infty}^{\infty} A_k e^{ik\frac{2\pi}{d}y} \quad (\text{cgs units}) \quad (56)
 \end{aligned}$$

A_k is the Fourier coefficient and is evaluated in Equation 57.

$$\begin{aligned}
 A_k &= \frac{1}{d} \frac{\phi_0}{2\pi\lambda\xi_V} \frac{1}{K_1(\xi_V/\lambda)} \int_0^d e^{-ik\frac{2\pi}{d}y} \sum_{n=-\infty}^{\infty} \left\{ K_0 \left(\frac{\sqrt{x^2 + (y-nd)^2 + \xi_V^2}}{\lambda} \right) \right\} dy = \\
 &= \frac{1}{d} \frac{\phi_0}{2\pi\lambda\xi_V} \frac{1}{K_1(\xi_V/\lambda)} \sum_{n=-\infty}^{\infty} \int_0^d e^{-ik\frac{2\pi}{d}y} \left\{ K_0 \left(\frac{\sqrt{x^2 + (y-nd)^2 + \xi_V^2}}{\lambda} \right) \right\} dy \quad (\text{cgs units}) \quad (57)
 \end{aligned}$$

Let $Y=y-nd$ to get

$$A_k = \frac{1}{d} \frac{\phi_0}{2\pi\lambda\xi_V} \frac{1}{K_1(\xi_V/\lambda)} \int_{-\infty}^{\infty} e^{-ik\frac{2\pi}{d}Y} K_0 \left(\frac{\sqrt{x^2 + Y^2 + \xi_V^2}}{\lambda} \right) dY \quad (\text{cgs units}) \quad (58)$$

Now use $K_0(z) = K_0(-z)$ to get

$$\begin{aligned}
 A_k &= \frac{1}{d} \frac{\phi_0}{2\pi\lambda\xi_V} \frac{1}{K_1(\xi_V/\lambda)} \int_{-\infty}^{\infty} \cos(2\pi\frac{k}{d}Y) K_0 \left(\frac{\sqrt{x^2 + Y^2 + \xi_V^2}}{\lambda} \right) dY \\
 &= \frac{1}{d} \frac{\phi_0}{2\pi\lambda\xi_V} \frac{1}{K_1(\xi_V/\lambda)} \frac{1}{\sqrt{\frac{1}{\lambda^2} + (\frac{2\pi k}{d})^2}} \exp \left\{ -\sqrt{x^2 + \xi_V^2} \sqrt{\frac{1}{\lambda^2} + (\frac{2\pi k}{d})^2} \right\} \quad (\text{cgs units}) \quad (59)
 \end{aligned}$$

And so the flux density may be written as in Equation 60 where

$$\xi_V' = \xi_V/\lambda, \quad x' = x/\lambda, \quad y' = y/\lambda, \quad \text{and } d' = d/\lambda.$$

$$\vec{b}(x,y) = \frac{\phi_o^2}{2\xi_V d K_1(\xi_V')} \left\{ \exp \left[-\sqrt{x'^2 + \xi_V'^2} \right] + \right. \quad (\text{cgs units}) \quad (60)$$

$$\left. + 2 \sum_{k=1}^{\infty} \frac{\exp \left[-\sqrt{1 + \left(\frac{2\pi k}{d'} \right)^2} \sqrt{x'^2 + \xi_V'^2} \right]}{\sqrt{1 + \left(\frac{2\pi k}{d'} \right)^2}} \cos \left(\frac{2\pi k}{d'} y' \right) \right\}$$

Then using Equation 53 and 61 we find the x component of the force per unit length to be given by Equation 62.

$$\vec{J} = \frac{c}{4\pi} \vec{\nabla} \times \vec{b} \quad (\text{cgs units}) \quad (61)$$

$$F_x = - \frac{\phi_o}{4\pi} \frac{\partial b}{\partial x} = \frac{\phi_o^2}{8\pi \xi_V d K_1(\xi_V')} \left\{ \frac{x' \exp \left[-\sqrt{x'^2 + \xi_V'^2} \right]}{\sqrt{x'^2 + \xi_V'^2}} + \right. \quad (\text{cgs units}) \quad (62)$$

$$\left. + 2 \sum_{k=1}^{\infty} \frac{x' \exp \left[-\sqrt{1 + \left(\frac{2\pi k}{d'} \right)^2} \sqrt{x'^2 + \xi_V'^2} \right]}{\sqrt{x'^2 + \xi_V'^2}} \cos \left(\frac{2\pi k}{d'} y' \right) \right\}$$

Looking at Equation 51 we see a natural unit in which to measure current densities per unit length in this approach is given by Equation 63.

$$\frac{c\phi_o}{8\pi^2 \lambda^2 \xi} = \frac{c\phi_o \kappa}{8\pi^2 \lambda^3} \quad (\text{cgs units}) \quad (63)$$

ξ is the Ginzburg-Landau coherence length and this choice then implies that the force per unit length is measured in the units given in Equation 64.

$$\left(\frac{c\phi_0\kappa}{8\pi^2\lambda^3} \right) \left(\frac{\phi_0}{c} \right) = \frac{\phi_0^2\kappa}{8\pi^2\lambda^3} \quad (\text{cgs units}) \quad (64)$$

Unfortunately this choice of reduced units does not turn out to be the same as the Ginzburg-Landau reduced units. If we call this choice of units the electromagnetic units (since we are allowing only for the electromagnetic interaction) and let F'_{em} denote the reduced force per unit length in electromagnetic units and F'_{GL} the reduced force per unit length in Ginzburg-Landau units, it is easily shown that the two sets of units are related by

$$F'_{GL} = \frac{4\pi}{\kappa} F'_{em} \quad (65)$$

All our modeling work will be done in these so-called electromagnetic units. This will not present the handicap that one might at first fear and it will still be possible to measure fields in Ginzburg-Landau units.

Now we are able to evaluate the force on a vortex due to a whole row of vortices by either direct vector addition or by the Fourier series expression. The sums are done by computer and it is found that in most cases it requires less time to sum the Fourier series expression since it involves simple exponentials while the vector addition expression requires evaluation of the modified Bessel functions. For some values

of x and d , though, it is faster to use the vector addition expression, and we have written our programs in such a way as to always use the most efficient method of calculating the force.

Since we are dealing with a slab of finite width, there will be required an infinite number of both positive and negative images to satisfy the boundary condition that no current flow through the surface. If a vortex is placed at x_0 the positive images must be placed at

$$x_0 + 2W, x_0 + 4W, x_0 + 6W, \dots$$

$$x_0 - 2W, x_0 - 4W, x_0 - 6W, \dots$$

and the negative images must be placed at

$$-x_0 + 2W, -x_0 + 4W, -x_0 + 6W, \dots$$

$$-x_0, -x_0 - 2W, -x_0 - 4W, -x_0 - 6W, \dots^{13}$$

Since the effect of the positive images of a given vortex cancel at the core of that vortex but not at other positions in the slab, they must be included in the calculation. The total force per unit length from a row of vortices in a slab is then the sum of the force from the actual vortices and the force from all the images and may be calculated by simply superimposing the contributions of each and using Equations 54 and 55 or Equation 62, whichever is the more efficient. We are now able to evaluate the two functions $FI(x, y, x_0)$ and $FIV(x, y, x_0)$. $FI(x, y, x_0)$ gives the electromagnetic force per unit length measured in electromagnetic units at the point (x, y) due to only the images of a row of vortices located in the slab at x_0 . $FIV(x, y, x_0)$ gives the electromagnetic force per unit length measured in electromagnetic units at the

point (x,y) due to a row of vortices located in the slab at x_0 and its images. Both expressions are implicit functions of the vortex spacing d , the slab width W and κ .

In a slab of width W in an applied field H the London theory predicts the magnetic field penetrates the slab as given by Equation 66.³⁶

$$b(x) = (H) \cosh\left(\frac{x}{\lambda} - \frac{w}{2\lambda}\right) / \cosh(w/2\lambda) \quad (\text{cgs units}) \quad (66)$$

This field results in a Meissner screening current given by

$$\vec{j} = \frac{c}{4\pi} \vec{\nabla} \times \vec{b} = - \frac{cH}{4\pi\lambda} \frac{\sinh\left(\frac{x}{\lambda} - \frac{w}{2\lambda}\right)}{\cosh(w/2\lambda)} \hat{y} \quad (\text{cgs units}) \quad (67)$$

Measuring the magnetic field in Ginzburg-Landau units and using Equation 53, one finds that the Meissner force per unit length in electromagnetic units is given by

$$- H \frac{\sinh(x-w/2)}{\cosh(w/2)} \quad (68)$$

The geometry is as shown in Figure 4. Now we are able to make contact with the Ginzburg-Landau work done earlier, for we see that, if one row of vortices is entering the slab from the left and another from the right in the staggered configuration, the electromagnetic force per unit length on the vortices entering from the left is given by

$$F'_{em}(x) = - \frac{H \sinh(x-w/2)}{\cosh(w/2)} + F_I(x,0,x) + F_{IV}(x,P/2,w-x) . \quad (69)$$

$P/2$ is the periodicity of the entering vortices in units of the penetration depth. The term $F_I(x,0,x)$ is the force on the row entering from the left by its own images and the term $F_{IV}(x,P/2,w-x)$ is the force from the row of vortices entering on the right and all its images. Setting Equation 69 equal to zero and solving for H , one obtains the field necessary to maintain one row of vortices at x and another at $w-x$.

In the Clem model (as in an exact Ginzburg-Landau solution) the supercurrent actually increases initially with distance from the vortex core. The peak occurs at about a coherence length and at this separation the vortex-image attraction will be greatest. Thus if a vortex and its image were held apart by an applied field, the field necessary to hold them about a coherence length apart would be the greatest field. Then if we set Equation 69 equal to zero and solve for H and then plot this as a function of x for some given value of κ and P a peak will occur at an x of about one half of a coherence length. This peak value of H will be the superheating field necessary to push the zero of the order parameter over the entry barrier caused by the vortex-image attraction.

Setting $w=4.0$, $P=5.6$, and $\kappa=2.0$ we find the superheating field to be 0.534 in Ginzburg-Landau units with this peak value of the field occurring at $x=0.30$. An x of 0.30 means that the vortex-image separation is 0.60, about a coherence length in these units. This superheating

field of 0.534 is well below the value of 0.932 found by integrating the Ginzburg-Landau equations, but it required only a few seconds of computer time and a relatively simply computer program. If we maintain the slab width to be 4.0 but let P go to infinity, the superheating field is lowered to 0.527. Recall that in the Ginzburg-Landau theory increasing the period also lowered the superheating field. This lowered superheating field is attributed to the decreased effectiveness of the images in attracting the entering vortices. The images are spaced further apart and the force of attraction is then less. Letting both P and W go to infinity the superheating field is further lowered to 0.501. This would be the superheating field for an isolated vortex in a bulk specimen.

CHAPTER 6. MODELING VORTEX DYNAMICS

We would like to use the model developed in the previous chapter to model the motion of vortices when a transport current is applied. Ideally one would like to integrate some sort of time-dependent Ginzburg-Landau equations, but such a procedure would be found to require more numerical work than was the case for the vortex nucleation work we did earlier. With the model developed in Chapter 5 we will be able to explain qualitatively many of the experimentally observed facts about flux flow.

At the simplest level we would like to apply a magnetic field and allow vortices to enter the slab freely and come to rest in an equilibrium lattice. We define the parameter $d_{\parallel}$ to be the distance between vortices in a given row; this distance is parallel to the surface of the slab. The parameter $d_{\perp}$ is the distance between rows of vortices and is perpendicular to the surface of the slab. At equilibrium the vortex lattice in the bulk of the slab is assumed to be an equilateral triangle³⁴ and this then forces $d_{\perp}$ and $d_{\parallel}$ to be related by

$$d_{\parallel} = 2d_{\perp}\sqrt{3} . \quad (70)$$

We next assume that the motion may be described by a viscous drag equation, so that, if $\vec{F}$ is the total electromagnetic force per unit length on a given vortex, the equation of motion of that vortex is given by

$$\vec{F} = \eta \vec{v} = \eta \frac{dx}{dt} \hat{x} \quad (\text{cgs units}) . \quad (71)$$

The force will have only an x component. η is the viscous drag coefficient and $\vec{v}$ is the velocity. We allow the various rows of vortices to move freely in the x direction and fix $d_{\parallel}$ to be the same for all rows of vortices. This fixed value of $d_{\parallel}$ is determined by Equation 70 and the value of $d_{\perp}$ for the rows of vortices in the middle of the slab. $d_{\perp}$ will have a different value depending upon where in the slab it is measured. We measure it in the middle and use this value to fix $d_{\parallel}$ for all the rows of vortices in the slab. Thus during the approach to equilibrium $d_{\perp}$ as measured in the middle of the slab will be constantly changing, resulting in a constantly changing value for $d_{\parallel}$, with $d_{\parallel}$ always of such a value as to create an equilateral triangular lattice in the middle of the slab.

Letting primes denote reduced quantities for the moment and inserting our electromagnetic reduced units, we obtain the equation of motion shown in Equation 72.

$$F' = \frac{8\pi^2 \lambda^3}{\phi_0^2 \kappa} \eta \frac{\lambda}{\tau} \frac{dx'}{dt'} \quad (72)$$

Time is measured in units of τ where $t' = t/\tau$. We then choose the unit of time as

$$\tau = \frac{8\pi^2 \lambda^4 \eta}{\phi_0^2 \kappa} . \quad (73)$$

We assume that the rows of vortices always enter the slab a complete row at a time and that they are not broken up during the motion. Then if there were three rows of vortices in the slab, the equations of motion in reduced units would be as given in Equations 74, 75, and 76.

$$\frac{dx_1}{dt} = - \frac{H \sinh(x_1 - w/2)}{\cosh(w/2)} + FI(x_1, 0, x_1) \quad (74)$$

$$+ FIV(x_1, d_{\parallel/2}, x_2) + FIV(x_1, 0, x_3)$$

$$\frac{dx_2}{dt} = - \frac{H \sinh(x_2 - w/2)}{\cosh(w/2)} + FI(x_2, 0, x_2) \quad (75)$$

$$+ FIV(x_2, d_{\parallel/2}, x_1) + FIV(x_2, d_{\parallel/2}, x_3)$$

$$\frac{dx_3}{dt} = - \frac{H \sinh(x_3 - w/2)}{\cosh(w/2)} + FI(x_3, 0, x_3) \quad (76)$$

$$+ FIV(x_3, d_{\parallel/2}, x_2) + FIV(x_3, 0, x_1)$$

During the motion we take $d_{\perp} = (x_1 - x_3)/2$. If there were four rows we would take $d_{\perp} = x_2 - x_3$. All three rows move independently and Equations 74, 75, and 76 must be integrated simultaneously. The integration is done by replacing dx/dt with $\Delta x/\Delta t$. A Δt of 0.1 is usually sufficiently small to give a smooth solution. If Δt is chosen too large, the vortices will overshoot their equilibrium position and will then bounce back and forth during the motion.

This method of integration is the crudest possible way to integrate the equations and the question of accuracy needs to be answered. This will be considered later when motion under the influence of a transport current is treated and it will be seen at that time that the accuracy is surprisingly good. If the applied field is fixed at a reduced strength of 0.50 for a slab of width 4 and a kappa of 10.0, the above method predicts that the equilibrium lattice will have four rows of vortices at 3.08, 2.02, 0.962, and 0.0188. We only allow newly entering vortices on the left of the slab because later when we apply a transport current it will be in such a direction as to nucleate vortices on this side.

We decide when to allow a new row of vortices to enter by constantly testing the force a new row of vortices would experience at the surface of the slab. If we test the force at $x=0$, the newly entering vortex feels no attraction for its closest image and the Meissner force is enough to indicate that it is favorable for another row of vortices to enter. The effect is to predict a double row of vortices sitting close to the surface. If the vortices in the bulk have periodicity P we would expect to find the newly entering vortices sitting at the surface with y coordinates of $P/2, 3P/2, 5P/2, \dots$ when the vortices in the bulk that are closest to the surface have y coordinates of $0., P, 2P, \dots$. Testing the force at $x=0$ predicts that the entering vortices would be found at $0., P/2, P, 3P/2, \dots$. Our Ginzburg-Landau work tells us that the extra row with y coordinates $0., P, 2P, \dots$ should not be there and that their presence is just a model anomaly. We would like to mimic the

Ginzburg-Landau results as much as possible and so seek a way to test for admission of new vortices which predicts only a single row of new vortices. It is found that, if we test the force a new vortex would experience at $x=1/\kappa$, a coherence length in these reduced units, and then admit the vortex from the surface of the slab when the force at $x=1/\kappa$ indicates it is favorable there, this procedure results in a single row of new vortices along the surface. We should note that there are no drastic changes in the results if a double row of vortices at the surface is allowed, since the close proximity of the images across the surface will nearly cancel any effects the vortices would have on other vortices in the bulk. Allowing only a single row of vortices along the surface reduces the number of interaction terms in the equations of motion and thus saves computer time while mimicking the Ginzburg-Landau results and so seems the favorable approach.

If a transport current is driven down the slab in the y direction, the London theory says that the spatial distribution of the current across the slab is

$$\vec{j} = \frac{JW}{2\lambda} \frac{\cosh(x/\lambda - w/2\lambda)}{\sinh(w/2\lambda)} \quad (\text{cgs units}). \quad (77)$$

J is related to the total transport current per unit length by

$$\int_0^w dx \frac{JW}{2\lambda} \frac{\cosh(x/\lambda - w/2\lambda)}{\sinh(w/2\lambda)} = JW \quad (\text{cgs units}). \quad (78)$$

In our reduced units this results in an additional force per unit length on the vortex given by

$$\frac{JW}{2} \frac{\cosh(x-w/2)}{\sinh(x/2)} \quad (79)$$

This additional force drives the vortices across the slab from left to right and such flux motion is the loss mechanism when the critical current of a superconductor is exceeded. At a given field there is some current density at which flux motion will begin to occur, and the superconductor is no longer able to carry the transport current without any losses. The higher the applied field the lower the current density at which flux motion begins to occur.

In these reduced units the reduced force is equal to the reduced velocity. As a given row of vortices travels across the slab, only the transport current should do any net work on the vortices. Thus the total work done on a given row in crossing the slab should always be the same and will be given by the integral across the slab of Equation 79, JW . For a given Δt we calculate a Δx at each position in the slab when we solve the equations of motion, so that for a given row of vortices we may also construct a graph of its velocity as a function of its position in the slab. We may then numerically integrate the area under this curve and it should be equal to JW . This gives us a numerical check on the accuracy of the work and it is typically found that we get agreement to within $\frac{1}{2}\%$.

We then model flux flow under the influence of a transport current in the following way. We fix the applied field and allow vortices to enter and come to rest in an equilibrium lattice configuration. During this part of the motion $d_{||}$ is determined as a function of $d_{\perp}$ and varies during the approach to equilibrium. When equilibrium is reached we fix $d_{||}$ at this equilibrium value and apply a transport current. During the resulting flux motion $d_{\perp}$ is allowed to vary freely. Quantities which will be of interest during the resulting motion are the average vortex velocity as it travels across the slab and the electric field along the slab resulting from the flux motion.

The average vortex velocity is taken as $\langle v \rangle = d_{\perp} \nu$ where ν is the rate at which vortices pass the middle of the slab and $d_{\perp}$ is the row separation of the vortices in the middle of the slab. ν is also the nucleation rate of vortices at the surface of the slab. The electric field along the slab may be obtained from the Josephson relation $2e\Delta V = \hbar \nu$.³⁷ Then the electric field is

$$E = \frac{\Delta V}{d_{||}} = \frac{\hbar}{2e} \frac{\nu}{d_{||}} = \frac{\phi_0}{c} \frac{\nu}{d_{||}} = \frac{\phi_0}{c} \frac{\langle v \rangle}{d_{\perp} d_{||}} \quad (\text{cgs units}). \quad (80)$$

If everything except E is measured in reduced units, this may be written as

$$E = \frac{\phi_0}{c} \frac{1}{\tau \lambda} \frac{\langle v \rangle'}{d_{\perp} d_{||}} \quad (81)$$

Primes denote reduced units and will be deleted in the future with the understanding that we are in reduced units. The natural choice of units for E is seen to be $\phi_0/c\tau\lambda$, and so in reduced units we have

$$E = \langle v \rangle / d_{\perp} d_{\parallel} . \quad (82)$$

At a given applied field $d_{\parallel}$ will remain the same for all transport current densities, while $\langle v \rangle$ and $d_{\perp}$ will be functions of the current density.

Now let us look at the results of this approach. Figure 36 is a plot of the vortex trajectories as they move under the influence of a current density of $J=0.05$ at a reduced field strength of $H=0.50$. The plot shows one period of motion after the steady state flux flow has been reached. Figure 37 shows the resulting velocity graph. On the velocity graph we have labeled entry and exit peaks. The entry peak occurs when the newly entering vortices break away from the images just across the surface and shoot rapidly into the bulk for a short distance. This rapid entrance causes the vortices in the bulk to shift over to accommodate the new row and shows up on the velocity graph as a sympathetic response to the entry peak. Note that the size of the sympathetic response depends upon how close to the entering row the responding vortices are. The more distant vortices response more weakly. The exit peak occurs when the exiting vortices begin to interact strongly with their images across the surface. When they are separated by about a coherence length the force of attraction is the greatest and they are

Figure 36. Vortex position as a function of time. There are four rows of vortices in the slab and one period of steady state motion is shown. $\text{Kappa}=10.0$, $W=4.0$, $J=0.05$, and $H=0.50$.

pulled rapidly out of the slab. When they get closer than about a coherence length the force of attraction dies out and only the transport current is effective in forcing them out of the slab. As shown in the trajectory plot the exiting vortices may sit for a long period of time very close to the surface before the transport current succeeds in pushing them out. The higher the current density the sooner the exiting vortices will be pushed out. This exit peak also produces a sympathetic response from the vortices in the bulk and as with the entry peak the amount of response depends upon how close the responding vortices are to the exiting vortices.

The velocity plot also shows something we have called a model anomaly. Recall that we allow vortices to enter when it is favorable at a distance of $1/\kappa$ from the surface but we introduce the vortices at the surface. When the force is favorable at $1/\kappa$ from the surface it is much more than favorable right at the surface where the image attraction is zero and so the vortices quickly shoot into the slab for a distance of about $1/\kappa$ at which point the image attraction slows them down. This model anomaly is the penalty for devising a model in which there is only a single row of surface vortices. In the velocity plot we have suppressed the full height of the anomaly peak since it turns out to be large enough to cause the other details to be suppressed when it is plotted on the same graph. This suppression of the anomaly peak is why the velocity plot does not extend up to the surface of the slab but rather begins at about 0.050.

The general features of all trajectories and velocity plots investigated were the same as the ones shown here. Numerical integration of the area under the curve shown in Figure 37 shows it to be 0.201 while $JW = 0.200$ for an error of $\frac{1}{2}\%$. This rather crude method of integrating the equations of motion is surprisingly good.

Experimentally one usually measures the voltage resulting from flux flow. The electric field is the voltage per unit length and may be easily calculated from this theory. Figure 38 is a plot of the average velocity and of the electric field as a function of the current density for the two field strengths 0.50 and 1.0. Increasing the field strength just shifts the velocity line with the slope remaining about the same while the electric field line is shifted and the slope is increased when the field is increased. This means that in a higher field less current can flow without losses and once losses begin they increase faster in the higher field. This behavior was first discussed in detail and given a phenomenological interpretation by Kim, Hempstead, and Strnad^{38,39,40} and is by now well known experimentally. An up-to-date review of the subject of vortex motion and the resulting resistivity has been done by Gorkov and Kopnin.⁴¹ Schelten, Ullmaier and Lippmann⁴² used neutron diffraction measurements to determine various properties of the vortex motion and concluded that "the periodic arrangement of flux lines was found to persist up to transport currents 20 times larger than the critical current". We use this finding to justify our treating the motion as being due to whole rows of vortices

Figure 37. Vortex velocity as a function of position when steady state motion has been reached. $\text{Kappa}=10.0$, $W=4.0$, $J=0.05$, and $H=0.50$.

Figure 38. Average vortex velocity and the resulting electric field as a function of the transport current density for two different values of the applied field. $\kappa=10.0$ and $W=4.0$.

moving across the slab, rather than considering the electric field as arising from isolated vortices moving more or less independently of each other.

By using the Clem model of an isolated vortex and by considering only surface pinning (that is, the interaction of vortices with their surface images) we are able to obtain electric field versus current density characteristics which bear a good qualitative resemblance to those found experimentally in specimens for which bulk pinning does not dominate. At $H=0.50$, for example, we found that if we applied $J=0.03$ no vortices had entered or left the slab after a time of 150.0, while vortex motion still occurred at a $J=0.02$ when the field was increased to 1.0. This model thus has the property that the critical current at which vortex motion begins is lowered with an increased field strength, in qualitative agreement with experiment.

Of all solutions investigated, the least accurate occurred when $H=1.0$ and $J=0.07$. For this case the area under the velocity curve differed from JW by 0.71%. At this high current density the period of the flux motion was 11.6, the shortest period investigated, and thus it was not surprising to find this solution to be the least accurate. Better accuracy could be obtained by decreasing Δt in the solution of the equations of motion.

CHAPTER 7. SUMMARY

In the first four chapters of this work we have considered the Ginzburg-Landau theory of vortex nucleation. By numerically integrating the Ginzburg-Landau equations, we calculated $H_{c1}(\kappa, W, P)$ and the superheating and supercooling fields. Tunnelling current measurements then gave an experimental test of the theory. The numerical integration was done over a grid of finite size, thus limiting the accuracy of the solutions. This inaccuracy is particularly important in the evaluation of $H_{c1}(\kappa, W, P)$, which we know only to about 200 G. To evaluate $H_{c1}(\kappa, W, P)$ with more accuracy would require a smaller grid size. Unfortunately our computer facilities are not capable of handling a smaller grid size in a reasonable amount of time.

Another limitation placed on our work is the use of a time-independent theory to describe a time-dependent process. Ideally one would like to integrate a set of time-dependent equations and watch the vortex form as a function of time. Such a set of equations would be more complicated, requiring larger computer facilities than we have available. We are thus limited to relatively inaccurate values of $H_{c1}(\kappa, W, P)$ and to a time-independent theory.

One could extend our work by applying a transport current in the presence of an applied field and watching vortices nucleate. This would entail a change in the boundary conditions at the surface of the slab and would not be expected to require substantially larger amounts of computer time if the grid size were kept relatively rough and the time-independent equations were used.

In Chapters 5 and 6 we considered a simple model for vortex nucleation and dynamics. The goal in these two chapters was to arrive at relatively simple equations of motion which would give qualitative agreement with experiment. The various interaction terms in the equations of motion are easily understandable and the equations require only simple computer programs for solution. Although the model gave a superheating field that was not in good quantitative agreement with the value obtained from the Ginzburg-Landau equations, the results for the flux-flow velocity and electric field versus current density are in good qualitative agreement with the behavior of these quantities seen experimentally.

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