

DOE/ER/25175--71

Final Technical Report for

**ANALYSES, ALGORITHMS, AND COMPUTATIONS FOR
MODELS OF HIGH-TEMPERATURE SUPERCONDUCTIVITY**

Max D. Gunzburger and Janet S. Peterson

Interdisciplinary Center for Applied Mathematics

Virginia Tech

Blacksburg, VA 24061-0531

Abstract

Under the sponsorship of the Department of Energy, we have achieved significant progress in the modeling, analysis, and computation of superconducting phenomena. Our work has focused on mesoscale models as typified by the celebrated Ginzburg-Landau equations; these models are intermediate between the microscopic models (that can be used to understand the basic structure of superconductors and of the atomic and sub-atomic behavior of these materials) and the macroscale, or homogenized, models (that can be of use for the design of devices). The models we have considered include a time dependent Ginzburg-Landau model, a variable thickness thin film model, models for high values of the Ginzburg-Landau parameter, models that account for normal inclusions and fluctuations and Josephson effects, and the anisotropic Ginzburg-Landau and Lawrence-Doniach models for layered superconductors, including those with high critical temperatures. In each case, we have developed or refined the models, derived rigorous mathematical results that enhance the state of understanding of the models and their solutions, and developed, analyzed, and implemented finite element algorithms for the approximate solution of the model equations.

Introduction

Under the sponsorship of the Department of Energy, we have achieved significant progress in the modeling, analysis, and computation of superconducting phenomena. Our work has focused on mesoscale models as typified by the celebrated Ginzburg-Landau equations; these models are intermediate between the microscopic models (that can be used to understand the basic structure of superconductors and of the atomic and sub-atomic behavior of these materials) and the macroscale, or homogenized, models (that can be of use for the design of devices). Mesoscale models are of great use in understanding important phenomena in superconductors such as pinning, vortex motion, critical currents, Josephson effects, fluctuations, vortex glass and vortex fluid structures, resistivity, etc.

The goals of our efforts in superconductivity center on the following aspects:

- to develop or refine mesoscale and macroscale models for superconductivity so to enlarge the range of physical problems for which such models are valid;
- to analyze these models in order to gain further understanding of the properties of these models and of their solutions, and also to determine their validity and usefulness for solving physically interesting problems;

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED



MASTER

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

DISCLAIMER

Portions of this document may be illegible electronic image products. Images are produced from the best available original document.

- to develop, analyze, and implement algorithms for the numerical simulation of solutions of the various models; and
- to use our algorithms and codes to study superconducting phenomena.

We have accomplished much towards meeting these goals. We now give an outline, roughly divided by problem characteristics, of the progress we have made under DOE sponsorship.

Time dependent Ginzburg-Landau model - New theoretical results have been obtained, and finite element algorithms have been defined, analyzed, and implemented. In addition, we have developed a code for approximate solutions of this model which forms the basis for all of our computational studies. We have, for example, incorporated the ability to handle applied voltages and currents, and other intrinsically transient superconducting phenomena.

Variable thickness thin film model - A new model for thin films having variable thickness has been developed; this model simplifies our own previous model for this situation. Theoretical results have been obtained, and finite element algorithms have been defined, analyzed, and implemented. Computational simulations showing the effectiveness of thin regions in the pinning of vortices have been carried out.

Models for high values of κ - Simplified models have been developed and analyzed that are valid for large values of the Ginzburg-Landau parameter κ . Since high- T_c superconductors are known to have large values of κ , this model has become one of our basic tools in the study of such materials. For example, our Lawrence-Doniach code is based on a high- κ version of the model.

Lawrence-Doniach model - The connection between this model for layered superconductors and the anisotropic Ginzburg-Landau model has been rigorously established. New theoretical results have been obtained, and finite element algorithms have been defined. Preliminary computational simulations have been carried out.

Models accounting for normal inclusions and fluctuations - Models that can account for normal materials such as impurities or layers co-existing with superconducting materials have been developed and analyzed. Computational simulations showing the effectiveness of normal impurities in the pinning of vortices have been carried out. The same code has been used to show how the model we have developed can be used for the study of Josephson junctions and of fluctuation and de-pinning phenomena. Some preliminary calculations for these effects have been carried out.

An amplification of the above outline is given in the next section; details may be found in the papers [1]-[12] listed in the Bibliography.

In recognition of our contributions to the study of superconductivity, we were invited to give a plenary talk, as well as to organize a minisymposium, at the SIAM Conference on Emerging Issues in the Material Sciences held in Pittsburgh in April 1994. We were also invited to give the main talk at the Conference on Applied Mathematics held in Korea during February, 1993. We have also been invited to organize a minisymposium on superconductivity at the ICIAM Conference in Hamburg, Germany in July 1995. On numerous occasions, we have been invited to give talks on our

work in superconductivity at universities, laboratories, and conferences. We have also co-organized (with Professor John Ockendon of Oxford) the *AMS-SIAM-IMS Summer Research Conference* on the *Mathematics of Superconductivity* which was held in Seattle during July-August 1993. This conference, which was partially sponsored by DOE, was a major international gathering of scientists, engineers, and mathematicians actively engaged in superconductivity research. Finally, we have written (with John Ockendon) an invited article on superconductivity for an upcoming issue of *SIAM News*.

Accomplishments

Time dependent Ginzburg-Landau models

We now discuss our work on the time dependent Ginzburg-Landau (TDGL) equations. Details may be found in [6], [7], and [11]. There is by now a substantial literature about TDGL models. For the case of a constant applied magnetic field \mathbf{H} and in the absence of applied voltages and currents, the governing equations may be found in Gor'kov and Éliashberg [13]; see also [14]. After a suitable nondimensionalization, these equations for the order parameter ψ and magnetic potential \mathbf{A} are given by

$$\eta \left(\frac{\partial \psi}{\partial t} + i\kappa \Phi \psi \right) + \left(\frac{i}{\kappa} \nabla + \mathbf{A} \right)^2 \psi - \psi + |\psi|^2 \psi = 0 \quad \text{in } \Omega \quad (1)$$

and

$$\frac{\partial \mathbf{A}}{\partial t} + \nabla \Phi + \operatorname{curl} \operatorname{curl} \mathbf{A} = -\frac{i}{2\kappa} (\psi^* \nabla \psi - \psi \nabla \psi^*) - |\psi|^2 \mathbf{A} \quad \text{in } \Omega \quad (2)$$

along with the boundary conditions

$$\left(\frac{i}{\kappa} \nabla + \mathbf{A} \right) \cdot \mathbf{n} = 0 \quad \text{on } \Gamma \quad (3)$$

and

$$\operatorname{curl} \mathbf{A} \times \mathbf{n} = \mathbf{H} \times \mathbf{n} \quad \text{on } \Gamma, \quad (4)$$

where \mathbf{n} denotes the unit normal vector of the boundary, and initial conditions

$$\psi(\mathbf{x}, 0) = \psi_0(\mathbf{x}) \quad \text{in } \Omega \quad (5)$$

and

$$\mathbf{A}(\mathbf{x}, 0) = \mathbf{A}_0(\mathbf{x}) \quad \text{in } \Omega, \quad (6)$$

where we assume that $\operatorname{div} \mathbf{A}_0 = 0$ and also that $|\psi_0(\mathbf{x})| \leq 1$, a.e., which means that the magnitude of the initial order parameter does not exceed its value at the superconducting state. Solutions of (1)-(6) are unique only up to a gauge transformation; for problems wherein the applied field \mathbf{H} is constant, we usually work with the gauge choice

$$\mathbf{A} \cdot \mathbf{n} = 0 \quad \text{on } \Gamma \quad \text{and} \quad \Phi = 0 \quad \text{in } \Omega. \quad (7)$$

Also, in (1)-(7), the Ginzburg-Landau parameter κ and the relaxation parameter η are positive constants.

We had previously shown the global existence and uniqueness of appropriately defined weak solutions of (1)-(7). We have also showed that the solution depends continuously on the initial data and other related results. We have also devised and analyzed discretization algorithms for the TDGL equations. First, semi-discrete Galerkin finite dimensional approximations were examined. (Here, by semi-discrete, we mean only the discretization in spatial variables is considered.) In this case, under the usual approximation theoretic assumptions, we proved the convergence of the approximations as the dimension of the approximating spaces tend to ∞ . This result was also specialized to the concrete case of finite element approximations. We have also considered a backward Euler based fully discrete approximating scheme as well as a second-order accurate in time scheme. In both cases, rigorous error estimates were derived.

These schemes are used in a two-dimensional code we have developed. Spatial discretization is effected using piecewise biquadratic polynomials. Typical results of our computational simulations are given in Figures 1 and 2. The Ginzburg-Landau parameter κ is set equal to 5 and the external field H , which points perpendicular to the plane, is set equal to 2.5. Figure 1 shows the time evolution of the level curves of the magnitude of the order parameter for the phenomena of vortex formation. The sample is a square having sides equal to 20 coherence lengths. Initial conditions correspond to a perfect superconducting state. Vortices first start to form at the edges and then settle down into the interior. Since the applied field is a constant and there are no external currents or voltages applied to the sample, the vortices approach a steady state configuration which is depicted in Figure 2.

The TDGL code we have developed forms the basis for our other codes that we use to obtain approximations of solutions of the variants of the Ginzburg-Landau model discussed below. The results obtained from this code are time accurate so that they can be used to simulate both transient and steady state phenomena. In particular, we have incorporated the ability to handle applied currents and applied voltages. More details will be given below when we discuss our proposed work. Here, we present some preliminary results from the computational simulation of the motion of vortices in the presence of a constant applied current that is directed in the vertical direction. In Figure 3, a sequence of contour plots of the magnitude of the order parameter is given at various time steps. Corresponding to the applied current, the applied magnetic field varies linearly in the horizontal direction. Due to the Lorentz force, vortices are moving from the left of the box towards the right edge of the box and eventually disappear; meanwhile, more vortices are created at the left edge. Similar simulations have produced strong numerical evidence for the annihilation of vortices that are of opposite signs.

A variable thickness thin film model

We now turn to a description of a model we have derived for variable thickness thin films. Thin-films of superconducting material are often modeled as two-dimensional objects. The third dimension, i.e., that across the film, is eliminated by an averaging procedure. If the material, viewed as a three-dimensional object, is homogeneous, and the thickness of the film is invariant with position, then the result of the averaging process will be a two-dimensional model having constant material properties. Variations in thickness can have significant effects on the electromagnetic behavior of the superconductor, e.g., there is evidence that vortices can be trapped within narrow (thin) regions.

One would like to develop a two-dimensional model that can account for thickness variations. Any such model would result from some sort of averaging process across the film. This averaging process will vary from point-to-point in the plane of the film, and introduce the variable thickness into the coefficients of the resulting two-dimensional model. We had previously developed such a model; see [5]. However, in the interim we have developed a simpler, yet equally valid model which we now briefly discuss. Details concerning the derivation of this model, as well as a variety of results concerning the model, may be found in [12].

We consider the case where a three-dimensional thin layer in \mathbf{R}^3 is symmetric with respect to the (x, y) -plane. The z -axis is thus perpendicular to the symmetry plane of the film. Thus, the thin-film Ω_ϵ can be defined by

$$\Omega_\epsilon = \{ (x, y, z) \in \mathbf{R}^3 \mid (x, y) \in \Omega_0 \subset \mathbf{R}^2, z \in (-\epsilon a(x, y), \epsilon a(x, y)) \},$$

where ϵ is small parameter and $a(x, y)$ is assumed to satisfy $a(x, y) \geq a_0 > 0$ for all $(x, y) \in \Omega_0$. The external field is directed perpendicular to the center-plane of the film, i.e., $\mathbf{H} = (0, 0, H)^T$. The platform of the film is denoted by Ω_0 and its boundary by Γ_0 .

In order to formally derive the model we assume that

$$\psi(x, y, z) = \sum_{j=0} \psi_j(x, y) z^j \quad \mathbf{A}(x, y, z) = \sum_{j=0} \mathbf{A}_j(x, y) z^j$$

for z small, i.e., ϵ small. One then obtains, to leading order, that

$$\left(\frac{i}{\kappa} \tilde{\nabla} + \tilde{\mathbf{A}}_0 \right) \cdot a \left(\frac{i}{\kappa} \tilde{\nabla} + \tilde{\mathbf{A}}_0 \right) \psi_0 + a(|\psi_0|^2 - 1) \psi_0 = 0 \quad \text{in } \Omega_0 \quad (8)$$

and

$$\left(\frac{i}{\kappa} \tilde{\nabla} \psi_0 + \tilde{\mathbf{A}}_0 \psi_0 \right) \cdot \mathbf{n} = 0 \quad \text{on } \Gamma_0, \quad (9)$$

where $\tilde{\mathbf{A}}_0 = (\tilde{A}_{01}, \tilde{A}_{02})^T$ is a magnetic potential such that $\text{curl}(\tilde{\mathbf{A}}_0, 0) = \mathbf{H}$ and $\tilde{\nabla}$ denotes the 2D gradient. Thus, to leading order, the magnetic field is unaffected by the presence of the thin film. We have also derived equations that determine the first-order correction to the magnetic field.

We have derived various results concerning the solution of the variable thickness thin film equations (8) and (9). In particular, we have established the rigorous connection between solutions of (8)-(9) and solutions of the three-dimensional steady state Ginzburg-Landau equations. For example, we have the following consistency result. For any $\epsilon > 0$, we denote by $(\psi_\epsilon, \mathbf{A}_\epsilon)$ the solution of the constant coefficient, three-dimensional, steady state Ginzburg-Landau equations over the three-dimensional domain Ω_ϵ . We let

$$\bar{\psi}_\epsilon(x, y) = \frac{1}{2\epsilon a} \int_{-\epsilon a}^{\epsilon a} \psi_\epsilon(x, y, z) dz, \quad \forall (x, y) \in \Omega_0$$

and

$$\bar{\mathbf{A}}_\epsilon(x, y) = \frac{1}{2\epsilon a} \int_{-\epsilon a}^{\epsilon a} \mathbf{A}_\epsilon(x, y, z) dz, \quad \forall (x, y) \in \Omega_0.$$

Thus, for any $(x, y) \in \Omega_0$, $\bar{\psi}_\epsilon$ and $\bar{\mathbf{A}}_\epsilon$ are the averages across the film of the solutions of the three-dimensional Ginzburg-Landau equations in the film, the latter viewed as a three-dimensional object. We then have shown the following consistency result.

The sequence $\{(\bar{\psi}_\epsilon, \bar{\mathbf{A}}_\epsilon)\}$ of solutions of the three-dimensional Ginzburg-Landau equations converges strongly (in appropriate function spaces) to a solution (ψ_0, \mathbf{A}_0) of the variable thickness thin film equations (8)-(9).

We have developed a code for determining finite element approximations to the solution of the variable thickness thin film equations (8) and (9). Piecewise biquadratic finite element functions are used. A typical result is given in Figure 4. The parameters for this calculation are the same as that for Figure 2 for the homogeneous Ginzburg-Landau model. The small boxes in Figure 4 denote regions where the film is thinner; specifically, $a = 1/5$ within the small boxes and $a = 1$ otherwise. Comparing Figures 2 and 4, one clearly sees that vortices are attracted to the thin regions, i.e., they are pinned by these regions.

A model accounting for normal/superconducting junctions

Models that can account for normal inclusions, or more generally, normal/superconducting junctions, are of considerable practical interest. For examples, normal impurities can be used to pin vortices and Josephson junctions consist of thin layers of normal material sandwiched between superconducting materials. We have developed a two-parameter model that can account for such situations; it may be viewed as a generalization of a model given in [15] and [16]. Details concerning the derivation and analysis of our model may be found in [8].

To understand the model we have developed, we need to write down the Ginzburg-Landau functional in dimensional form, which, to within a constant additive factor, is given by

$$\mathcal{G}(\psi, \mathbf{A}) = \int_{\Omega} \left[\alpha |\psi|^2 + \frac{\beta}{2} |\psi|^4 + \frac{1}{2m} \left| \left(i\hbar \nabla + \frac{2e\mathbf{A}}{c} \right) \psi \right|^2 + \frac{|\mathbf{h} - \mathbf{H}|^2}{8\pi} \right] d\Omega.$$

Here, ψ denotes the complex-valued order parameter, \mathbf{h} the magnetic field, $\mathbf{A} = \text{curl } \mathbf{h}$ the magnetic potential, \mathbf{H} the applied magnetic field, e the electron charge, c the speed of light, and $2\pi\hbar$ Plank's constant. For a superconducting material, the parameter α changes sign at the critical temperature T_c , with $\alpha < 0$ for $T < T_c$ and $\alpha > 0$ for $T > T_c$. (The parameter $\beta \geq 0$ always.) In our model, we choose $\alpha < 0$ in the superconducting material and $\alpha \geq 0$ in the normal material. Whenever $\alpha \geq 0$, the role of the parameter β becomes unimportant, so that we choose $\beta = 0$ in the normal material. We also allow for the arbitrary choice for the mass parameter m in the two materials and also allow for different permeabilities in the two materials. Thus, we define a free energy

$$\begin{aligned} & \int_{\Omega_s} \left\{ \alpha_s |\psi|^2 + \frac{\beta_s}{2} |\psi|^4 + \frac{1}{2m_s} \left| \left(i\hbar \nabla + \frac{2e\mathbf{A}}{c} \right) \psi \right|^2 + \frac{\mu_s}{8\pi} |\mathbf{h} - \mathbf{H}|^2 \right\} d\Omega \\ & + \int_{\Omega_n} \left\{ \alpha_n |\psi|^2 + \frac{1}{2m_n} \left| \left(i\hbar \nabla + \frac{2e\mathbf{A}}{c} \right) \psi \right|^2 + \frac{\mu_n}{8\pi} |\mathbf{h} - \mathbf{H}|^2 \right\} d\Omega, \end{aligned}$$

where Ω_n and Ω_s denote the regions occupied by the normal and superconducting materials, respectively. Minimizers of this functional must satisfy the equations (appropriate nondimensionalizations

have been introduced)

$$\left(\frac{i}{\kappa}\nabla + \mathbf{A}\right)^2 \psi - \psi + |\psi|^2 \psi = 0 \quad \text{in } \Omega_s, \quad (10)$$

$$(\mathbf{curl})^2 \mathbf{A} = -\frac{i}{2\kappa} (\psi^* \nabla \psi - \psi \nabla \psi^*) - |\psi|^2 \mathbf{A} \quad \text{in } \Omega_s, \quad (11)$$

$$\frac{1}{m} \left(\frac{i}{\kappa}\nabla + \mathbf{A}\right)^2 \psi + \alpha \psi = 0 \quad \text{in } \Omega_n, \quad (12)$$

$$\frac{1}{\mu} (\mathbf{curl})^2 \mathbf{A} = -\frac{1}{m} \left(\frac{i}{2\kappa} (\psi^* \nabla \psi - \psi \nabla \psi^*) + |\psi|^2 \mathbf{A}\right) \quad \text{in } \Omega_n, \quad (13)$$

$$[\mathbf{A}] = 0, \quad [\psi] = 0, \quad (14)$$

$$\left[\mathbf{n} \cdot \frac{1}{m} \left(\frac{i}{\kappa}\nabla + \mathbf{A}\right) \psi\right] = 0, \quad (15)$$

and

$$\left[\frac{1}{\mu} \mathbf{curl} \mathbf{A} \times \mathbf{n}\right] = 0, \quad (16)$$

where $m = m_n/m_s$, $\mu = \mu_n/\mu_s$, $\alpha = m_n \alpha_n / (m_s |\alpha_s|)$ and $[\cdot]$ denotes the jump across Γ , and \mathbf{n} denotes the unit normal vector of Γ . In general, we have no control over the values of the permeabilities μ_n and μ_s . Likewise, the Ginzburg-Landau parameter κ is fixed by the choice of superconducting material. Thus, we have two constants at our disposal in defining the model, namely, m and α . The freedom afforded by these two parameters enables the model (10)-(16) to account for a variety of normal/superconducting phenomena. We now describe how our model accounts for some of these.

For the model of (10)-(16), the order parameter and the supercurrent in the normal region does not vanish; the latter is given by

$$\mathbf{J} = -\frac{1}{m} \left(\frac{i}{2\kappa} (\psi^* \nabla \psi - \psi \nabla \psi^*) + |\psi|^2 \mathbf{A}\right).$$

Thus, the model can be used to describe the proximity effect.

In one dimension and in the absence of a potential it can be shown that on the superconducting side of a superconducting/normal interface the order parameter satisfies the relation

$$\psi' = -\frac{\kappa\sqrt{\alpha}}{m_n} \psi.$$

Thus, we retrieve the de Gennes boundary condition (see [17])

$$\psi' = -\gamma \psi$$

with $\gamma = \kappa\sqrt{\alpha}/m$. The corresponding boundary condition for a superconducting/vacuum interface should be $\psi' = 0$. This boundary condition is recovered from the model (10)-(16) if we let $\alpha \rightarrow \infty$ and $m \rightarrow \infty$ in such a way that $\sqrt{\alpha}/m \rightarrow 0$.

The model (10)-(16) can also account for the de Gennes relations across a Josephson junction; see [17]. Here we have a normal region sandwiched between two superconducting regions. We denote

by $(\cdot)^+$ and $(\cdot)^-$ evaluation of a quantity in the superconducting material at the left and right-hand interfaces with the normal material. De Gennes then gave the relation

$$\left(\mathbf{n} \cdot \left(\frac{1}{\kappa} \nabla - i\mathbf{A} \right) \psi \right)^+ = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} \left(\mathbf{n} \cdot \left(\frac{1}{\kappa} \nabla - i\mathbf{A} \right) \psi \right)^- \quad (17)$$

for the order parameter and its gauge invariant normal derivative across the junction. Here, the M_{ij} are real and are determined by the particular junction and depend on its thickness, the type of material, etc. de Gennes postulates that for an insulating material M_{11} and M_{22} are close to unity, and M_{12} and M_{21} are small. The junction is symmetric, i.e., has the same type of superconductor on each side of the junction, if and only if $M_{11} = M_{22}$. In this case, de Gennes shows that

$$M_{11}M_{22} - M_{12}M_{21} = 1. \quad (18)$$

Finally, the supercurrent across the junction is given by

$$J = \frac{1}{M_{12}} |\psi^+ \psi^-| \sin(\chi^+ - \chi^-), \quad (19)$$

where χ denotes the phase of the order parameter. All of these relations are directly recoverable from the model (10)-(16). In fact, if we assume that the normal layer has thickness d , and that we have different superconductors on each side of the junction, then our model yields that (17) is satisfied with

$$\begin{aligned} M_{11} &= \cosh(2\kappa d \sqrt{\alpha}) & M_{12} &= (m_n / \sqrt{\alpha}) \sinh(2\kappa d \sqrt{\alpha}) \\ M_{21} &= (m_{s_2} \sqrt{\alpha} / m_n) \sinh(2\kappa d \sqrt{\alpha}) & M_{22} &= m_{s_2} \cosh(2\kappa d \sqrt{\alpha}). \end{aligned} \quad (20)$$

Here, we have nondimensionalized with respect to one of the superconductors, so that m_n and m_{s_2} denote the nondimensionalized masses of the normal material and the other superconductor. Note that the junction is symmetric if and only if $m_{s_2} = 1$, i.e., only if the superconductors are the same material, and that in this case (18) is satisfied. Also, our model yields that the supercurrent in the junction is given by

$$J = \frac{\sqrt{\alpha}}{m_n \sinh(2\kappa d \sqrt{\alpha})} |\psi^+ \psi^-| \sin(\chi^+ - \chi^-)$$

which, using (20), recovers the de Gennes relation (19). Note that, as expected, J decreases exponentially as d increases and as α increases. Furthermore, J also decreases as m_n increases. Since large m_n corresponds to a highly insulating material, this is in agreement with the experimental observation that junctions made from insulating materials need to be thinner than junctions made from metals, in order to obtain the same tunneling current.

In summary, it is important to note that our model recovers all the well-known conditions at normal/superconducting interfaces, including the de Gennes formula for the tunneling current. Such agreement is not possible with previous models having only one parameter at one's disposal.

We have also developed a biquadratic finite element code for the variable α , variable m model of equations (10)-(16). Some typical computational results obtained from the code are found in Figures 5 and 6. For Figure 5, the same conditions are in effect as for Figure 2 for the homogeneous

Ginzburg-Landau model, except that some normal impurities are introduced at the locations denoted by the small boxes. Comparing Figures 2 and 5 we see that our model clearly can account for the pinning of vortices by normal impurities. In Figure 6 we have a Josephson junction type configuration; a thin vertical strip of normal material is sandwiched between superconducting material. Otherwise, the conditions are the same as that for Figure 2. We see that vortices are attracted to the strip of normal material.

A model accounting for large values of κ

Superconductors are largely characterized by the value of the Ginzburg-Landau parameter κ . The recently discovered high critical temperature superconductors are known to have values of κ in excess of 50. Thus, for technological reasons, there is interest in exploring the behavior of superconductors in the limit of large κ . For the same reasons, high magnetic fields are also of interest. Thus, we have developed, analyzed, and computed with simplified models of the Ginzburg-Landau type that are valid in the limit of high κ and high applied fields. The discussion below is in the context of the homogeneous, isotropic Ginzburg-Landau model. We have effected analogous simplifications to other models for superconductivity such as the anisotropic Ginzburg-Landau and Lawrence-Doniach models for layered high critical temperature superconductors. Details can be found in [9] and [10].

We assume that the (nondimensionalized) applied field $\mathbf{H} = \kappa \mathbf{H}_0$, where \mathbf{H}_0 is independent of κ . Note that this does not imply that \mathbf{H} is near the upper critical field $H_{c2} = \kappa$; for example, we could take $|\mathbf{H}_0| = 1/2$. To derive the model, we formally expand the order parameter and magnetic potential in powers of κ :

$$\psi = \sum_{j=0} \frac{1}{\kappa^{2j}} \psi_j \quad \mathbf{A} = \kappa \sum_{j=0} \frac{1}{\kappa^{2j}} \mathbf{A}_j \quad (21)$$

and then substitute these expansions into the full steady state Ginzburg-Landau equations. Equating powers of κ yields, to leading order, the system for \mathbf{A}_0 :

$$\operatorname{curl} \operatorname{curl} \mathbf{A}_0 = 0 \quad \text{in } \Omega \text{ and } \Omega_e, \quad (22)$$

$$[\mathbf{A}_0 \times \mathbf{n}] = 0 \quad \text{on } \Gamma, \quad (23)$$

$$[\operatorname{curl} \mathbf{A}_0 \times \mathbf{n}] = 0 \quad \text{on } \Gamma, \quad (24)$$

and

$$\operatorname{curl} \mathbf{A}_0 \rightarrow \mathbf{H}_0 \quad \text{as } |\mathbf{x}| \rightarrow \infty \quad (25)$$

and the system for ψ_0 :

$$(i\nabla + \mathbf{A}_0)^2 \psi_0 - \psi_0 + |\psi_0|^2 \psi_0 = 0 \quad \text{in } \Omega, \quad (26)$$

and

$$\mathbf{n} \cdot (i\nabla + \mathbf{A}_0) \psi_0 = 0 \quad \text{on } \Gamma, \quad (27)$$

where Ω denotes the region occupied by the superconducting material, Ω_e the region external to the superconductor, and Γ the boundary of the superconductor. We have also derived governing systems for the corrections \mathbf{A}_1 and ψ_1 .

Note that the system (22)-(25) for \mathbf{A}_0 is uncoupled from the system (26)-(27), i.e., one may solve the former set of equations for \mathbf{A}_0 and then use this solution in the latter set in order to determine ψ_0 . Furthermore, the system (22)-(25) implies that to leading order, the magnetic potential is exactly the same as that would be obtained if the superconducting sample were not present. In many cases, these equations may be easily solved. Thus, the main task to be performed in solving the high- κ , high field equations is to solve (26)-(27) for the leading order term of the order parameter ψ_0 . This tremendous simplification, e.g., uncoupling, is not possible with the full Ginzburg-Landau model for which the order parameter and magnetic potential are fully coupled.

On the theoretical side, we have shown that as $\kappa \rightarrow \infty$, solutions of the full Ginzburg-Landau equations converge strongly (in an appropriate function space) to solutions of the leading order equations (22)-(27). We can actually show that the convergence is quadratic, i.e., that $\mathbf{A}_\kappa - \kappa \mathbf{A}_0 = O(\kappa^{-2})$ and $\psi_\kappa - \psi_0 = O(\kappa^{-2})$ as $\kappa \rightarrow \infty$, where $(\psi_\kappa, \mathbf{A}_\kappa)$ denotes the solution of the Ginzburg-Landau equations for a given value of κ . This provides partial justification for the expansions (21) in terms of powers of $1/\kappa^2$.

We have also developed a biquadratic finite element code for finding solutions of the simplified equations (26)-(27). Here, in Figure 7, we compare results obtained using this code with the results found by using our code for the full, coupled, Ginzburg-Landau equations. As in the previous figures, the sides of the square superconducting samples are of length equal to 20 coherence lengths. The non-dimensional applied field is perpendicular to the sample and has magnitude equal to $\kappa/2$. The plots labeled with finite values of κ were obtained from the full Ginzburg-Landau model with the indicated values of κ . The plot labeled with an infinite value of κ was obtained using the simplified model (22)-(27). It is evident from the plots that there is very little difference between the results for the full Ginzburg-Landau equations for values of $\kappa \geq 5$, and that these are also indistinguishable from the results obtained using the leading order equations. Thus, it seems that the simplified model (22)-(27) yields accurate approximations to solutions of the full Ginzburg-Landau model even for moderate values of κ and of the applied field.

The Lawrence-Doniach model for layered superconductors

One of the features of high- T_c superconductors is their layered structure, comprising of alternating layers of superconducting and non- (or weakly) superconducting materials. In planes parallel to the layers, the material is isotropic. However, there is a strong anisotropy present when one compares material properties parallel and perpendicular to the layers. The homogeneous, isotropic Ginzburg-Landau model cannot account for the anisotropy of layered superconductors. In its place, alternative models have been proposed. One of these is the *anisotropic Ginzburg-Landau model* or *effective mass model* introduced by Ginzburg in 1952; see [18] and [19] and the references cited therein. In this model, the effects of the microscopic layered structure are averaged out so that the anisotropic nature of the material appears only in the form of a mass tensor with unequal principal values. The model itself is only a slight variant of the Ginzburg-Landau model. Another model for layered superconductors (which is thought to be a better model for high- T_c superconductors) is the *Lawrence-Doniach model* introduced in [20]; see also [21] and [22]. In this model, the material is treated as a stack of superconducting planes, each pair of which is separated by a vacuum or

insulating material. Furthermore, in this model, the coupling between the superconducting planes is similar to that that occurs in a Josephson junction. One may also consult [23] and the references cited therein for a discussion of these models and the physical circumstances necessary for their validity.

We have analyzed both the anisotropic Ginzburg-Landau and Lawrence-Do-niach models showing, for example, that appropriately defined free energy functionals have minimizers in suitable function spaces. We have also rigorously established the connection between the two models. Specifically, we have shown that minimizers of the Lawrence-Doniach equations converge, as the interlayer spacing tends to zero, to a solution of the anisotropic Ginzburg-Landau equations. We have also derived simplified versions of both models that are valid for high values of κ and applied fields of $O(\kappa)$. Details may be found in [10].

We have also developed biquadratic finite element codes for both models. The anisotropic Ginzburg-Landau model can be used not only for studying anisotropic, homogeneous superconductors, but also superconductor samples containing twin boundaries. This code is in the final stages of testing. Likewise, the Lawrence-Doniach code is in the final stages of testing. This code takes advantage of the simplifications that can be effected for high values of κ ; these simplifications are similar to those that were described in the previous subsection. Most notably, the computation of the magnetic potential uncouples from that of the order parameter. Using this simplified model, we are able to "easily" simulate three-dimensional layered superconductors on workstations. Here, we present some preliminary results obtained using our Lawrence-Doniach code. In Figure 8, we have surface plots of the magnitude of the order parameters for a two-layer superconducting sample. In these simulations, we first choose the applied magnetic field to be perpendicular to the layer, i.e., along the z -axis; in this case, the vortices align themselves vertically (see the picture on the left). Then, we tilt the applied magnetic field slightly towards the right, (i.e., it has a nonzero y -component). Specifically, we keep the z -component of the applied field fixed at 1.5, and choose the three different values 0.0, 0.6, and 1.5 for the y -component. The vortices shift and turn to try to align themselves with the applied magnetic field. If the applied field is tilted further, the vortex locations in two layers also shift more.

BIBLIOGRAPHY

- [1] Q. Du, M. Gunzburger and J. Peterson: Analysis and approximation of Ginzburg-Landau models for superconductivity, *SIAM Review* **34**, 1992, 54-81.
- [2] Q. Du, M. Gunzburger and J. Peterson: Solving the Ginzburg-Landau equations by the finite element method, *Phys. Review B* **46**, 1992, 9027-9034.
- [3] Q. Du, M. Gunzburger and J. Peterson: Modeling and analysis of a periodic Ginzburg-Landau model for type-II superconductivity, *SIAM J. Appl. Math.* **53**, 1993, 689-717.
- [4] Q. Du, M. Gunzburger and J. Peterson: Finite element approximation of a periodic Ginzburg-Landau model for type-II superconductors, *Numer. Math.* **64**, 1993, 85-114.
- [5] Q. Du and M. Gunzburger: A model for superconducting thin films having variable thickness,

Physica D **69**, 1993, 215-231.

- [6] Q. Du: Global existence and uniqueness of solutions of the time-dependent Ginzburg-Landau model for superconductivity, to appear in *Applicable Anal.*
- [7] Q. Du: Finite element methods for the time-dependent Ginzburg-Landau model of superconductivity, *Comp. Math. & Appl.* **27** 1994, 119-133.
- [8] J. Chapman, Q. Du, and M. Gunzburger: A Ginzburg-Landau type model of superconducting/normal junctions including Josephson junctions, to appear in *Europ. J. Appl. Math.*
- [9] J. Chapman, Q. Du, M. Gunzburger, and J. Peterson: Simplified Ginzburg-Landau models for superconductivity valid for high kappa and high fields, to appear in *Adv. Math. Sciences Appl.*
- [10] J. Chapman, Q. Du, and M. Gunzburger: On the Lawrence-Doniach and anisotropic Ginzburg-Landau models for layered superconductors, to appear in *SIAM J. Appl. Math.*
- [11] Q. Du, M. Gunzburger, and J. Peterson: Models and computations for superconducting vortices including pinning mechanisms, in preparation.
- [12] J. Chapman, Q. Du, and M. Gunzburger: A variable thickness thin film model for superconductivity, in preparation.
- [13] L. Gor'kov and G. Éliashberg: Generalization of the Ginzburg-Landau equations for non-stationary problems in the case of alloys with paramagnetic impurities, *Sov. Phys. JETP* **27**, 1968, 328-334.
- [14] L. Gor'kov and N. Kopnin: Viscous flow of vortices in type-II superconducting alloys, *Sov. Phys. JETP* **38**, 1974, 195-201.
- [15] A. Larkin: Effects of inhomogeneities on the structure of the mixed state of superconductors, *Sov. Phys. JETP* **31**, 1971, 784-786.
- [16] K. Likharev: Superconducting weak links, *Rev. Modern Phys.* **51**, 1979, 101-159.
- [17] P. de Gennes: *Superconductivity in Metals and Alloys*, Benjamin, New York, 1966.
- [18] R. Klemm and J. Clem: Lower critical field of an anisotropic type-II superconductor, *Phys. Rev. B* **21**, 1980, 1868-1875.
- [19] D. Tilley: Critical fields and flux penetration pattern in anisotropic type-II superconductors, *Proc. Phys. Soc. London* **85**, 1965, 1177-1184.
- [20] W. Lawrence and S. Doniach: Theory of layer structure superconductors, in *Proc. 12th Inter. Conf. on Low Temperature Physics*, Academic Press of Japan, Kyoto, 1971.
- [21] L. Bulaevskii: Magnetic properties of layered superconductors with weak interaction between the layers, *Zh. Eksperim. i Teor. Fiz.* **64**, 1973, 2241-2247. [English translation: *Sov. Phys.-JETP* **37**, 1973, 1133-1136.]
- [22] R. Klemm, A. Luther, and M. Beasley: Theory of the upper critical field in layered superconductors, *Phys. Rev. B*, **12**, 1975, 877-891.
- [23] Y. Iye: How anisotropic are the cuprate high T_c superconductors?, *Comments Cond. Mat. Phys.* **16** 1992, 89-111.

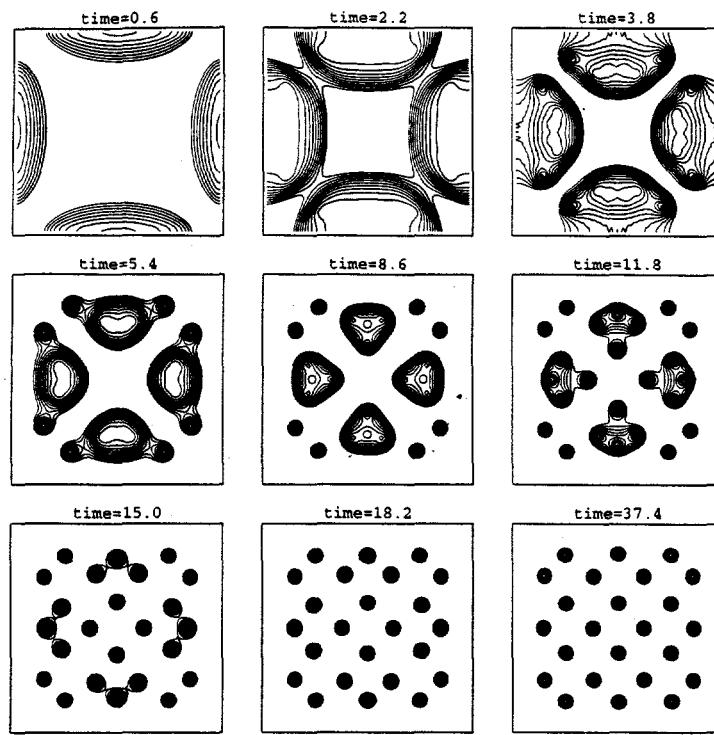


Figure 1. Time evolution of vortices for a type-II superconductor.

Ginzburg-Landau Model

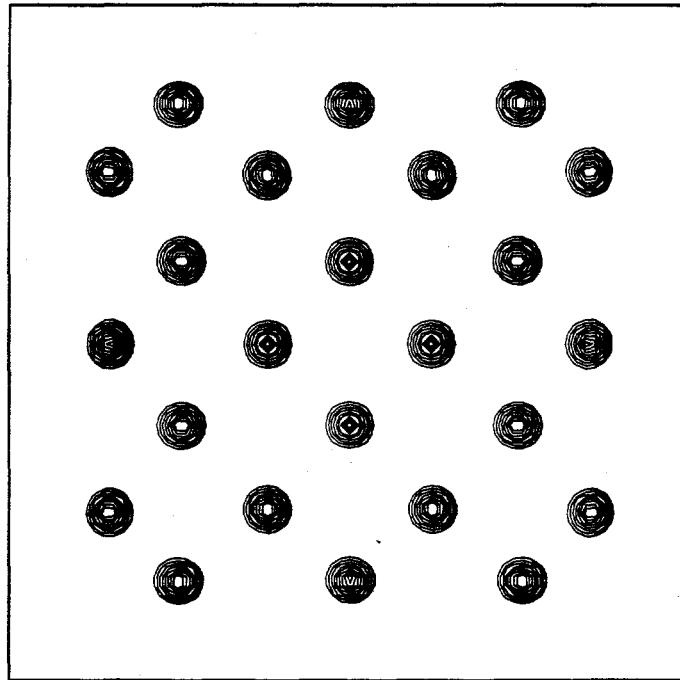


Figure 2. Steady state vortex configuration for a type-II superconductor.

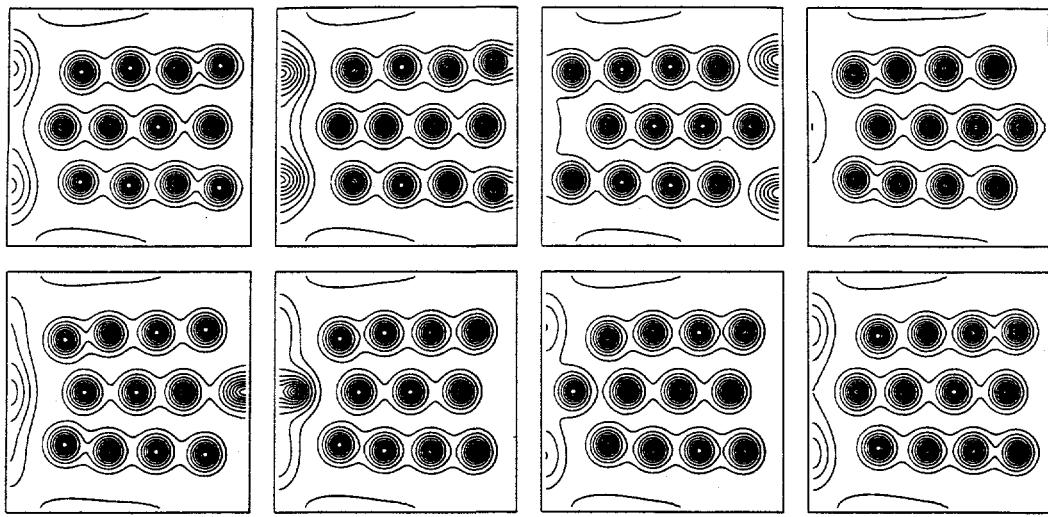


Figure 3. Motion of vortices in the presence of an applied current.
Variable Thickness Model

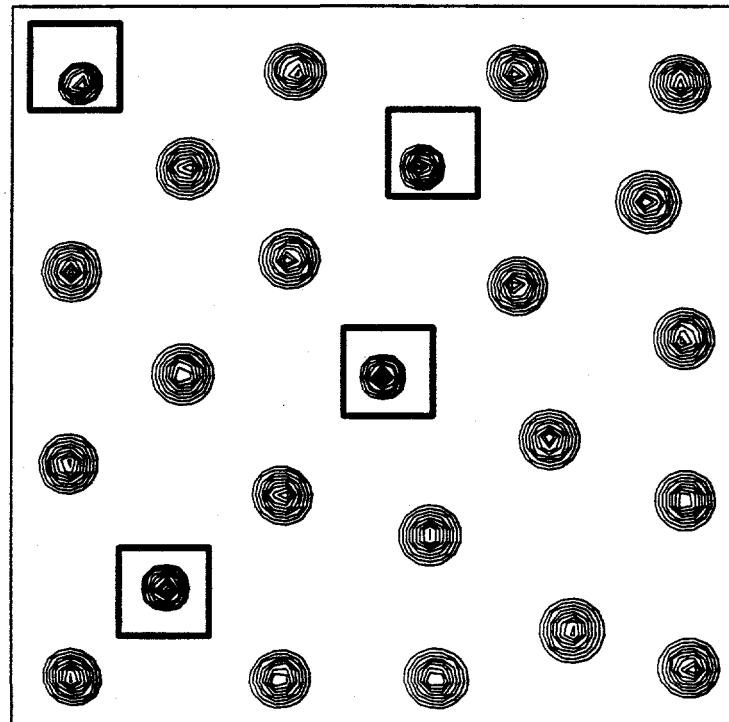


Figure 4. Pinning of vortices by thin regions (small boxes)
in a variable thickness thin film.

Normal Inclusion Model

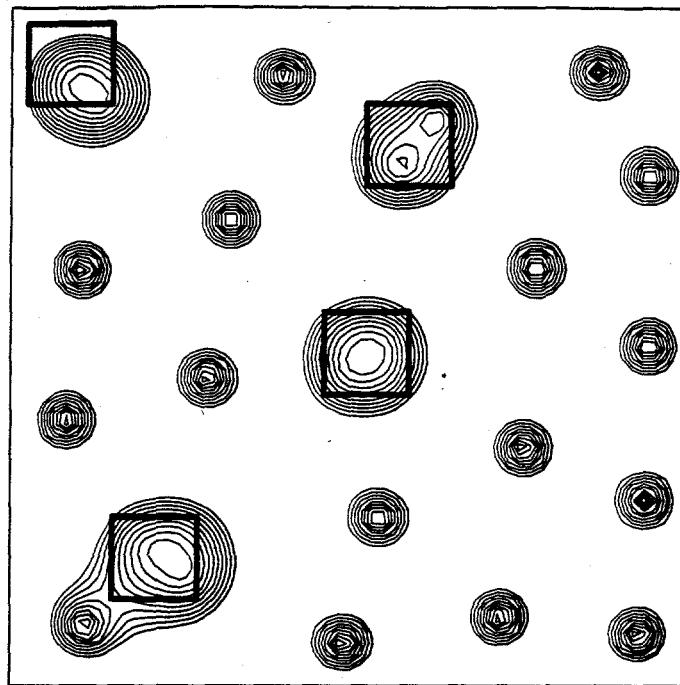


Figure 5. Pinning of vortices by normal inclusions (small boxes).

Normal Inclusion Model

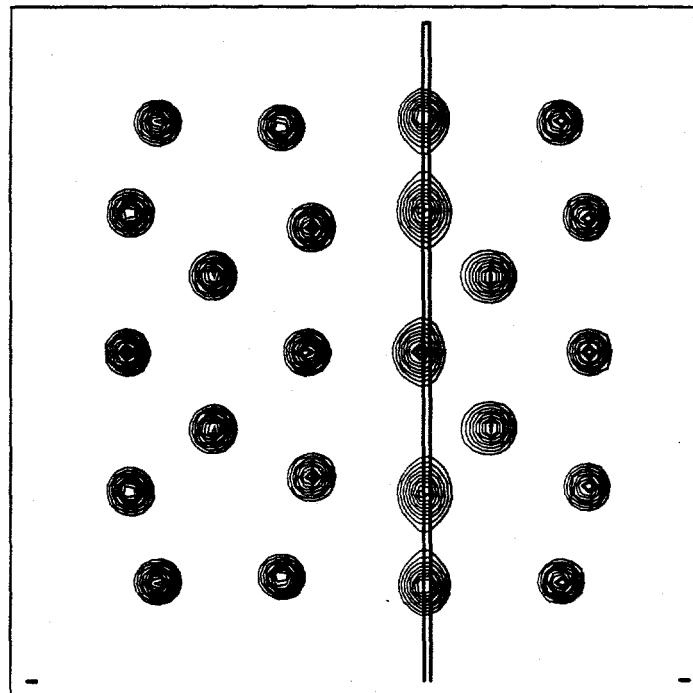


Figure 6. Vortices in a Josephson junction type configuration.
(The thin strip denotes the location of the normal material.)

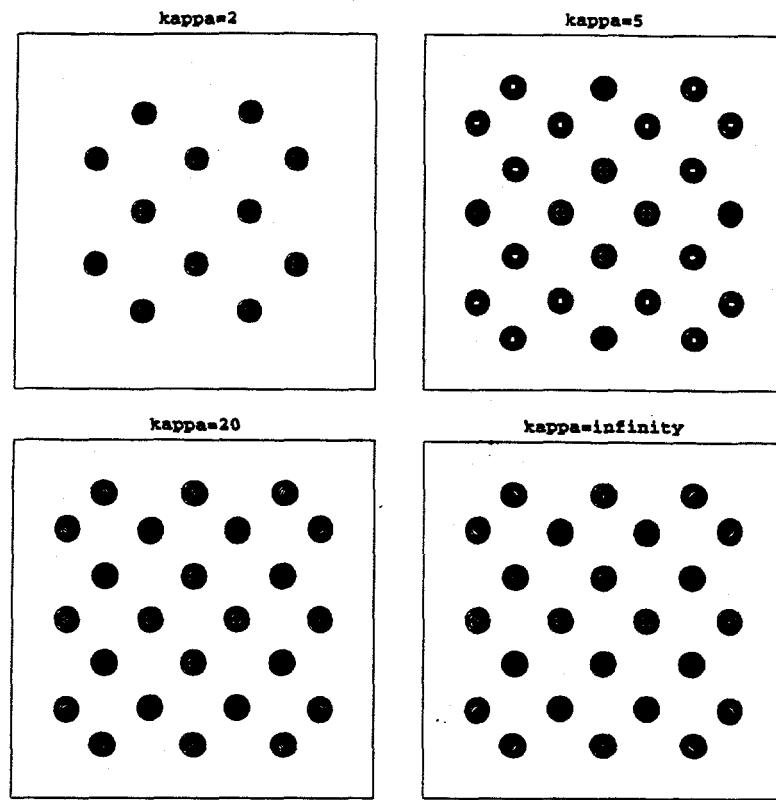


Figure 7. Vortices for different values of κ and for the simplified high- κ model.

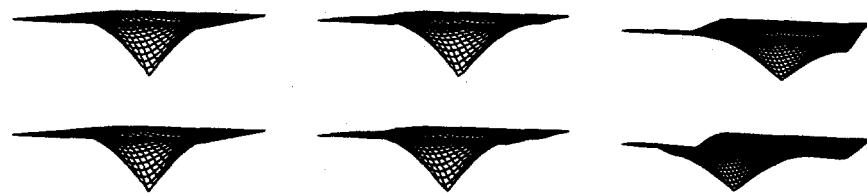


Figure 8. Vortices in two layers (top and bottom) vs. tilt of the applied field.
 left: $H_y = 0.0$ (no tilt), middle: $H_y = 0.6$, right: $H_y = 1.5$