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The recent discovery of certain ceramic materials that turns into superconductors at relatively high temperatures has stimulated much activities in the subject area. We strongly believe that mathematics can play a significant role by helping physicists to understand the basic theory of the phenomenon, by testing existing models with numerical simulation, and by suggesting modifications of the models.

Since the original discovery of superconductivity by Kamerlingh Onnes in 1911, theoretical physicists have proposed several models to explain the phenomena. The first successful one was given by the brothers F. and H. London. In 1950, Ginzburg and Landau suggested to explain superconductivity as a new type of phase transition. They hypothesized that the global minimizer of the Helmholtz energy, calculated from an order parameter and a vector potential, determines the electromagnetic state of the material. The energy functional contains coefficients that depend on the temperature, in such a way that below the critical temperature, a bifurcation occurs and a new branch of solutions takes over as the minimizer. Applying the calculus of variation to the energy functional yields the

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famous Ginzburg-Landau equations that are the subject matter of all the articles in this section.

The newly discovered superconductors belong to the class of Type-II superconductors, characterized by a large value for a certain parameter, κ, that appears in the Ginzburg-Landau equations. Typically, κ is in the range of 100 and above. Back in 1957, Abrikosov showed the existence of vortices of supercurrent in Type-II superconductors. The practical implication of these vortices is the one of the most active topic of investigation in the study of superconductors.

The papers in this section represent recent efforts by mathematicians to study the Ginzburg-Landau model. Du, Gunzburger, and Peterson discuss various variations of the classical model. Chapman investigates the development of the interface between normal and superconducting regions in a Type-I material. Kwong describes some numerical experiments in solving the static Ginzburg-Landau equations. Du and E each looks at the time-dependent Ginzburg-Landau equations and studies the dynamics of vortices. The authors, M. Jones, P. Plassmann, and S. Wright, of the talk "Inexact Newtons methods and the Ginzburg-Landau model for Type-II superconductors" would like to refer the readers to their recent article "Solution of large, sparse systems of linear equations in massively parallel applications", Proceedings of Supercomputing '92, Minneapolis, Nov. 16–22, pp. 551–560, IEEE Computer Society Press, Los Alamitos, California.

The most current findings in experimental physics indicate that modifications to the original Ginzburg-Landau theory is needed to adequately describe the phenomena exhibited by the new superconductors, which have a layered structure at the atomic level and possess high anisotropy. Impurities in the material act as pinning centers for vortices and random thermal noise tends to depin them. Theoretical physicists have even suggested the existence of more phases: the vortex-liquid and vortex-glass phases, but the debate is still going on.

The papers presented here serve to give a better understanding of the classical model and will surely shed some light on how to modify it to accommodate the newer theories.

Asymptotic Analysis of the Ginzburg-Landau Model of Superconductivity: Reduction to a Free Boundary Model

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Abstract. A formal asymptotic analysis of the Ginzburg-Landau model of superconductivity is performed and it is found that the leading order solution satisfies a vectorial version of the Stefan problem for the melting or solidification of a pure material. The first order correction to this solution is found to contain terms analogous to those of surface tension and kinetic undercooling in the scalar Stefan model. However, the "surface energy" of a superconducting material is found to take both positive and negative values, defining type I and type II superconductors respectively, leading to the conclusion that the free boundary model is only appropriate for type I superconductors.

1991 Mathematics Subject Classification: 35R35, 82D55.

1. Introduction

It is observed experimentally that the magnetic field in the interior of a material in the superconducting state is zero, even though there may be a non-zero field in the region adjacent to the superconductor (this effect is usually known as the Meissner effect). However, a superconductor can only exclude fields below a certain magnitude, known as the critical magnetic field H_c. If the field in the adjacent region exceeds the critical magnetic field, then superconductivity will be destroyed and the sample will gradually be converted back to the normally conducting (normal) state, with the field gradually penetrating it. While this conversion is occurring the superconductor might consist of an expanding normal region separated from the remaining superconducting region by a smooth boundary Γ.

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The following free boundary model for this situation was derived in [6]:

$$\frac{\partial \mathbf{H}}{\partial t} = \nabla^2 \mathbf{H} \qquad \text{in the normal region,} \tag{1}$$

$$\mathbf{H} = \mathbf{0} \qquad \text{in the superconducting region,} \tag{2}$$

$$|\mathbf{H}| = H_c \qquad \text{on } \Gamma_N, \tag{3}$$

$$\text{curl } \mathbf{H} \wedge \mathbf{n} = -v_n \mathbf{H} \qquad \text{on } \Gamma_N, \tag{4}$$

together with suitable initial and boundary conditions, where Γ_N denotes the interface Γ approached from the normal region, and v_n is the normal velocity of the interface. This model is derived from Maxwell's equations, neglecting the displacement current. Latent heat and Joule heating effects are also neglected, so that the conversion is assumed to occur under isothermal conditions. Equation (2) describes the Meissner effect, equation (3) describes the critical magnetic field, and equation (4) follows from flux conservation across the interface Γ.

The model (1)-(4) is similar in form to a one-phase Stefan problem, albeit in a vectorial form, which is itself the simplest macroscopic model that could be written down for the evolution of a phase boundary in the theory of the melting or solidification of a pure material [7] (in certain two-dimensional situations (1)-(4) reduces exactly to a one-phase Stefan model [16]. In its simplest dimensionless two-phase form, the Stefan model is

$$\frac{\partial T}{\partial t} = \nabla^2 T \qquad \text{in both solid and liquid phases,} \tag{5}$$

$$T = T_m \qquad \text{on } \Gamma, \tag{6}$$

$$\left[\frac{\partial T}{\partial n}\right]_{Solid}^{Liquid} = -L v_n, \tag{7}$$

where T is the temperature, T_m is the melting temperature, L is the latent heat, and [ ] denotes the jump in the enclosed quantity across the phase boundary Γ. When the melting temperature is constant this model is know to be well-posed just as long as neither superheating nor supercooling occurs, i.e. $T_{solid} < T_m$, $T_{liquid} > T_m$ [15]. In the superconductivity problem this corresponds to $|\mathbf{H}| > H_c$ in the normal region. If either of these conditions is violated the model is ill-posed and thus needs to be regularised [8]. A popular way of doing this is to include surface tension (Gibbs-Thompson) and/or kinetic undercooling effects [19] so that T_m is not constant, but given by

$$T_m = -\sigma\tilde{\kappa} - \beta v_n, \tag{1.8}$$

where $\tilde{\kappa}$ is the mean curvature of the interface, with a suitable sign, and σ and β are positive constants; σ is known as the surface energy. An analogous regularisation of the model (1)-(4) was proposed in [17] in which it was suggested that the interface condition (4) should be modified to

$$|\mathbf{H}| = H_c - \frac{H_c}{2}\sigma\tilde{\kappa}, \tag{1.9}$$

as Γ is approached from the normal region, where σ is the surface energy of a normal/superconducting interface. The physical justification for the addition of such a term in the superconductivity model is not as clear as that for the solidification model.

An alternative regularisation of the Stefan model is the phase field model [1] in which the free boundary is smoothed out altogether by the introduction of an order parameter $F \in [-1, 1]$, such that (5) is replaced by

$$\frac{\partial T}{\partial t} + \frac{L}{2}\frac{\partial F}{\partial t} = \nabla^2 T. \tag{1.10}$$

The order parameter represents the mass fraction of material to have changed phase from solid ($F = -1$) to liquid ($F = 1$). Equation (10) is coupled with an evolution equation for F, obtained by equating the time variation of F to the variational derivative of a suitably chosen free energy functional, in the form

$$\alpha\frac{\partial F}{\partial t} = \alpha\xi^2\nabla^2 F + \frac{1}{2a}(F - F^3) + 2T; \tag{1.11}$$

here α, ξ and a are all positive constants. Numerical simulations of (10)-(11) have been performed which seem to indicate their well-posedness [3]. Their most intriguing feature from the present point of view however, is their ability to reduce formally to the classical and modified Stefan models as a, ξ and in some cases α tend to zero [2].

We aim here to perform a similar analysis of the superconductivity problem. We first introduce the Ginzburg-Landau equations of superconductivity, in which the phase boundary is smoothed as in the phase field model. We then perform an asymptotic analysis as certain parameters in the model tend to zero, and retrieve the vectorial Stefan model at leading order. An examination of the magnitude of the magnetic field at first order will reveal the emergence of "surface tension" and "kinetic undercooling terms", as in the modified Stefan model. However, the "surface energy" of a normal/superconducting interface can take both positive and negative values, defining type I and type II superconductors respectively, and so is not always a stabilizing influence.

2. Asymptotic Analysis

For a more complete introduction to the Ginzburg-Landau theory of superconductivity the reader is referred to [6,9,13,14] and the references therein. Here we merely state the dimensionless, time-dependent Ginzburg-Landau equations as

$$-\alpha\xi^2\frac{\partial\Psi}{\partial t} - \frac{\alpha\xi i}{\lambda}\Psi\phi + \left(\xi\nabla - \frac{i}{\lambda}\mathbf{A}\right)^2\Psi = \Psi(|\Psi|^2 - 1), \tag{12}$$

$$-\lambda^2(\mathrm{curl})^2\mathbf{A} = \lambda^2\left(\frac{\partial\mathbf{A}}{\partial t} + \nabla\phi\right) + \frac{i\xi\lambda}{2}\left(\Psi^*\nabla\Psi - \Psi\nabla\Psi^*\right) + |\Psi|^2\,\mathbf{A}, \tag{13}$$

where Ψ is the (in this case complex) superconducting order parameter (with Ψ^* denoting its complex conjugate), and $\mathbf{A}$ and ϕ are the magnetic vector and electric scalar potential respectively, which are such that

$$\mathbf{H} = \text{curl } \mathbf{A}, \qquad \mathbf{E} = -\frac{\partial \mathbf{A}}{\partial t} - \nabla\phi; \tag{14}$$

$\mathbf{A}$ is unique up to the addition of a gradient; once $\mathbf{A}$ is given ϕ is unique up to the addition of a function of t. Here α, λ and ξ are positive material constants; λ is known as the penetration depth, ξ as the coherence length. The ratio of these lengthscales is the Ginzburg-Landau parameter $\kappa = \lambda/\xi$.

Equations (12)-(14) are gauge invariant, in the sense that they are invariant under transformations of the type

$$\mathbf{A} \to \mathbf{A} + \nabla\omega, \qquad \phi \to \phi - \frac{\partial \omega}{\partial t}, \qquad \Psi \to \Psi e^{i\omega/\xi\lambda}.$$

We may write the equations in terms of real variables by introducing the new, gauge invariant potentials

$$\mathbf{Q} = \mathbf{A} - \xi\lambda\nabla\chi, \qquad \Phi = \phi + \xi\lambda\frac{\partial \chi}{\partial t}, \tag{15}$$

where $\Psi = fe^{i\chi}$. We then obtain the following equations for f, $\mathbf{Q}$ and Φ:

$$-\alpha\xi\frac{\partial f}{\partial t} + \xi^2\nabla^2 f = f^3 - f + \frac{f\,|\mathbf{Q}|^2}{\lambda^2} \tag{10}$$

$$\alpha f^2\Phi + \text{div}\left(f^2\mathbf{Q}\right) = 0, \tag{17}$$

$$-\lambda^2(\text{curl})^2\mathbf{Q} = \lambda^2\left(\frac{\partial \mathbf{Q}}{\partial t} + \nabla\Phi\right) + f^2\mathbf{Q}. \tag{18}$$

We seek limiting behaviour as λ, $\xi \to 0$. We have the following proposition.

Proposition. *In the formal asymptotic limit of the Ginzburg-Landau model (16)-(18) as λ, $\xi \to 0$, with $\kappa = \lambda/\xi$ fixed, the leading order solution satisfies the free-boundary model (1)-(4).*

We assume that the solution comprises normal and superconducting domains separated by thin transition regions. Away from any transition regions we seek asymptotic expansions of the form

$$f \sim f^{(0)} + \lambda f^{(1)} + \cdots, \tag{19}$$

$$\mathbf{Q} \sim \mathbf{Q}^{(0)} + \lambda\mathbf{Q}^{(1)} + \cdots, \tag{20}$$

$$\mathbf{H} \sim \mathbf{H}^{(0)} + \lambda\mathbf{H}^{(1)} + \cdots, \tag{21}$$

$$\Phi \sim \Phi^{(0)} + \lambda\Phi^{(1)} + \cdots. \tag{22}$$

We then find that either $f^{(0)} = 0$ or $\mathbf{Q}^{(0)} = \mathbf{0}$, corresponding to normal and superconducting regions respectively. Proceeding to second order in these outer expansions we find that $f^{(1)} = 0$ in the normal region, and hence

$$\frac{\partial \mathbf{Q}^{(0)}}{\partial t} + \nabla\Phi^{(0)} = -(\text{curl})^2\mathbf{Q}^{(0)}, \qquad \mathbf{H}^{(0)} = \text{curl } \mathbf{Q}^{(0)},$$

so that

$$\frac{\partial \mathbf{H}^{(0)}}{\partial t} = \nabla^2 \mathbf{H}^{(0)}, \tag{23}$$

there, as in (1). In the superconducting region we find $\mathbf{H}^{(0)} = 0$, and $f^{(0)} = 1$.

It remains to consider a local analysis of a transition layer between two such regions. When local coordinates parallel and perpendicular to the transition region are introduced, as in [4] we find that the leading order solution corresponds to a stationary, one-dimensional transition, providing the velocity and curvature of the 'interface' are not too large. We find that the magnetic field and the potential are both parallel to the interface, and that at leading order

$$f'' = \kappa^2(f^3 - f + fQ^2), \tag{24}$$

$$Q'' = f^2 Q, \tag{25}$$

$$H = Q', \tag{26}$$

where H and Q are the magnitudes of the magnetic field $\mathbf{H}$ and vector potential $\mathbf{Q}$ respectively, and $' = d/dz$ where z is the (stretched) coordinate normal to the transition layer. In order for the solution to these equations to match with the previously derived outer solutions in the normal and superconducting regions, we require

$$f \to 1, \quad Q \to 0, \quad \text{as} \quad z \to -\infty \text{ (superconducting)}, \tag{27}$$

$$f \to 0, \quad \text{as} \quad z \to \infty \quad \text{(normal)}. \tag{28}$$

Integrating (24)-(25) once it is now easy to deduce[1]

$$H \to \frac{1}{\sqrt{2}} \text{ as } z \to \infty. \tag{29}$$

By matching, this means that, as we approach the phase boundary from the normal region, the magnitude of the magnetic field tends to $1/\sqrt{2}$, which is equal to the critical magnetic field in these units. Thus we have recovered the free-boundary condition (3).

Beyond this level the asymptotic analysis becomes more intricate. By proceeding to first order in the transition layer equations it is possible to show that

$$\lim_{z\to\infty} \left\{ \frac{\partial H_i^{(1)}}{\partial z} + \tilde{\kappa}_i^{(0)} H_i^{(0)} \right\} = -v_n^{(0)} \lim_{z\to\infty} H_i^{(0)}, \qquad i = 1, 2, \tag{30}$$

where, to leading order, $v_n^{(0)}$ is the normal velocity of the phase boundary, $\tilde{\kappa}_1^{(0)}$ and $\tilde{\kappa}_2^{(0)}$ are the principal curvatures of the phase boundary, and $H_1^{(0)}$ and $H_2^{(0)}$ are the components of the magnetic field in the principal directions. By matching with the outer normal region these conditions can be shown to imply (4).

We have thus arrived at the free-boundary model (1)-(4) at leading order.

1 For a rigirous demonstration of this result see [5].

If we continue with the asymptotic analysis we find that up to second order the matching condition for the magnitude of the magnetic field as the phase boundary is approached from the normal region is

$$|\mathbf{H}| \to H_c - \lambda \frac{H_c}{2} \left\{ \beta v_n^{(0)} + \sigma(\tilde{\kappa}_1^{(0)} + \tilde{\kappa}_2^{(0)}) \right\}, \tag{31}$$

where β and σ are constants determined by the structure of the solutions to (24)-(25) (σ is the 'surface energy' of a normal/superconducting interface). As expected there is a correction proportional to the normal velocity and a correction proportional to the mean curvature of the interface. However, the surface energy σ may take both positive and negative values according to whether $\kappa < 1/\sqrt{2}$ or $\kappa > 1/\sqrt{2}$, defining type I and type II superconductors respectively. The constant β also depends on the size of α in (16)-(18), but again may take positive and negative values.

We recall that when the corresponding constants were positive in the modified Stefan model, they stabilised what would have been an ill-posed problem in their absence. Here it seems that the second term at least is only stabilising when $\kappa < 1/\sqrt{2}$, i.e. for type I superconductors. Even in this case, because the stabilizing terms appear only at first order they will not appreciably affect the solution until the interface curvature or normal velocity becomes very large. Thus we expect quite intricate morphologies, even for solutions to the Ginzburg-Landau equations. Numerical simulations and experimental results seem to support this conjecture [11,18,10,20].

For type II superconductors the correction terms are destabilizing, and thus even in situations in which the free-boundary model is well posed, it may not accurately represent the solution to the Ginzburg-Landau equations. A common observation for type II superconductors is that the normal regions form 'cores' of size comparable to the thickness of a domain boundary [12]. In such a situation the preceding asymptotic analysis, and therefore the free-boundary model, is not valid.

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Time-dependent Ginzburg-Landau models for superconductivity

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Abstract. We discuss analytical and numerical results for the initial-boundary value problems of the time-dependent nonlinear Ginzburg-Landau equations which are evolutionary macroscopic models of superconductivity. We present theorems on the well-posedness of the equations and the convergence of semidiscrete finite dimensional Galerkin approximations. Fully-discrete schemes are also studied here together with numerical experiments.

1991 Mathematics Subject Classification: 82D55, 35A05, 35A40, 81J05.

0. Introduction

The time-dependent Ginzburg-Landau equations for superconductivity were derived by Gor'kov and Eliashberg [15] based on an averaging of the BCS theory (see also [2] and [25]). The equations are nonlinear evolutionary differential equations for the complex order parameter ψ, the real vector magnetic potential $\mathbf{A}$ and the real scalar electric potential Φ. These models have been widely used to study the dynamics of the superconducting transition, especially for the *type-II* superconductors [1] where the generation and the interaction of "flux vortices" are of great interests.

Here, we briefly discuss some recent works on the time dependent Ginzburg-Landau (TDGL) equations. The paper is organized as follows: first, we present some analytical results concerning the well-posedness of the initial boundary value problems for the TDGL equations. Then, we consider the finite dimensional approximations. Both semi-discrete and fully-discrete approximations will be discussed. Finally, we present some preliminary results from our numerical experiments. Due to space limitations, our discussion is not complete and proofs are omitted. For more discussion, we refer to [6] and future reports.

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1. Time dependent Ginzburg-Landau equations

The time dependent Ginzburg-Landau models of superconductivity are closely related to the steady state Ginzburg-Landau models. The latter can be found in many classic books on superconductivity, e.g., [2,25]. For a recent survey on the steady state models, we refer to [7]. More results and references on the steady state models may be found in [4,5,8-11,13,18,19] and [26]. The relations between the time dependent equations and the basic hypotheses of the Ginzburg-Landau theory of superconductivity were discussed in [6]. In [22] and its subsequent works, J. Neu studied the asymptotic behavior of the vortex structure and its dynamics for similar time-dependent G-L equations. For time-dependent models, see also [4,5,12,17,21] and [23].

In order to present the models with simplicity, let us introduce a nondimensionalized form of the free energy functional given by

$$\mathcal{G}(\psi, \mathbf{A}) = \int_\Omega \left[\left| -\frac{i}{\kappa}\nabla\psi - \mathbf{A}\psi \right|^2 + \frac{1}{2}(|\psi|^2 - 1)^2 + |\mathbf{curl}\,\mathbf{A} - \mathbf{H}|^2 \right] d\Omega\,. \tag{1.1}$$

where κ is the Ginzburg-Landau parameter and $\mathbf{H}$ the external field. For simplicity, $\mathbf{H}$ is assumed to be constant here.

The steady-state Ginburg-Landau equations are the Euler-Lagrange equations for the minimizers of the functional $\mathcal{G}$. The time dependent equations may be formulated as

$$\eta\frac{\partial\psi}{\partial t} + i\eta\kappa\Phi\psi + \left(-\frac{i}{\kappa}\nabla - \mathbf{A}\right)^2 \psi - \psi + |\psi|^2\psi = 0 \quad \text{in } \Omega\,, \tag{1.2}$$

$$\mathbf{curl}\,\mathbf{curl}\,\mathbf{A} = -\mathbf{E} - \frac{i}{2\kappa}(\psi^*\nabla\psi - \psi\nabla\psi^*) - |\psi|^2\mathbf{A} \quad \text{in } \Omega\,, \tag{1.3}$$

where

$$\mathbf{E} = \frac{\partial \mathbf{A}}{\partial t} + \nabla\Phi\ . \tag{1.4}$$

The boundary conditions are

$$\left(\frac{i}{\kappa}\nabla\psi + \mathbf{A}\psi\right) \cdot \mathbf{n} = 0 \quad \text{on } \Gamma\,, \tag{1.5}$$

$$\mathbf{curl}\,\mathbf{A} \times \mathbf{n} = \mathbf{H} \times \mathbf{n} \quad \text{on } \Gamma \tag{1.6}$$

and

$$\mathbf{E} \cdot \mathbf{n} = 0 \quad \text{on } \Gamma\,. \tag{1.7}$$

The initial conditions are

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

and

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

We assume that $|\psi_0(x)| \leq 1, a.e.$, which means that the magnitude of the initial order parameter does not exceed the value at superconducting state.

One can naturally rewrite the equations as

$$\eta \frac{\partial \psi}{\partial t} + i\eta\kappa\Phi\psi = -\frac{\delta \mathcal{G}}{\delta \psi} ,$$

$$\frac{\partial \mathbf{A}}{\partial t} = -\frac{\delta \mathcal{G}}{\delta \mathbf{A}}$$

where δ denotes the first variation of the functional. The term $i\eta\kappa$ maintains the gauge invariance of the equations [6].

A more general system of mathematical equations than (1.2-1.4) is given by:

$$\eta \frac{\partial \psi}{\partial t} + i\alpha\Phi\psi + \left(\frac{i}{\kappa}\nabla + \mathbf{A}\right)^2 \psi - \sigma(1 - |\psi|^2)\psi = 0 , \tag{1.8}$$

$$\beta \frac{\partial \mathbf{A}}{\partial t} - \gamma\nabla \mathbf{div}\ \mathbf{A} + \mathbf{curl}\ \mathbf{curl}\ \mathbf{A} + \theta\nabla\Phi = -\frac{i}{2\kappa}(\psi^*\nabla\psi - \psi\nabla\psi^*) - |\psi|^2\mathbf{A} , \tag{1.9}$$

and, often, augmented by $\mathbf{div}\ \mathbf{A} = 0$. The parameters β, γ, θ and κ are usually real while η, α, σ may take either real or complex values. Various special cases have been studied in many areas. For example, (1.8) gives the complex Landau-Ginzburg equations in the hydrodynamic stability theory when $\mathbf{A}$ and Φ are set to be zero. In the context of superconductivity, J. Neu studied cases where $\alpha = \beta = 0, \sigma = 1, \theta \neq 0$, and $\eta = 1$ or i, corresponding to either irreversible or reversible processes. We shall study the above general equations and their physical meanings in the future. However, here we focus on (1.2-1.4), which is the only possible form of (1.8-1.9) where the so called gauge invariance of the equations is perserved.

Throughout, for any non-negative integer s, $H^s(\mathcal{D})$ denotes the Sobolev space of real-valued functions having square integrable spatial derivatives of order up to s in a domain $\mathcal{D}$. The corresponding spaces of complex-valued or vector-valued functions are denoted by $\mathcal{H}^s(\mathcal{D})$ and $\mathbf{H}^s(\mathcal{D})$ respectively. A similar notational convention holds for other Sobolev spaces [3]. The following subspaces of $\mathbf{H}^1(\Omega)$ are also used:

$$\mathbf{H}^1_n(\Omega) = \{\ \mathbf{Q} \in \mathbf{H}^1(\Omega)\ :\ \mathbf{Q}\cdot\mathbf{n} = 0 \text{ on } \Gamma\ \} ,$$

$$\mathbf{H}^1_n(\mathbf{div}\ ;\Omega) = \{\ \mathbf{Q} \in \mathbf{H}^1(\Omega)\ :\ \mathbf{div}\ \mathbf{Q} = 0 \text{ in } \Omega \text{ and } \mathbf{Q}\cdot\mathbf{n} = 0 \text{ on } \Gamma\ \} .$$

To take into account the time-dependence, we let $\mathbf{S} = \mathbf{L}^2(0,T;\mathbf{L}^2(\Omega))$ and

$$\mathbf{V} = \mathbf{L}^\infty(0,T;\mathbf{H}^1_n(\Omega)) \cap \mathbf{H}^1(0,T;\mathbf{L}^2(\Omega)) .$$

Also, we let $\mathcal{S} = \mathcal{L}^2(0,T;\mathcal{L}^2(\Omega))$ and

$$\mathcal{V} = \mathcal{L}^\infty(0,T;\mathcal{H}^1(\Omega)) \cap \mathcal{H}^1(0,T;\mathcal{L}^2(\Omega)) .$$

For convenience of study finite element approximations, we assume that Ω is a bounded convex polygon or convex polyhedron in $\mathbb{R}^d$, where $d = 2$ or 3. Results can be extended to domains with smooth boundary if curved finite element spaces are used.

2. Well-posed gauge choices

The time-dependent Ginzburg-Landau equations (1.2)-(1.6) with the prescribed boundary conditions have the gauge invariant property, see [6,25]. Consequently, it indicates that the time-dependent Ginzburg-Landau equations given above lack uniqueness and thus are not well-posed. One must fix the gauge in order to obtain mathematically well-posed equations. Such a procedure was done in [6]. Several possible gauge choices were given, corresponding to one of the following conditions on the solutions:

- $\mathbf{div}\ \mathbf{A} = 0$; or
- $\mathbf{div}\ \mathbf{A} = \Phi$; or
- $\Phi = 0$.

Here, we focus our attention to the third gauge which eliminates the electric potential Φ. This is one of the most frequently used gauge choice in numerical simulations, see, for example, [21]. All results apply to other gauges by means of gauge transformations. In this gauge, the equations become:

$$\eta \frac{\partial \psi}{\partial t} + \left(-\frac{i}{\kappa} \nabla - \mathbf{A} \right)^2 \psi - \psi + |\psi|^2 \psi = 0 \quad \text{in } \Omega\,, \tag{2.1}$$

$$\frac{\partial \mathbf{A}}{\partial t} + \mathbf{curl\ curl\ A} = -\frac{i}{2\kappa}(\psi^* \nabla \psi - \psi \nabla \psi^*) - |\psi|^2 \mathbf{A} \quad \text{in } \Omega\,. \tag{2.2}$$

The boundary conditions are

$$\nabla \psi \cdot \mathbf{n} = 0 \quad \text{on } \Gamma\,, \tag{2.3}$$

$$\mathbf{curl\ A} \times \mathbf{n} = \mathbf{H} \times \mathbf{n} \quad \text{on } \Gamma\,, \tag{2.4}$$

$$\mathbf{A} \cdot \mathbf{n} = 0 \quad \text{on } \Gamma\,, \tag{2.5}$$

and at $t = 0$, $\mathbf{div}\ \mathbf{A} = 0$ in Ω.

First, the solution $(\psi, \mathbf{A}) \in \mathcal{V} \times \mathbf{V}$ of equations (2.1)-(2.5) satisfies the following weak formulation:

$$\begin{aligned} &\eta \frac{d}{dt}(\psi, \tilde{\psi}) + \left(\left[-\frac{i}{\kappa} \nabla \psi - \mathbf{A}\psi \right], \left[-\frac{i}{\kappa} \nabla \tilde{\psi} - \mathbf{A}\tilde{\psi} \right] \right) \\ &\quad + ([|\psi|^2 - 1]\psi, \tilde{\psi}) = 0\,, \quad \forall\, \tilde{\psi} \in \mathcal{H}^1(\Omega)\,; \end{aligned} \tag{2.6}$$

$$
\begin{aligned}
&\frac{d}{dt}(\mathbf{A},\tilde{\mathbf{A}})+(\mathbf{curl}\ \mathbf{A},\mathbf{curl}\ \tilde{\mathbf{A}})+(|\psi|^2\mathbf{A},\tilde{\mathbf{A}})\\
&\quad+(\frac{i}{2\kappa}(\psi^*\nabla\psi-\psi\nabla\psi^*),\tilde{\mathbf{A}})=(\mathbf{H},\mathbf{curl}\ \tilde{\mathbf{A}})\ ,\quad\forall\ \tilde{\mathbf{A}}\in\mathbf{H}^1_n(\Omega)\,.
\end{aligned}
\tag{2.7}
$$

Concerning the weak form, we have

Theorem 1. *Given $T>0$, if $\psi_0\in\mathcal{H}^1(\Omega)$, $\mathbf{A}_0\in\mathbf{H}^1_n(\mathbf{div}\ ;\Omega)$ and $|\psi_0(x)|\le 1$, a.e., then there exists a unique solution $(\psi,\mathbf{A})\in\mathcal{V}\times\mathbf{V}$ to the equations (2.1-2.3). Moreover, it satisfies*

$$
\mathcal{G}(\psi(t),\mathbf{A}(t))+\int_0^t\left[\left\|\frac{\partial\mathbf{A}}{\partial t}(\tau)\right\|_0^2+\eta\left\|\frac{\partial\psi}{\partial t}(\tau)\right\|_0^2\right]\,d\tau=\mathcal{G}(\psi_0,\mathbf{A}_0)\ ,\ \ \forall\ t\in(0,T),
$$

and there exists a constant $c>0$, only depend on the initial condition, such that

$$
||\mathbf{div}\ \mathbf{A}(t)||_{L^\infty(0,T;L^2(\Omega))}\le c\ ,
$$

$$
|\psi|\le 1\ ,\ a.e.\ ,
$$

$$
||\psi||_{\mathcal{L}^2(0,T;\mathcal{H}^2(\Omega))}\le c\ ,
$$

$$
||\mathbf{curl}\ \mathbf{A}||_{\mathbf{L}^2(0,T;\mathbf{H}^1(\Omega))}\le c\ ,
$$

and

$$
\left\|\mathbf{div}\ \frac{\partial\mathbf{A}}{\partial t}\right\|_{L^2(0,T;L^2(\Omega))}\le c\ .
$$

□

The above results were first proved in [6] (Theorem 3.13 and Lemma 3.14) using techniques in [20,24]. They were also presented in [11]. Continuous dependence on the initial data and other related results may also be found in [6]*. To study the existence and uniqueness of the solutions of the above system, the following modified problem was introduced [6]:

Find $(\psi^\epsilon,\mathbf{A}^\epsilon)\in\mathcal{V}\times\mathbf{V}$ such that

$$
\begin{aligned}
&\eta\frac{d}{dt}(\psi^\epsilon,\tilde{\psi})+(\left[-\frac{i}{\kappa}\nabla\psi^\epsilon-\mathbf{A}^\epsilon\psi^\epsilon\right],\left[-\frac{i}{\kappa}\nabla\tilde{\psi}-\mathbf{A}^\epsilon\tilde{\psi}\right])\\
&\quad+([|\psi^\epsilon|^2-1]\psi^\epsilon,\tilde{\psi})=0\quad\forall\ \tilde{\psi}\in\mathcal{H}^1(\Omega)\,;
\end{aligned}
\tag{2.6$_\epsilon$}
$$

$$
\begin{aligned}
&\frac{d}{dt}(\mathbf{A}^\epsilon,\tilde{\mathbf{A}})+(\mathbf{curl}\ \mathbf{A}^\epsilon,\mathbf{curl}\ \tilde{\mathbf{A}})+\epsilon(\mathbf{div}\ \mathbf{A}^\epsilon,\mathbf{div}\ \tilde{\mathbf{A}})+(|\psi^\epsilon|^2\mathbf{A}^\epsilon,\tilde{\mathbf{A}})\\
&\quad+\Re\left\{\left(\frac{i}{\kappa}\nabla\psi^\epsilon,\psi^\epsilon\tilde{\mathbf{A}}\right)\right\}=(\mathbf{H},\mathbf{curl}\ \tilde{\mathbf{A}})\quad\forall\ \tilde{\mathbf{A}}\in\mathbf{H}^1_n(\Omega)
\end{aligned}
\tag{2.7$_\epsilon$}
$$

* After the Congress, the author received a similar existence result given by Z. Chen, K.H. Hoffmann and J. Liang for the TDGL equations in the second gauge $\Phi=\mathbf{div}\ \mathbf{A}$ on domains with C^2 boundary. They obtained an interesting H^2 regularity result for those domains and used techniques that are different from those in [6].

and the initial conditions are the same as the original equations, so that they are independent of ϵ.

Here, $\epsilon > 0$ is an arbitrary parameter. Note that the above modified system reduces to the original system (2.6)-(2.7) when $\epsilon = 0$.

3. Semi-discrete finite dimensional approximation

Here, we present the semi-discrete Galerkin finite dimensional approximation of the time-dependent Ginzburg-Landau equations in the zero electric potential gauge. By semi-discrete, we mean only the discretization in spatial variables is considered.

In [6], we have studied abstract finite dimensional Galerkin approximations for the system $(2.6_\epsilon), (2.7_\epsilon)$. Let $\mathbf{\Lambda}_n$ and $\mathcal{Z}_n$ be n-dimensional subspaces of $\mathbf{H}^1_n(\Omega)$ and $\mathcal{H}^1(\Omega)$ respectively such that

$$\bigcup \mathbf{\Lambda}_n \quad \text{is dense in } \mathbf{H}^1_n(\Omega), \text{ and } \quad \bigcup \mathcal{Z}_n \quad \text{is dense in } \mathcal{H}^1(\Omega)\ .$$

The standard Galerkin finite dimensional approximation may be given by:

Find $(\psi^\epsilon_n(t), \mathbf{A}^\epsilon_n(t)) \in \mathcal{Z}_n \times \mathbf{\Lambda}_n$ such that

$$(\nabla\psi^\epsilon_n(0), \nabla\tilde{\psi}_n) + (\psi^\epsilon_n(0), \tilde{\psi}_n) = (\nabla\psi(0), \nabla\tilde{\psi}_n) + (\psi(0), \tilde{\psi}_n) \quad \forall\tilde{\psi}_n \in \mathcal{Z}_n\ , \tag{3.1_ϵ}$$

$$(\nabla\mathbf{A}^\epsilon_n(0), \nabla\tilde{\mathbf{A}}_n) + (\mathbf{A}^\epsilon_n(0), \tilde{\mathbf{A}}_n) = (\nabla\mathbf{A}(0), \nabla\tilde{\mathbf{A}}_n) + (\mathbf{A}(0), \tilde{\mathbf{A}}_n) \quad , \tag{3.2_ϵ}$$

for any $\tilde{\mathbf{A}}_n \in \mathbf{\Lambda}_n$ and

$$\begin{aligned} &\eta\frac{d}{dt}(\psi^\epsilon_n, \tilde{\psi}_n) + (\left[-\frac{i}{\kappa}\nabla\psi^\epsilon_n - \mathbf{A}^\epsilon_n\psi^\epsilon_n\right], \left[-\frac{i}{\kappa}\nabla\tilde{\psi}_n - \mathbf{A}^\epsilon_n\tilde{\psi}_n\right]) \\ &\quad + ([|\psi^\epsilon_n|^2 - 1]\psi^\epsilon_n, \tilde{\psi}_n) = 0 \quad \forall\ \tilde{\psi}_n \in \mathcal{Z}_n\ ; \end{aligned} \tag{3.3_ϵ}$$

$$\begin{aligned} &\frac{d}{dt}(\mathbf{A}^\epsilon_n, \tilde{\mathbf{A}}_n) + (\mathbf{curl}\ \mathbf{A}^\epsilon_n, \mathbf{curl}\ \tilde{\mathbf{A}}_n) + \epsilon(\mathbf{div}\ \mathbf{A}^\epsilon_n, \mathbf{div}\ \tilde{\mathbf{A}}_n) + (|\psi^\epsilon_n|^2\mathbf{A}^\epsilon_n, \tilde{\mathbf{A}}_n) \\ &\quad + \Re\left\{\left(\frac{i}{\kappa}\nabla\psi^\epsilon_n, \psi^\epsilon_n\tilde{\mathbf{A}}_n\right)\right\} = (\mathbf{H}, \mathbf{curl}\ \tilde{\mathbf{A}}_n) \quad \forall\ \tilde{\mathbf{A}}_n \in \mathbf{\Lambda}_n\ . \end{aligned} \tag{3.4_ϵ}$$

The following result was proved in [6].

Theorem 2. *Given $T > 0$, if $\psi_0 \in \mathcal{H}^1(\Omega)$, $|\psi_0(x)| \le 1$, a.e. and $\mathbf{A}_0 \in \mathbf{H}^1_n(\mathbf{div}\ ;\Omega)$, then for $\epsilon \ge 0$,, $\{(\psi^\epsilon_n, \mathbf{A}^\epsilon_n)\}$ converges weakly in $\mathcal{L}^2(0,T;\mathcal{H}^1(\Omega)) \times \mathbf{L}^2(0,T;\mathbf{H}^1(\Omega))$ to the unique solution $(\psi^\epsilon, \mathbf{A}^\epsilon)$ of $(2.6_\epsilon) - (2.7_\epsilon)$ as $n \to \infty$. In addition, for $\epsilon > 0$, $(\psi^\epsilon_n, \mathbf{A}^\epsilon_n)$ converges strongly in $\mathcal{L}^2(0,T;\mathcal{H}^1(\Omega)) \times \mathbf{L}^2(0,T;\mathbf{H}^1(\Omega))$ to the solution $(\psi^\epsilon, \mathbf{A}^\epsilon)$ of $(2.6_\epsilon) - (2.7_\epsilon)$ as $n \to \infty$.* □

In [6], it was also shown that solutions of the modified problems converge to the solution of the original system as $\epsilon \to 0$. Note also the first part of the conclusion applies to the original TDGL where $\epsilon = 0$.

If we replace $\mathbf{\Lambda}_n$ and $\mathcal{Z}_n$ by $\mathbf{\Lambda}_h$ and $\mathcal{Z}_h$, where $\mathbf{\Lambda}_h$ and $\mathcal{Z}_h$ are C^0 finite element subspaces of $\mathbf{H}^1_n(\Omega)$ and $\mathcal{H}^1(\Omega)$ respectively, defined on a regular quasi-uniform mesh, parametrized by a parameter h that tends to zero, the corresponding solution sequence $(\psi^\epsilon_n, \mathbf{A}^\epsilon_n)$ becomes a sequence of semi-discrete finite element solution $(\psi^\epsilon_h, \mathbf{A}^\epsilon_h)$. Assume that the spaces $\mathbf{\Lambda}_h$ and $\mathcal{Z}_h$ are constructed in a standard way and h is some measure of the size of the finite elements in the mesh. We assume that the subspaces satisfy the following approximation properties:

$$\inf_{\psi_h \in \mathcal{Z}_h} \|\psi - \psi_h\|_1 \to 0 \quad \text{ as } h \to 0 \quad \forall\, \psi \in \mathcal{H}^1(\Omega)\,, \tag{3.5}$$

$$\inf_{\mathbf{A}_h \in \mathbf{\Lambda}_h} \|\mathbf{A} - \mathbf{A}_h\|_1 \to 0 \quad \text{ as } h \to 0 \quad \forall\, \mathbf{A} \in \mathbf{H}^1_n(\Omega)\,, \tag{3.6}$$

One may consult [14] for conditions on the finite element partitions such that (3.5)-(3.6) are satisfied.

Therefore, by the theorem, we have

Corollary 3. *Under the conditions of the previous theorem, for any $\epsilon \geq 0$, the semi-discrete finite element approximation $(\psi^\epsilon_h, \mathbf{A}^\epsilon_h)$ exists in $[0,T]$. Moreover, $(\psi^\epsilon_h, \mathbf{A}^\epsilon_h)$ is uniformly bounded in $\mathcal{V} \times \mathbf{V}$, independent of h and ϵ. Furthermore, for any $\epsilon \geq 0$, , the sequence $(\psi^\epsilon_h, \mathbf{A}^\epsilon_h)$ converges weakly or weakly * in $\mathcal{V} \times \mathbf{V}$ (and therefore strongly in $\mathcal{S} \times \mathbf{S}$) to the unique solution $(\psi^\epsilon, \mathbf{A}^\epsilon)$ of $(2.6_\epsilon) - (2.7_\epsilon)$ as $n \to \infty$. In addition, for $\epsilon > 0$, $(\psi^\epsilon_h, \mathbf{A}^\epsilon_h)$ converges strongly in $\mathcal{L}^2(0,T;\mathcal{H}^1(\Omega)) \times \mathbf{L}^2(0,T;\mathbf{H}^1(\Omega))$ to $(\psi^\epsilon, \mathbf{A}^\epsilon)$ as $n \to \infty$.* □

The finite dimensional dynamical system $(3.3_\epsilon) - (3.4_\epsilon)$ is a gradient system [16], since the functional $\mathcal{G}_\epsilon$ serves as a Lyapunov functional. Hence, we have

Theorem 4. *Under the conditions of the previous theorem and the above assumptions, the ω-limit set of the system $(3.3_\epsilon) - (3.4_\epsilon)$ is a subset of the equilibrium points which consists of solutions of the following equations:*

$$\begin{aligned}&\left(\left[-\frac{i}{\kappa}\nabla\psi^\epsilon_h - \mathbf{A}^\epsilon_h\psi^\epsilon_h\right], \left[-\frac{i}{\kappa}\nabla\tilde{\psi}^h - \mathbf{A}^\epsilon_h\tilde{\psi}^h\right]\right)\\ &\qquad\qquad + ([|\psi^\epsilon_h|^2 - 1]\psi^\epsilon_h, \tilde{\psi}^h) = 0\,, \quad \forall\, \tilde{\psi}^h \in \mathcal{Z}^h\,;\end{aligned} \tag{3.7_ϵ}$$

$$\begin{aligned}&(\mathbf{curl}\,\mathbf{A}^\epsilon_h - \mathbf{H}, \mathbf{curl}\,\tilde{\mathbf{A}}^h) + \epsilon(\mathbf{div}\,\mathbf{A}^\epsilon_h, \mathbf{div}\,\tilde{\mathbf{A}}^h) + (|\psi^\epsilon_h|^2\mathbf{A}^\epsilon_h, \tilde{\mathbf{A}}^h)\\ &\quad + \Re\left\{\left(\frac{i}{\kappa}\nabla\psi^\epsilon_h, \psi^\epsilon_h\tilde{\mathbf{A}}^h\right)\right\} = 0\,, \quad \forall\, \tilde{\mathbf{A}}^h \in \mathbf{\Lambda}^h\,.\end{aligned} \tag{3.8_ϵ}$$

□

Solutions of $(3.7_\epsilon) - (3.8_\epsilon)$ are the finite element approximations of the steady state Ginzburg-Landau equations. For a complete analysis, see [7] and [9].

4. Fully-discrete approximations

Semi-discrete approximations only deal with spatial discretization and the resulting equations form a system of ODEs. Fully discrete approximations may indicate how the ODEs can be solved. Here, we use the implicit Euler method as an illustration. A interesting feature is the existence of a discrete Lyapunov like functional corresponding to such type of approximations which may be very useful for long time integration.

Let $t_0 = 0$, and $t_{n+1} = t_n + \Delta t_n$ where Δt_n is the step size at the step n. The initial approximation is given by H^1 projection. Define $(\psi_0^h, \mathbf{A}_0^h) \in \mathcal{Z}^h \times \mathbf{\Lambda}^h$ by

$$(\nabla\psi_0^h, \nabla\tilde{\psi}^h) + (\psi_0^h, \tilde{\psi}^h) = (\nabla\psi(0), \nabla\tilde{\psi}^h) + (\psi(0), \tilde{\psi}^h) \quad \forall\tilde{\psi}_n \in \mathcal{Z}_n \ , \tag{4.1}$$

$$(\nabla\mathbf{A}_0^h, \nabla\tilde{\mathbf{A}}^h) + (\mathbf{A}_0^h, \tilde{\mathbf{A}}^h) = (\nabla\mathbf{A}(0), \nabla\tilde{\mathbf{A}}^h) + (\mathbf{A}(0), \tilde{\mathbf{A}}^h) \quad \forall\tilde{\mathbf{A}}^h \in \mathbf{\Lambda}^h \ . \tag{4.2}$$

For $n \geq 0$, we have the implicit Euler scheme:

$$\begin{gathered}\eta\left(\frac{\psi_{n+1}^h - \psi_n^h}{\Delta t}, \tilde{\psi}^h\right) + \left(\left[-\frac{i}{\kappa}\nabla\psi_{n+1}^h - \mathbf{A}_{n+1}^h\psi_{n+1}^h\right], \left[-\frac{i}{\kappa}\nabla\tilde{\psi}^h - \mathbf{A}_{n+1}^h\tilde{\psi}^h\right]\right) \\ + ([|\psi_{n+1}^h|^2 - 1]\psi_{n+1}^h, \tilde{\psi}^h) = 0 \ , \quad \forall\ \tilde{\psi}^h \in \mathcal{Z}^h \ ;\end{gathered} \tag{4.3}$$

$$\begin{gathered}\left(\frac{\mathbf{A}_{n+1}^h - \mathbf{A}_n^h}{\Delta t}, \tilde{\mathbf{A}}^h\right) + (\mathbf{curl}\ \mathbf{A}_{n+1}^h - \mathbf{H}, \mathbf{curl}\ \tilde{\mathbf{A}}^h) \\ + \epsilon(\mathbf{div}\ \mathbf{A}_{n+1}^h, \mathbf{div}\ \tilde{\mathbf{A}}^h) + (|\psi_{n+1}^h|^2\mathbf{A}_{n+1}^h, \tilde{\mathbf{A}}^h) \\ + \left(\frac{i}{2\kappa}(\psi_{n+1}^{h*}\nabla\psi_{n+1}^h - \psi_{n+1}^h\nabla\psi_{n+1}^{h*}), \tilde{\mathbf{A}}^h\right) = 0 \ , \quad \forall\ \tilde{\mathbf{A}}^h \in \mathbf{\Lambda}^h \ .\end{gathered} \tag{4.4}$$

Let us define

$$\mathcal{J}_n^h(\psi, \mathbf{A}) = \mathcal{G}(\psi, \mathbf{A}) + \int_\Omega \left(\epsilon|\mathbf{div}\ \mathbf{A}|^2 + \frac{(\psi - \psi_n^h)^2}{\Delta t} + \frac{(\mathbf{A} - \mathbf{A}_n^h)^2}{\Delta t}\right) d\Omega \ . \tag{4.5}$$

One may show that $\mathcal{J}_n^h$ has at least one minimizer in $\mathcal{Z}^h \times \mathbf{\Lambda}^h$ which, in fact, is a solution of (4.3)-(4.4). Hence,

Theorem 5. *For any $h > 0$, $\Delta t > 0$ and $\epsilon \geq 0$, there exists a solution to the system (4.3)-(4.4) for any n. Moreover, $\forall\ n = 0, 1, ...$,*

$$\mathcal{J}_n^h(\psi_{n+1}^h, \mathbf{A}_{n+1}^h) \leq \mathcal{J}_n^h(\psi_n^h, \mathbf{A}_n^h) \ .$$

Lemma 6. *Let $C > 0$ be a constant. If Δt and $\Delta t h^{-d/2}$ are sufficiently small, then for any $\epsilon \geq 0$, the functional $\mathcal{J}_n^h$ is convex for any $(\psi^h, \mathbf{A}^h)$ in the set*

$$\begin{aligned}\mathcal{M} = \{(\psi^h, \mathbf{A}^h) \in \mathcal{Z}^h \times \mathbf{\Lambda}^h \mid \|\psi^h\|_{0,4} \leq C \ , \ \|\mathbf{A}^h\|_0 \leq C \ , \\ \textit{and} \quad \left\|\frac{i}{\kappa}\nabla\psi_{n+1}^h + \mathbf{A}_{n+1}^h\psi_{n+1}^h\right\|_0 \leq C\} \ .\end{aligned}$$

$\square$

From theorem 5, uniform a priori estimates can be obtained for $\|\psi^h\|_{0,4}$, $\|\mathbf{A}^h\|_0$ and $\|\frac{i}{\kappa}\nabla\psi^h_{n+1} + \mathbf{A}^h_{n+1}\psi^h_{n+1}\|_0$. Using the convexity of the functional, we can get

Theorem 7. *If $\Delta t h^{-d/2}$ is sufficiently small, then for any $\epsilon \geq 0$, the functional $\mathcal{J}^h_n$ has a unique global minimizer which is a solution of (4.3) and (4.4).* □

Remark. In case ϵ is taken to be a positive constant, independent of h, then, the proof of the above theorem may be modified to show that if Δt is small enough, then the global minimizer of $\mathcal{J}^h_n$ is unique for any $h > 0$, i.e., we do not need to assume that $\Delta t h^{-d/2}$ is small. Detailed discussion will be given in future reports.

Remark. In fact, the same proof is valid for the solution of the following problem which, by itself, is a time-discretized version of the original time-dependent G-L equations:

$$\eta\left(\frac{\psi_{n+1}-\psi_n}{\Delta t}, \tilde{\psi}\right) + \left(\left[-\frac{i}{\kappa}\nabla\psi_{n+1} - \mathbf{A}_{n+1}\psi_{n+1}\right], \left[-\frac{i}{\kappa}\nabla\tilde{\psi} - \mathbf{A}_{n+1}\tilde{\psi}\right]\right)$$
$$+ ([|\psi_{n+1}|^2 - 1]\psi_{n+1}, \tilde{\psi}) = 0\,, \quad \forall\, \tilde{\psi} \in \mathcal{H}^1(\Omega)\,;$$

$$\left(\frac{\mathbf{A}_{n+1}-\mathbf{A}_n}{\Delta t}, \tilde{\mathbf{A}}\right) + (\mathbf{curl}\ \mathbf{A}_{n+1} - \mathbf{H}, \mathbf{curl}\ \tilde{\mathbf{A}})$$
$$+ \epsilon(\mathbf{div}\ \mathbf{A}_{n+1}, \mathbf{div}\ \tilde{\mathbf{A}}) + (|\psi_{n+1}|^2\mathbf{A}_{n+1}, \tilde{\mathbf{A}}^h)$$
$$+ \left(\frac{i}{2\kappa}(\psi^*_{n+1}\nabla\psi_{n+1} - \psi_{n+1}\nabla\psi^*_{n+1}), \tilde{\mathbf{A}}\right) = 0\,, \quad \forall\, \tilde{\mathbf{A}} \in \mathbf{H}^1_n(\Omega)\,.$$

Further analysis also gives the following result that is useful in implementing numerical methods.

Corollary 8. *There is no local maxima for the functional $\mathcal{J}^h_n$.* □

For given $h, \Delta t, \epsilon > 0$, the asymptotic behavior of the finite element solution $(\psi^h_n, \mathbf{A}^h_n)$ can be studied. Using compactness, it is straightforward to get

Lemma 9. *If Δt is small enough, the limit set of the sequence $\{(\psi^h_n, \mathbf{A}^h_n)\}$ is a subset of the solution of $(3.7_\epsilon) - (3.8_\epsilon)$.* □

The solution set of $(3.7_\epsilon) - (3.8_\epsilon)$ does not consist of only isolated points, even with $\epsilon > 0$ because of the $U(1)$ symmetry in the order parameter. One can show, however, for almost all κ, there are only finite number of isolated solutions to $(3.7_\epsilon) - (3.8_\epsilon)$, modulus the $U(1)$ symmetry. It remains to be seen whether this will imply that the sequence $\{(\psi^h_n, \mathbf{A}^h_n)\}$ is convergent for almost all κ.

5. Numerical experiments

Some preliminary numerical experiments have been performed on a Sun Sparcstation using a two-dimensional finite element code similar to the one developed in [9] and [10]. The code may be used to study the formation and evolution of the vortices as well as flux pinning in inhomogeneous media. More extensive reports on the experiments will be given in a joint report with M. Gunzburger and J. Peterson. Here, let us describe a simple experiments in which the TDGL equations are solved using the above fully discrete schemes on a two-dimensional square box. The code uses piecewise biquadratic polynomials on a uniform spatial mesh. The Ginzburg-Landau parameter is $\kappa = 3$ with external field at $H = 1.5$. The solution should correspond to a vortex state in this setting. The penetration depth is taken to be three-tenth of the box size. For the particular experiment described here, initial conditions correspond to a pecfect superconducting state. We hereby include a few plots. Figure 1 shows the decay of the free energy and the magnetization in time. Figure 2 and Figure 3 give contour plots of the magnitude of the order parameter. Vortices first start to form near the midpoint of the boundary and then settle down in the interior.

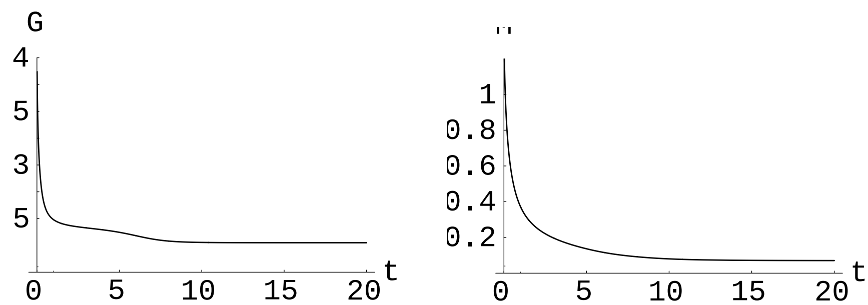

Figure 1. *Free energy vs. time and Magnetization vs. time.*

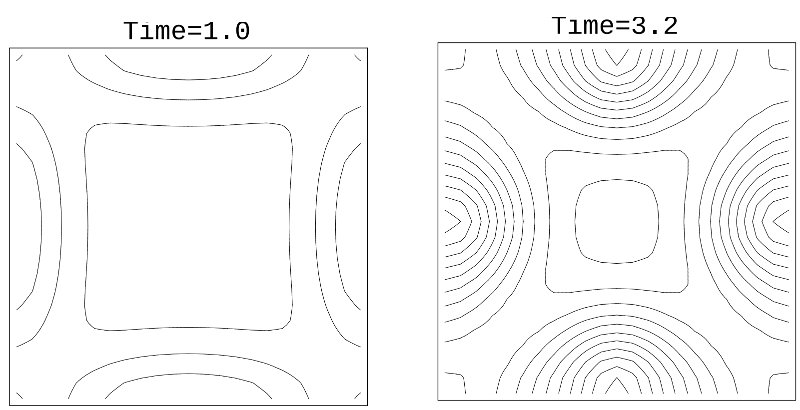

Figure 2. *Magnitude of the order parameter*

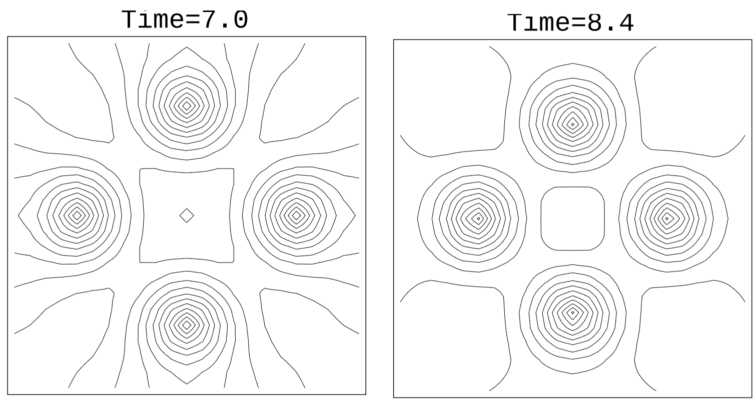

Figure 3. *Magnitude of the order parameter*

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Ginzburg-Landau type models for superconductivity†

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Abstract. Three different models for superconductivity are presented. All are based on the first, the Ginzburg-Landau model for superconductivity in bounded, homogeneous, isotropic samples. The second is a periodic model for which the physical variables are asssumed to be periodic with respect to some prescribed lattice in the plane. The third model is for variable thickness thin-films; this model may be useful in the study of flux pinning mechanisms.

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1. Introduction

The Ginzburg-Landau model for superconductivity, introduced in 1950, has met with great success in describing macroscopic physical phenomena in superconducting materials. The model introduced by Ginzburg and Landau pertained to samples of finite size that, insofar as their material properties were concerened, were isotropic and homogeneous. In Section 2, we briefly describe this model.

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For various reasons, variations to the basic model introduced by Ginzburg and Landau are neceesary in order to successfully describe phenomena in superconductors. For example, for type-II superconductors, the appearance of vortex-like sructures over length scales of a few hundred Angstroms obviates the use of finite size samples in a computational simulation. For this reason, the great majority of such simulations have been carried out using periodic models for superconductivity; these models have also been extensively used in analytical studies. Here, in Section 3, we describe a periodic model for superconductivity in the plane.

Real superconducting thin-films are not necessarily of constant thickness, and indeed, there are reasons why one may want to purposely introduce thickness variations in such samples. In Section 4, we describe a variable thikness thin-film model.

We should mention that there are other variants of the basic Ginzburg-Landau model that have been proposed and studied. For example, there are models for anisotropic superconductors such as the Lawrence-Doniach layered model and the anisotropic mass model. We do not cnsider these here, nor do we cosider time dependent models. Also, we assume that the reader has some familiarity with the basic Ginzburg-Landau model for bounded samples.

2. The finite sample Ginzburg-Landau model

There are many avaiable expositions of the Ginzburg-Landau model for superconductivity in finite samples; see, *e.g.*, [1], [3], [4], [8], [14], [17], and [18]. Here, for the sake of completeness, we simply state the governing equations for the model.

The dependent variables of the Ginzburg-Landau model are the complex and scalar-valued order parameter ψ and the real and vector-valued magnetic potential $\mathbf{A}$. The nondimensionalized physical variables of interest are the magnetic field $\mathbf{h} = \operatorname{curl}\mathbf{A}$, the current $\mathbf{j} = \operatorname{curl}\mathbf{h}$, and the density of superconducting charge carriers $N_s = |\psi|^2$. The sample occupies the domain Ω whose boundary is denoted by Γ. The Ginzburg-Landau equations are given by

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

and

$$\mathbf{j} = \operatorname{curl}\mathbf{h} = \operatorname{curl}\operatorname{curl}\mathbf{A} = -\frac{i}{2\kappa}(\psi^*\nabla\psi - \psi\nabla\psi^*) - |\psi|^2\mathbf{A} + \operatorname{curl}\mathbf{H} \quad \text{in } \Omega\,,$$

where $\mathbf{H}$ denotes the applied field and κ denotes the Ginzburg-Landau parameter. We have the boundary conditions

$$(\frac{i}{\kappa}\nabla\psi + \mathbf{A}\psi)\cdot\mathbf{n} = 0 \quad \text{on } \Gamma\,, \tag{2.1}$$

and

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

We note that these equations may be derived by minimizing the Gibbs free energy

$$\mathcal{G}(\psi, \mathbf{A}) = \int_\Omega \left(f_n - |\psi|^2 + \frac{1}{2}|\psi|^4 + \left| \left(\frac{i}{\kappa}\nabla + \mathbf{A} \right) \psi \right|^2 + |\mathbf{h}|^2 - 2\mathbf{h}\cdot\mathbf{H} \right) d\Omega$$

over a suitable function space. We note that generalizations of the boundary condition (2.1) have also been proposed; these stipulate that the vanishing right-hand side be replaced by a term proportional to the order parameter.

3. A periodic Ginzburg-Landau model

We now turn to a periodic Ginzburg-Landau type model for superconductivity. This model, or variants of it, has been extensively used in analytical and computational studies of superconductivity. See, *e.g.*, [2], [6], [9], [10], [11]-[13], [15], and [16]. Details concerning the presentation given below may be found in [9] and [10].

Given two arbitrary vectors $\mathbf{t}_1$ and $\mathbf{t}_2$ that span $\mathbb{R}^2$, we say that a function $f(\mathbf{x})$ is *periodic with respect to the lattice determined by* $\mathbf{t}_1$ *and* $\mathbf{t}_2$ if

$$f(\mathbf{x}+\mathbf{t}_k) = f(\mathbf{x}) \qquad \text{for } k = 1, 2 \text{ and } \forall\, \mathbf{x} \in \mathbb{R}^2 .$$

Given any point $\mathbf{P} \in \mathbb{R}^2$, a *cell of the lattice with respect to the point* $\mathbf{P}$ is the open parallelogram $\Omega_P \subset \mathbb{R}^2$ having a vertex at $\mathbf{P}$ and two sides aligned with the lattice vectors $\mathbf{t}_1$ and $\mathbf{t}_2$. We assume that the ectermal field is directed normal to the plane of the lattice so that $\mathbf{H} = (0,\, 0,\, H)^T$ and then also $\mathbf{h} = (0,\, 0,\, h)^T$.

The basic assumption of the periodic Ginzburg-Landau model for superconductivity concerns the periodic nature of the physical attributes of the superconductor, *i.e.*,

> the density of superconducting charge carriers N_s, the magnetic field h, the current $\mathbf{j}$, and the free energy density are periodic with respect to the lattice vectors $\mathbf{t}_1$ and $\mathbf{t}_2$.

In terms of the magnetic potential $\mathbf{A}$ and order parameter ψ, these infer that

$$\operatorname{curl}\mathbf{A}\,, \quad |\psi|\,, \quad \text{and} \quad \left(\frac{1}{\kappa}\,\mathbf{grad}\,\phi - \mathbf{A} \right) \quad \text{are periodic}\,, \tag{3.1}$$

where ϕ denotes the phase of the order parameter, *i.e.*, $\psi = |\psi|e^{i\phi}$. Note that the magnetic potential and order parameter themselves are not assumed to be periodic.

Another important notion is that of *fluxoid quantization*. In the present context, we have that

$$\kappa \bar{B} |\Omega| = 2\pi n\,, \tag{3.2}$$

where n denotes the integer number of fluxoids associated with the lattice cell Ω_P, $|\Omega|$ is the area of the lattice cell, and $\bar{B} = (1/|\Omega|)\int_{\Omega_P} h\, d\Omega$ denotes the average magentic field over the lattice cell.

The pairs $(\psi, \mathbf{A})$ and $(\zeta, \mathbf{Q})$ are said to be *gauge equivalent* if there exists a $\chi \in H^2_{\rm loc}(\mathbb{R}^2)$ such that

$$\zeta = \psi e^{i\chi} \quad \text{and} \quad \mathbf{Q} = \mathbf{A} + \frac{1}{\kappa}\mathbf{grad}\,\chi\,.$$

We then have the following result which allows one to deal with a periodic reduced magnetic potential.

Proposition 3.1 *Let* $\mathbf{A}$ *and* $\psi = |\psi|e^{i\phi}$ *satisfy* (3.1)*. Let*

$$\mathbf{A}_0 = \frac{\bar{B}}{2}\begin{pmatrix} x_2 \\ -x_1 \end{pmatrix}.$$

Let $\mathbf{Q}$ *be defined by*

$$\Delta\mathbf{Q} = -\mathbf{curl}\,\mathrm{curl}\,\mathbf{A} \quad \forall\, \mathbf{x} \in I\!R^2 \quad \textit{and} \quad \mathbf{Q} \textit{ periodic}$$

and let

$$\zeta = \psi e^{i\chi} = |\psi|e^{i(\phi+\chi)} = |\psi|e^{i\omega}\,,$$

where $\omega = \phi + \chi$ *and* $\chi \in H^2_{\rm loc}(\mathbb{R}^2)$ *satisfies*

$$\frac{1}{\kappa}\mathbf{grad}\,\chi = \mathbf{Q} - \mathbf{A} - \mathbf{A}_0\,.$$

Then, $(\psi, \mathbf{A})$ *is gauge equivalent to* $(\zeta, \mathbf{Q} - \mathbf{A}_0)$*. Moreover,* $\mathbf{Q}$ *and* $\mathrm{curl}\,\mathbf{Q}$ *are periodic,* $\mathbf{Q}$ *is uniquely determined,* $\mathrm{div}\,\mathbf{Q} = 0$*, and, if*

$$g_k(\mathbf{x}) = -\frac{\bar{B}}{2}(\mathbf{x} \times \mathbf{t}_k)\,, \quad k = 1, 2\,,$$

then

$$\mathbf{A}_0(\mathbf{x} + \mathbf{t}_k) - \mathbf{A}_0(\mathbf{x}) = -\mathbf{grad}\,g_k(\mathbf{x})\,, \quad k = 1, 2$$

and

$$\omega(\mathbf{x} + \mathbf{t}_k) - \omega(\mathbf{x}) = \kappa g_k(\mathbf{x})\,, \quad k = 1, 2\,.$$

Furthermore, the magnetic field h *and the density of superconducting charge carriers may be recovered from* ζ *and* $\mathbf{Q}$ *through the relations*

$$h = \mathrm{curl}\,\mathbf{A} = \mathrm{curl}\,\mathbf{Q} + \bar{B} \quad \textit{and} \quad N_s = |\psi|^2 = |\zeta|^2\,.$$

The Gibbs free energy is invariant to gauge transformations, so that, with repect to the lattice cell Ω_P, it may be written in the form

$$\begin{aligned}\mathcal{G}(\zeta, \mathbf{Q}) = \int_{\Omega_P} \Bigg(& f_0 - |\zeta|^2 + \frac{1}{2}|\zeta|^4 \\ & + \left|\left(\frac{i}{\kappa}\mathbf{grad} + \mathbf{Q} - \mathbf{A}_0\right)\zeta\right|^2 + |\mathrm{curl}\,(\mathbf{Q} - \mathbf{A}_0)|^2 \Bigg)\, d\Omega\,,\end{aligned} \tag{3.3}$$

where ζ, $\mathbf{Q}$, and $\mathbf{A}_0$ satisfy the results of Proposition 3.1.

Denote the right, left, top, and bottom sides of the parallelogram Ω_P by Γ_{+1}, Γ_{-1}, Γ_{+2}, and Γ_{-2}, resepctively. Note that for $k = 1$ or 2, Γ_{+k} is the locus of points $\mathbf{y} \in \mathbb{R}^2$ such that $\mathbf{y} = \mathbf{x} + \mathbf{t}_k$ for $\mathbf{x} \in \Gamma_{-k}$.

The "periodic" Ginzburg-Landau model is then to minimize the free energy (3.3) over all appropriate functions ζ and $\mathbf{Q}$, *i.e.*, functions having one square integrable derivative that also satisfy

$$\zeta(\mathbf{x} + \mathbf{t}_k) = \zeta(\mathbf{x}) e^{i\kappa g_k(\mathbf{x})} \quad \forall\, \mathbf{x} \in \Gamma_{-k},\, k = 1, 2\,, \tag{3.4}$$

$$\mathbf{Q}(\mathbf{x} + \mathbf{t}_k) = \mathbf{Q}(\mathbf{x}) \quad \forall\, \mathbf{x} \in \Gamma_{-k},\, k = 1, 2\,, \tag{3.5}$$

and

$$\operatorname{div} \mathbf{Q} = 0 \text{ in } \Omega_P\,. \tag{3.6}$$

These constraints are motivated by Proposition 3.1.

Standard techniques of the calculus of variations then yield the differential equations

$$\mathbf{curl}\, \operatorname{curl} \mathbf{Q} + |\zeta|^2 \mathbf{Q} + \Re \left\{ \zeta^* (\frac{i}{\kappa} \mathbf{grad} - \mathbf{A}_0) \zeta \right\} = \mathbf{0} \quad \text{in } \Omega_P$$

and

$$(\frac{i}{\kappa} \mathbf{grad} - \mathbf{A}_0) \cdot (\frac{i}{\kappa} \mathbf{grad} - \mathbf{A}_0) \zeta + (|\mathbf{Q}|^2 + |\zeta|^2 - 1) \zeta \\ + 2\mathbf{Q} \cdot (\frac{i}{\kappa} \mathbf{grad} - \mathbf{A}_0) \zeta = 0 \quad \text{in } \Omega_P$$

and the natural boundary conditions

$$\Big(\mathbf{grad}\, |\zeta| \Big) |_{\mathbf{x} + \mathbf{t}_k} = \Big(\mathbf{grad}\, |\zeta| \Big) |_{\mathbf{x}} \quad \forall\, \mathbf{x} \in \Gamma_{-k},\, k = 1, 2\,,$$

$$\operatorname{curl} (\mathbf{Q} - \mathbf{A}_0) |_{\mathbf{x} + \mathbf{t}_k} = \operatorname{curl} (\mathbf{Q} - \mathbf{A}_0) |_{\mathbf{x}} \quad \forall\, \mathbf{x} \in \Gamma_{-k},\, k = 1, 2\,,$$

and

$$|\zeta| \Big(\mathbf{grad}\, \hat{\omega} - \kappa (\mathbf{Q} - \mathbf{A}_0) \Big) |_{\mathbf{x} + \mathbf{t}_k} \\ = |\zeta| \Big(\mathbf{grad}\, \hat{\omega} - \kappa (\mathbf{Q} - \mathbf{A}_0) \Big) |_{\mathbf{x}} \quad \forall\, \mathbf{x} \in \Gamma_{-k},\, k = 1, 2\,,$$

where ω denotes the phase of ζ. Of course, $(\zeta, \mathbf{Q})$ also satisfy the essential conditions (3.4)-(3.6). The various boundary conditions imply that the magnetic field, the current, and the density of superconducting charge carriers are periodic across a lattice cell.

An examination of the periodic Ginzburg-Landau model indicates that the model is uniquely specified once κ, $\mathbf{A}_0$, $g_1(\mathbf{x})$, $g_2(\mathbf{x})$, and Ω_P are chosen. Note that $\mathbf{A}_0$ is determined once the average magnetic field $\bar{B}$ is specified and $g_k(\mathbf{x})$, $k = 1, 2$, are determined once $\bar{B}$ and the lattice vectors $\mathbf{t}_k$, $k = 1, 2$, are specified. Of course, these lattice vectors and a specification of the point $\mathbf{P}$ completely determine the lattice cell Ω_P. Thus, choosing particular values for κ, $\bar{B}$, $\mathbf{P}$, $\mathbf{t}_1$, and $\mathbf{t}_2$ suffices to uniquely specify the model. However, not all of these may be chosen independently; they are related through the fluxoid quantization condition (3.3) which contains the additional parameter n, the number of fluxoids associated with the lattice cell Ω_P.

It is known that an equilateral triangular arrangement of vortex-like structures having one fluxoid associated with each vortex yields the smallest value for the Gibbs free energy. Thus, the preponderance of calculations employing periodic Ginzburg-Landau models have been carried out for such an arrangement. For example, one could choose $n = 1$ and use lattice vectors corresponding to a equilateral tringular lattice, *i.e.*, $\mathbf{t}_1$ and $\mathbf{t}_2$ having the same length and having an angle of $\pi/3$ between them. Alternately, one could choose $n = 2$ and a rectangular lattice defined by orthogonal lattice vectors having lengths in the ratio of $\sqrt{3}$. In either case, the absolute lengths of the lattice vectors are then determined from κ, $\bar{B}$, n, and the fluxoid quantization condition (3.3).

Note that we are specifying the average field $\bar{B}$, and not the external field H; this is a matter of convenience. Note that once $(\zeta, \mathbf{Q})$ is determined (from a particular choice for $\bar{B}$), one may deduce the corresponing external field through a quadrature; see [5].

A variety of results concerning solution of the periodic Ginzburg-Landau model may be found in [9]. The analysis of finite element approximations for this model, as well as the results of some computational experiments are found in [10].

4. A variable thickness thin-film model

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 properties of the material, viewed as a three-dimensional object, are 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. This is exactly the type of situation addressed by the great majority of the analyses and approximations extant in the literature.

In practice, superconducting thin films are not of constant thickness. Variations in thickness have significant effects on the electromagnetics of the superconductor, *e.g.*, there is evidence that vortices can be trapped within narrow 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. Details concerning the derivaition of the model discussed below, as well as a variety of results concerning the model, may be found in [7].

Here, we consider the case where a three dimensional thin layer in $\mathbb{R}^3$ 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

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

where ϵ is small parameter and $a(x,y)$ is assumed to be smooth and $a(x,y) \geq a_0 > 0$ for all $(x,y) \in \Omega_0$. The external field is directed perpendicular to the plane of the film, *i.e.*, $\mathbf{H} = (0,\,0,\,H)^T$. Our interest is to study the G-L functional and its minimizers defined on Ω_ϵ as $\epsilon \to 0$.

We define the modified free energy for the film by

$$\mathcal{F}_\epsilon(\psi,\mathbf{A}) = \int_{\Omega_\epsilon} \left(\frac{1}{2}(|\psi|^2-1)^2 + \left| \left(-\frac{i}{\kappa}\nabla - \mathbf{A} \right)\psi \right|^2 \right) d\Omega + \int_{\Omega_\epsilon} \left(|\mathbf{curl}\,\mathbf{A} - \mathbf{H}|^2 + |\mathrm{div}\,\mathbf{A}|^2 \right) d\Omega\,.$$

We shall see that the inclusion of the last term merely designates a particular class of gauge choices for the magnetic potential. We also let

$$\mathcal{F}_0(\psi,\mathbf{A}) = \lim_{\epsilon\to 0} \frac{1}{2\epsilon}\mathcal{F}_\epsilon(\psi,\mathbf{A})\,.$$

Formally, we write

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

and

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

for z small, *i.e.*, ϵ small. In the sequel, we let $\tilde{\mathbf{V}}$ and $\hat{\mathbf{V}}$ denote the projections of a three-vector $\mathbf{V} \in \mathbb{R}^3$ onto the (x,y)-plane and the z-axis; note that $\tilde{\mathbf{V}} \cdot \hat{\mathbf{V}} = 0$ and $\tilde{\mathbf{V}} + \hat{\mathbf{V}} = \mathbf{V}$.

It can be shown that

$$\begin{aligned}\mathcal{F}_0(\psi,\mathbf{A}) &= \lim_{\epsilon\to 0}\frac{1}{2\epsilon}\mathcal{F}_\epsilon(\psi,\mathbf{A})\\ &= \int_\Omega a\left(\frac{1}{2}(|\psi_0|^2-1)^2+\left|\left(\frac{i}{\kappa}\tilde\nabla+\tilde{\mathbf{A}}_0\right)\psi_0\right|^2\right)\,d\Omega\\ &\quad+\int_\Omega a\left(|\mathrm{curl}\,\tilde{\mathbf{A}}_0-H|^2+|\tilde{\mathbf{A}}_1|^2+a^{-2}|\mathrm{div}\,a\tilde{\mathbf{A}}_0|^2\right)\,d\Omega\,.\end{aligned}$$

This result motivates us to define the functional

$$\begin{aligned}\tilde{\mathcal{F}}_0(\psi_0,\tilde{\mathbf{A}}_0) &= \int_{\Omega_0} a\left(\frac{1}{2}(|\psi_0|^2-1)^2+\left|\left(\frac{i}{\kappa}\tilde\nabla+\tilde{\mathbf{A}}_0\right)\psi_0\right|^2\right)\,d\Omega\\ &\quad+\int_{\Omega_0}\left(a|\mathrm{curl}\,\tilde{\mathbf{A}}_0-H|^2+a^{-1}|\mathrm{div}\,a\tilde{\mathbf{A}}_0|^2\right)\,d\Omega\,.\end{aligned}$$

Note that $\tilde{\mathcal{F}}_0$ involves only an integration over the two-dimensional planform Ω_0 of the film, and that it also depends only on a two-dimensional magnetic potential $\tilde{\mathbf{A}}_0(x,y)$. Formally, one can show that if $(\psi,\mathbf{A})$ is a minimizer of $\mathcal{F}_0$ in $\mathcal{H}^1(\Omega_\epsilon)\times\mathbf{H}^1_n(\Omega_\epsilon)$, then $(\psi_0,\tilde{\mathbf{A}}_0)$ is a minimizer of $\tilde{\mathcal{F}}_0$ in $\mathcal{H}^1(\Omega_0)\times\mathbf{H}^1_n(\Omega_0)$. Moreover,

$$\min_{\mathcal{H}^1(\Omega_\epsilon)\times\mathbf{H}^1_n(\Omega_\epsilon)}\mathcal{F}_0=\min_{\mathcal{H}^1(\Omega_0)\times\mathbf{H}^1_n(\Omega_0)}\tilde{\mathcal{F}}_0\,.$$

For a domain $\mathcal{D}$ in $\mathbb{R}^2$ or $\mathbb{R}^3$, let us introduce the function space

$$\mathbf{H}^1_n(\mathcal{D})=\{\,\mathbf{Q}\in\mathbf{H}^1(\mathcal{D})\;:\;\mathbf{Q}\cdot\mathbf{n}=0\text{ on }\partial\mathcal{D}\,\}\,.$$

Also, $\mathcal{H}^1(\mathcal{D})$ denotes the space of complex-valued functions whosse real and imaginary parts belong to $H^1(\mathcal{D})$. Then, we have the following results. First, we have a result about the equivalence of minimizers of $\mathcal{F}_0$ and $\tilde{\mathcal{F}}_0$.

Next, we have an existence result about minimizers of $\tilde{\mathcal{F}}_0$.

Theorem 4.1. *$\tilde{\mathcal{F}}_0$ has a minimizer $(\psi_0,\tilde{\mathbf{A}}_0)$ in $\mathcal{H}^1(\Omega_0)\times\mathbf{H}^1_n(\Omega_0)$. Moreover, every minimizing sequence of $\tilde{\mathcal{F}}_0$ in $\mathcal{H}^1(\Omega_0)\times\mathbf{H}^1_n(\Omega_0)$ has a subsequence which converges strongly to a minimizer of $\tilde{\mathcal{F}}_0$ in $\mathcal{H}^1(\Omega_0)\times\mathbf{H}^1_n(\Omega_0)$.*

One may now derive the Euler-Lagrange equation for the minimizer of $\tilde{\mathcal{F}}_0$ in $\mathcal{H}^1(\Omega_0)\times\mathbf{H}^1_n(\Omega_0)$; these constitute the variable-thickness Ginzburg-Landau equations and are given by

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

$$\begin{aligned}&\mathbf{curl}\,(a\mathrm{curl}\,\tilde{\mathbf{A}}_0)+a\nabla(\mathrm{div}\,\tilde{\mathbf{A}}_0)+a\nabla(a^{-1}\nabla a\cdot\tilde{\mathbf{A}}_0)\\ &\quad=-\frac{i}{2\kappa}a(\psi_0^*\nabla\psi_0-\psi_0\nabla\psi_0^*)-a|\psi_0|^2\tilde{\mathbf{A}}_0+\mathbf{curl}\,(aH)\quad\text{in }\Omega_0\,,\end{aligned}\tag{4.1}$$

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

and

$$\operatorname{curl}\tilde{\mathbf{A}}_0 = H \quad \text{on } \Gamma_0\,.$$

If we choose the the gague

$$\operatorname{div}(a\tilde{\mathbf{A}}_0) = 0$$

then (4.1) simplifies to

$$\mathbf{curl}\,(a\operatorname{curl}\tilde{\mathbf{A}}_0) = -\frac{i}{2\kappa}a(\psi_0^*\nabla\psi_0 - \psi_0\nabla\psi_0^*) - a|\psi_0|^2\tilde{\mathbf{A}}_0 + \mathbf{curl}\,(aH) \quad \text{in } \Omega_0\,.$$

A comparison of these equations with those of Section 2, the latter restricted to the planar case, reveals the role of the thickness function $a(x,y)$ in the variable thickness model. Note that if we set $a=1$ in the above equations we recover those of Section 2.

We now turn to the question of the consistincy of the variable thickness model. We have denoted a minimizer of $\tilde{\mathcal{F}}_0$, *i.e.*, a solution of the variable thickness Ginzburg-Landau equations by $(\psi_0,\tilde{\mathbf{A}}_0)$. For any $\epsilon > 0$ we denote a minimizer of the functional $\mathcal{F}_\epsilon$, i.e., a solution of the constant coefficient, three-dimensional Ginzburg-Landau equations over the three-dimensional domain Ω_ϵ, by $(\psi_\epsilon,\mathbf{A}_\epsilon)$. We want to show that, in an appropriate sense, $(\psi_0,\tilde{\mathbf{A}}_0)$ is the limit of the sequence of minimizers $\{(\psi_\epsilon,\mathbf{A}_\epsilon)\}$ as $\epsilon\to 0$.

To this end, let

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

and

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

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 the following consistency result.

Theorem 4.2. *The sequence* $\{(\bar{\psi}_\epsilon,\bar{\mathbf{A}}_\epsilon)\}$ *converges strongly to a minimizer* $(\psi_0,\tilde{\mathbf{A}}_0)$ *of* $\tilde{\mathcal{F}}_0$ *in* $\mathcal{H}^1(\Omega_0)\times\mathbf{H}^1_n(\Omega_0)$.

This shows that the average of the solution in a three-dimensional thin-film converges, as the thickness parameter ϵ goes to zero, to the solution of the two-dimensional variable thickness thin-film model we have derived.

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Dynamics of Vortices in Superconductors*

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Abstract. We study the dynamics of vortices in type-II superconductors from the point of view of time-dependent Ginzburg-Landau equations. We outline a proof of existence, uniqueness and regularity of strong solutions for these equations. We then derive reduced systems of ODEs governing the motion of the vortices in the asymptotic limit of large Ginzburg-Landau parameter.

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1. Introduction

In this paper, we report some of our results on the study of time-dependent Ginzburg-Landau (TDGL) equations with application to the modeling of superconductors. The present paper contains two topics: the well-posedness of TDGL (including existence, uniqueness and regularity) and the derivation of dynamical equations governing the evolution of vortex solutions.

The basic phenomenology of superconductivity is described by the Ginzburg-Landau free energy density [5]:

$$f = \frac{1}{2m^*}\left|\left(\frac{\hbar}{i}\nabla - \frac{e^*}{c}A\right)\varphi\right|^2 + \alpha|\varphi|^2 + \frac{\beta}{2}|\varphi|^4 + \frac{B^2}{8\pi} \tag{1.1}$$

Here m^* and e^* are the effective mass and charge of the "Cooper pairs", φ is a complex order parameter, with $|\psi|^2$ representing the density of super-electrons, B is the induced magnetic field, A is the vector potential: $B = \nabla \times A$. In the absence of fields and gradients, f is reduced to the condensation energy: $f = \alpha|\varphi|^2 + \frac{\beta}{2}|\varphi|^4$, where the temperature-dependent constants $\alpha(T)$ and $\beta(T)$ satisfy:

$$\alpha(T) \sim \alpha_0\left(\frac{T}{T_c} - 1\right), \quad \beta(T) > 0, \alpha_0 > 0. \tag{1.2}$$

Therefore for $T > T_c$, the minimum free energy occurs at $|\psi|^2 = 0$ (normal state), whereas for $T < T_c$, the minimum free energy occurs at $|\psi|^2 = -\alpha/\beta$ (superconducting state). T_c is the transition temperature.

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(1.1) defines two length scales: the penetration depth $\lambda(T)$ which is the characteristic length scale associated with the variation of the magnetic field, and the coherence length $\xi(T)$ which is associated with the variation of the order parameter ψ:

$$\xi^2(T) = \frac{\hbar^2}{2m^*|\alpha(T)|}, \quad \lambda^2(T) = \frac{m^*c^2}{4\pi|\varphi|^2 e^{*2}}. \tag{1.3}$$

These two length scales are typically temperature-dependent, and diverge as $T \to T_c$. However, their ratio

$$\kappa = \frac{\lambda(T)}{\xi(T)} \tag{1.4}$$

is a roughly temperature-independent quantity and characterize the property of the material. κ is called the Ginzburg-Landau parameter. It is known that if $\kappa < 1/\sqrt{2}$, the surface energy of a normal-superconducting interface is positive, and the material is called a type-I superconductor. If $\kappa > 1/\sqrt{2}$, then the surface energy is negative and the material is called a type-II superconductor.

Type-II superconductors exhibit an additional phase, called the mixed state, besides the usual normal and superconducting phases. This occurs when the external field H is between the lower and the upper critical fields H_{c_1} and H_{c_2}. In the mixed state, a superconducting bulk sample is shredded by tiny tubes of normal states where magnetic field penetrates. These tiny tubes are called vortices since there is a screening current flowing around each of the vortex.

When a transport current is applied to the sample, the vortices will move because of the various forces acting on them. From a phenomenological view point, the vortices typically experience the Lorentz force, the Magnus force and the viscous drag force. It is established that the motion of vortices causes resistance. Therefore, there is major theoretical as well as practical interest in studying the dynamics of vortices.

In this paper we derive reduced system of ODEs which govern the dynamics of the vortices in the asymptotic limit $\kappa \gg 1$. We remark that typical high temperature superconductors such as YBCO and BiSCCO have rather large values of κ (between 100 and 200). Although the Ginzburg-Landau equations have to be modified to describe the phenomenology of high T_c materials, the techniques we develop are sufficiently general that we expect similar results can also be derived for the high T_c materials, using for example the layered models [2].

2. Preliminaries

Our starting point for the dynamics of vortices is the TDGL equation:

$$\overline{\gamma}\left(\varphi_t + i\frac{e^*}{\hbar}V\varphi\right) = -\frac{\delta\int f d^3x}{\delta\overline{\varphi}} \tag{2.1}$$

together with Maxwell's equation

$$\frac{c}{4\pi}\nabla\times B = J. \tag{2.2}$$

Here V is the electric potential, J is the total current. The time-derivative of φ has to enter in the combination $\varphi_t + i\frac{e^*}{\hbar}V\varphi$ because of the requirement of gauge invariance: If (φ, A, V) is a solution of (2.1)-(2.2), then (φ', A', V') should also be a solution where

$$\varphi' = \varphi e^{-i\frac{e^*}{\hbar c}\eta}, A' = A - \nabla\eta, \quad V' = V + \frac{1}{c}\ \eta_t \tag{2.3}$$

and η is an arbitrary scalar function. The total current consists of two parts: the normal part J_n which obeys Ohm's law and a super-current J_s:

$$J = J_n + J_s = \sigma_n E + e^*|\varphi|^2 v_s \tag{2.4}$$

Here σ_n is the normal state conductivity, E is the electric field, v_s is the super-electron velocity:

$$E = -\frac{1}{c}\ A_t - \nabla V, \ \ v_s = \frac{1}{m^*}\left(\hbar\nabla\theta - \frac{e^*}{c}A\right) \tag{2.5}$$

θ is the phase of the order parameter φ.

We nondimensionalize these equations by choosing new variables: $x \longrightarrow \lambda x'$, $\varphi \longrightarrow \varphi_0\varphi'$, $A \longrightarrow \lambda H_0\sqrt{2}A'$, $t \longrightarrow t_0 t'$, $V \longrightarrow V_0 V'$, where $\varphi_0^2 = -\alpha/\beta$, $H_0 = (-4\pi\alpha)^{1/2}\varphi_0$, $t_0 = 4\pi\sigma_n\lambda^2/c^2$, $V_0 = \lambda^2 H_0\sqrt{2}/(t_0 c)$ The nondimensionalized equations are (omitting the primes)

$$\begin{cases} \gamma^*(\frac{1}{\kappa}\varphi_t + iV\varphi) = (\frac{1}{i\kappa}\nabla - A)^2\varphi + (1-|\varphi|^2)\varphi \\ A_t + \nabla V = -\nabla\times\nabla\times A + |\varphi|^2(\frac{\nabla\theta}{\kappa} - A) \end{cases} \tag{2.6}$$

where

$$\gamma^* = -\frac{\overline{\gamma}e^*V_0}{\hbar\alpha}$$

γ^* depends on the properties of the material been studied.

(2.6) holds inside the sample Ω. Naturally, we associate (2.6) with the following boundary conditions on $\partial\Omega$:

$$\left(\frac{i}{\kappa}\nabla\varphi + A\varphi\right)\cdot n = 0 \tag{2.7}$$

$$\nabla\times A\times n = H\times n \tag{2.8}$$

$$E\cdot n = 0 \tag{2.9}$$

Here n is the outnormal on $\partial\Omega$, H is the external field. (2.7) is a consequence of (2.1) in nondimensionalized variables. (2.8) is a statement that there is no surface current present at the boundary. Therefore the tangential component of the magnetic field should be continuous. We should also assign an initial data to (2.6)-(2.9):

$$\varphi = \varphi_0(x), A = A_0(x). \tag{2.10}$$

Clearly the solutions of (2.6) $\sim$ (2.10) cannot be unique because of the free choice of gauge. It is sometimes important to fix the gauge. It turns out that one convenient way of fixing the gauge, particularly for the purpose of numerical computations, is to make the electric potential zero.

In the rescaled variables, we have as $\kappa \longrightarrow +\infty$,

$$H_{c_1} \sim \frac{\ell_n \kappa}{\kappa}, \quad H_{c_2} \sim \kappa. \tag{2.11}$$

Therefore under a wide range of magnetic fields, the material is in the mixed state. Before studying the dynamics of vortices in this state, we will prove the basic well-posedness theorems for the initial-boundary value problem (2.6)-(2.10).

3. Existence, Uniqueness and Regularity

In this section we outline the argument and a priori estimates needed to establish existence, uniqueness and regularity of strong solutions for (2.6)-(2.10). The key to all of these is the observation that with the choice of gauge such that the scalar potential is zero, (2.6)-(2.9) can be written as

$$\begin{cases} A_t = -\dfrac{\delta F(A,\varphi)}{\delta A} \\ \dfrac{\gamma^* \varphi_t}{\kappa} = -\dfrac{\delta F(A,\varphi)}{\delta \overline{\varphi}} \end{cases} \tag{3.1}$$

where

$$\begin{aligned} F(A,\varphi) = \int \{ \left| (\frac{1}{i\kappa}\nabla - A)\varphi \right|^2 - |\varphi|^2 + \frac{1}{2}|\varphi|^4 + \\ + (\nabla \times A)^2 - 2(\nabla \times A)\cdot H \} d^3x \end{aligned} \tag{3.2}$$

(3.1) implies that

$$\frac{d}{dt}\int F(A,\varphi)d^3x + \frac{\kappa}{\gamma^*}\int \left|\frac{\delta F}{\delta \overline{\varphi}}\right|^2 d^3x + \int \left|\frac{\delta F}{\delta A}\right|^2 d^3x = 0. \tag{3.3}$$

If $F(A_0,\varphi_0) < +\infty$, we obtain from (3.3)

$$F(A(\cdot,t),\varphi(\cdot,t)) + \int_0^t \int \Big\{ \frac{\kappa}{\gamma^*}\Big|\frac{\delta F}{\delta\varphi}\Big|^2 + \Big|\frac{\delta F}{\delta A}\Big|^2 \Big\} d^3x\,dt \\ \leq F(A_0,\varphi_0). \tag{3.4}$$

This is the basic energy estimate.

Next let $\varphi = fe^{i\theta}, f > 0$. Using (2.6) we obtain an equation for f:

$$\begin{cases} \dfrac{\gamma^*}{\kappa} f_t = \dfrac{1}{\kappa^2}\Delta f + (1-f^2)f - \Big|\dfrac{\nabla\theta}{\kappa} - A\Big|^2 f \\ \dfrac{\partial f}{\partial n} = 0 \quad at\ \partial\Omega \end{cases} \tag{3.5}$$

where Ω is the domain occupied by the sample. A standard application of the maximum principle gives: If $0 \leq f(x,0) \leq 1$, then we have for $t > 0$,

$$0 \leq f(x,t) \leq 1. \tag{3.6}$$

(3.4) gives control on the L^2-norm of $B = \nabla \times A$. To control A, we also need to estimate $\nabla \cdot A$. From (2.6), we have

$$(\nabla\cdot A)_t = -(|\varphi|^2\nabla\cdot A + \nabla|\varphi|^2\cdot A) - \frac{i}{2\kappa}(\overline{\varphi}\Delta\varphi - \varphi\Delta\overline{\varphi}) \tag{3.7}$$

This, together with (3.4) and (3.6), gives an additional estimate for $\nabla \cdot A$

$$\max_{0\leq t\leq T}\int(\nabla\cdot A)^2 d^3x \leq C(T). \tag{3.8}$$

(3.4), (3.6) and (3.8) are the key a priori estimates needed to establish the existence and uniqueness of strong solutions. Since the rest of the details are more or less standard, we will omit them and refer the interested reader to the paper of Du [3] who has independently found these estimates and proved the following result:

Theorem *Assume that $\varphi_0, A_0, H \in H^1(\Omega)$. Then exists a unique solution (φ, A) of (2.6)-(2.10) (with $V = 0$), such that for any $T > 0, \varphi \in L^\infty(0,T;H^1(\Omega)) \cap L^2(0,T;H^2(\Omega))$, $A \in L^\infty(0,T;H^1(\Omega))$, $\nabla\times A \in L^\infty(0,T;L^2(\Omega)) \cap L^2(0,T;H^1(\Omega))$.*

4. Dynamics of Interacting Vortices

In this section we derive reduced systems of ODEs which govern the evolution of interacting vortices in the asymptotic limit as $\kappa \longrightarrow \infty$. One difficulty in this asymptotic analysis is the scaling of the different time scales. Since φ and A have different length scales, we expect that their typical time scales can also be very different. However, the relative time scale of φ and A is a material-dependent quantity, and it is difficult to decide how it should behave as $\kappa \longrightarrow +\infty$. Therefore we will take the relative time scale of φ and A as another parameter δ and study the distinguished limit as δ and $\frac{1}{\kappa} \longrightarrow 0$. Here we will only study the case when $\delta = O(1)$. We refer the interested reader to [4] for details of the other distinguished limits.

In this paper we will restrict ourselves to the following situation: an infinite cylindrical sample is placed in an external field parallel to the axis of the cylinder. In this case, the vortices are columnar and we only have to consider a two-dimensional problem in the plane perpendicular to the axis of the cylinder.

The basic phenomenology is the following. We have N vortices moving in the plane. Their core sizes are of $O(\frac{1}{\kappa})$, and they are $O(1)$ distance apart. Let $\epsilon = \frac{1}{\kappa}$, we write (2.6) as

$$\gamma\delta(\epsilon\varphi_t + iV\varphi) = (-i\epsilon\nabla - A)^2\varphi + (1 - |\varphi|^2)\varphi \tag{4.1}$$

$$A_t + \nabla V = -\nabla \times \nabla \times A + |\varphi|^2(\epsilon\nabla\theta - A) \tag{4.2}$$

where $\gamma = \gamma^*/\delta$.

We will restrict ourselves to the case when $\delta = 1$. Rescale time $t = \frac{t'}{\epsilon}\gamma$ and omit the primes we get

$$\begin{aligned} \epsilon^2\varphi_t + \gamma iV\varphi &= (-i\epsilon\nabla - A)^2\varphi + (1 - |\varphi|^2)\varphi \\ \frac{\epsilon}{\gamma}A_t + \nabla V &= -\nabla \times \nabla \times A + |\varphi|^2(\epsilon\nabla\theta - A). \end{aligned} \tag{(4.3)}$$

We proceed to analyze (4.3) using matched asymptotics. For simplicity we choose the zero-electric potential gauge. It can be checked easily that the procedure we follow does not depend on the gauge.

Outer solutions:

It is well-known that the flux carried by each vortex is quantized: Let us estimate the magnitude of the flux quanta. Away from the vortex core, the super-electron velocity is essentially zero. Therefore we have

$$\oint v_s \cdot d\ell = 0 \tag{4.4}$$

where the line integral is evaluated sufficiently far from the vortex core. Since $v_s = \epsilon\nabla\theta - A$, we get

$$\oint A \cdot d\ell = \epsilon \oint \nabla\theta \cdot d\ell = 2\pi n\epsilon. \tag{4.5}$$

Here $n = \frac{1}{2\pi} \oint \nabla\theta d\ell$ is the Poincare index of the vortex. It is known that if $\kappa > \frac{1}{\sqrt{2}}$, then vortices with multiple indices ($|n| > 1$) are unstable. Therefore we will assume that the Poincare index of the vortices satisfy $|n| = 1$.

Denote by $\xi_j(t)$ the location of the j-th vortex and n_j its Poincare index. The total magnetic flux

$$\int_\Omega H d^2x = \oint_{\partial\Omega} A \cdot d\ell = 2\pi\epsilon \sum_j n_j \tag{4.6}$$

is of $O(\epsilon)$. Based on this information, we make the following ansatz:

$$\begin{aligned} \varphi(x,t) &= \varphi_0(x,t) + \epsilon\varphi_1(x,t) + \epsilon^2\varphi_2(x,t) + \dots \\ A(x,t) &= \epsilon a_1(x,t) + \epsilon^2 a_1(x,t) + \dots \\ H(x,t) &= \epsilon h_1(x,t) + \epsilon^2 h_2(x,t) + \dots \end{aligned} \tag{(4.7)}$$

(4.7) should hold outside the cores of the vortices. Substituting (4.7) into (4.3) and collecting equal powers of ϵ, we get a hierarchy of equations. The $O(\epsilon^0)$ equation is:

$$(1 - |\varphi_0|^2)\varphi_0 = 0 \tag{4.8}$$

(4.8) implies that

$$|\varphi_0| = 1, \quad \varphi_0 = e^{i\theta_0(x,t)}. \tag{4.9}$$

The $O(\epsilon)$ equations are:

$$Re(\varphi_0\overline{\varphi}_1) = 0 \tag{4.10}$$

$$-\nabla \times \nabla \times a_1 - a_1 = 0 \tag{4.11}$$

or

$$\Delta h_1 - h_1 = 0 \tag{4.12}$$

(4.12) holds in the punctuated region outside the vortex cores. The boundary condition for h_1 near these cores are obtained from the inner solutions.

Inner solutions:

To study the inner solution in the core of the j-th vortex, we introduce the stretched coordinates $X = \frac{x-\xi_j(t)}{\epsilon}$, and expand the variables as follows:

$$\begin{aligned} \varphi &= \Phi_0(X,t) + \epsilon\ \Phi_1(X,t) + \dots \\ A &= \epsilon\ A_1(X,t) + \epsilon^2 A_2(X,t) + \dots \\ H &= \epsilon\ H_1(X,t) + \epsilon^2 H_2(X,t) + \dots \end{aligned} \tag{4.13}$$

We immediately see that A_1 should be zero since otherwise it will contribute to $O(1)$ terms in H. Substituting (4.13) into (4.3) and collecting equal powers of ϵ, we get, at $O(\epsilon^0)$:

$$\Delta\Phi_0 + \Phi_0(1 - |\Phi_0|^2) = 0 \tag{4.14}$$

$$-\nabla\times\nabla\times A_2-\frac{i}{2}\Big[\overline{\Phi}_0\nabla\Phi_0-\Phi_0\nabla\overline{\Phi}_0\Big]=0 \qquad (4.15)$$

or

$$\Delta H_1-\frac{i}{2}\nabla\times\Big[\overline{\Phi}_0\nabla\Phi_0-\Phi_0\nabla\overline{\Phi}_0\Big]=0. \qquad (4.16)$$

These equations describe the leading order core structure. We look for solutions which take the form:

$$\Phi_0(X,t)=f_0(R)e^{in_j\theta},\, H_1(X,t)=H_1(R,t) \qquad (4.17)$$

where (R,θ) is the polar coordinate of $X, n_j=\pm1$. (4.14) and (4.16) become:

$$f_0''+\frac{1}{R}f_0'+\Big(1-f_0^2-\frac{1}{R^2}\Big)f_0=0 \qquad (4.18)$$

$$H_1''+\frac{1}{R}H_1'+n_j\frac{2f_0f_0'}{R}=0. \qquad (4.19)$$

Since the order parameter should vanish at the center of the core, and match to the outer solution outside the core, f_0 satisfies the boundary conditions:

$$f_0(0)=0,\;\; f_0(+\infty)=1. \qquad (4.20)$$

It can be proved [1] that such solution exists and satisfies

$$1-f_0^2(R)-\frac{1}{R^2}=O(\frac{1}{R^4}),\quad \text{for } R\gg1. \qquad (4.21)$$

Since

$$\int_{R^2}\frac{2f_0f_0'}{R}d^2X=2\pi\int_0^{+\infty}2f_0f_0'dR=2\pi \qquad (4.22)$$

we have as $R\longrightarrow+\infty$,

$$H_1(R)=-n_j\log R+C^*+o(1) \qquad (4.23)$$

where C^* is a constant determined from matching to the outer solution.

We now turn to the $O(\epsilon)$ equations:

$$-\dot{\xi}_j\cdot\nabla\Phi_0=\Delta\Phi_1+\Phi_1(1-2|\Phi_0|^2)-\Phi_0^2\overline{\Phi}_1 \qquad (4.24)$$

$$-\nabla\times\nabla\times A_3-\frac{i}{2}\Big[\overline{\Phi}_1\nabla\Phi_0+\overline{\Phi}_0\nabla\Phi_1-\Big(\Phi_1\nabla\overline{\Phi}_0+\Phi_0\nabla\overline{\Phi}_1\Big)\Big]=0. \qquad (4.25)$$

Let $\Phi_1=f_1e^{in_j\theta}$. Then (4.24) becomes

$$\begin{aligned}&-\dot{\xi}_1(f_0'\cos\theta-in_j\frac{f_0}{R}\sin\theta)-\dot{\xi}_2(f_0'\sin\theta+in_j\frac{f_0}{R}\cos\theta)\\&\quad=\Delta f_1+2in_j\nabla f_1\cdot\nabla\theta-\frac{1}{R^2}f_1+(1-2f_0^2)f_1-f_0^2\overline{f}_1.\end{aligned} \qquad (4.26)$$

Let $f_1=A(R)\cos\theta+B(R)\sin\theta$ and separate real and imaginary parts:

$$A(R)=A_r(R)+iA_i(R),\quad B(R)=B_r(R)+iB_i(R),$$

we obtain the following equations for the real functions $A_r(R)$, $B_r(R)$, $A_i(R)$, and $B_i(R)$:

$$-\dot{\xi}_1 f_0' = A_r'' + \frac{1}{R}A_r' + \left(1 - 3f_0^2 - \frac{2}{R^2}\right) A_r - n_j \frac{2B_i}{R^2} \tag{4.27}$$

$$-\dot{\xi}_2 f_0' = B_r'' + \frac{1}{R}B_r' + \left(1 - 3f_0^2 - \frac{2}{R^2}\right) B_r + n_j \frac{2A_i}{R^2} \tag{4.28}$$

$$-n\dot{\xi}_2 \frac{f_0}{R} = A_i'' + \frac{1}{R}A_i' + \left(1 - f_0^2 - \frac{2}{R^2}\right) A_i + n_j \frac{2B_r}{R^2} \tag{4.29}$$

$$n\dot{\xi}_1 \frac{f_0}{R} = B_i'' + \frac{1}{R}B_i' + \left(1 - f_0^2 - \frac{2}{R^2}\right) B_i - n_j \frac{2A_r}{R^2}. \tag{4.30}$$

Here we have adopted a slight abuse of notation: $\xi_j = (\xi_1, \xi_2)$.

The solutions of these equations can be obtained through:

$$\begin{aligned} A_r &= \dot{\xi}_1 Z, \quad A_i = \dot{\xi}_2 n_j W \\ B_r &= \dot{\xi}_2 Z, \quad B_i = -\dot{\xi}_1 n_j W \end{aligned} \tag{4.31}$$

where Z and W satisfy

$$-f_0' = Z'' + \frac{1}{R}Z' + \left(1 - 3f_0^2 - \frac{2}{R^2}\right) Z + \frac{2W}{R^2} \tag{4.32}$$

$$-\frac{f_0}{R} = W'' + \frac{1}{R}W' + \left(1 - f_0^2 - \frac{2}{R^2}\right) W + \frac{2Z}{R^2} \tag{4.33}$$

As $R \longrightarrow +\infty$, the asymptotic behavior of W and Z is given by

$$W = -\frac{1}{2}R\log R + C_0 R + O(\log R) \tag{4.34}$$

$$Z = -\frac{1}{2R}\log R + O\left(\frac{1}{R}\right) \tag{4.35}$$

Here C_0 is a fixed constant which can be determined numerically from the profile of f_0.

Turning now to (4.25), we have

$$\begin{aligned} &\overline{\Phi}_1 \nabla \Phi_0 + \overline{\Phi}_0 \nabla \Phi_1 - (\Phi_1 \nabla \overline{\Phi}_0 + \Phi_0 \nabla \overline{\Phi}_1) \\ &= (\overline{f}_1 - f_1) f_0' \nabla R + 2in_j f_0 \nabla\theta(\overline{f}_1 + f_1) + f_0 \nabla(f_1 - \overline{f}_1) \end{aligned} \tag{4.36}$$

Therefore, we can write (4.25) as

$$\begin{aligned} \Delta H_2 &+ \frac{2}{R}\cos\theta\Big[f_0' B_i + n_j f_0' A_r + n_j f_0 A_r'\Big] \\ &+ \frac{2}{R}\sin\theta\Big[-f_0' A_i + n_j f_0' B_r + n_j f_0 B_r'\Big] = 0 \end{aligned} \tag{4.37}$$

Hence we have

$$H_2 = G_1(R)\cos\theta + G_2(R)\sin\theta, \tag{4.38}$$

where G_1 and G_2 satisfy

$$G_1'' + \frac{1}{R}G_1' - \frac{1}{R^2}G_1 + \frac{2}{R}\left[f_0' B_i + n_j f_0' A_r + n_j f_0 A_r'\right] \tag{4.39}$$

$$G_2'' + \frac{1}{R}G_2' - \frac{1}{R^2}G_2 + \frac{2}{R}\left[-f_0' A_i + n_j f_0' B_r + n_j f_0 B_r'\right] = 0 \tag{4.40}$$

Using (4.31), we obtain

$$G_1 = n_j \dot{\xi}_1 G, \quad G_2 = n_j \dot{\xi}_2 G \tag{4.41}$$

where G satisfies

$$G'' + \frac{1}{R}G' - \frac{1}{R^2}G + \frac{2}{R}\left[-f_0' W + f_0' Z + f_0 Z'\right] = 0 \tag{4.42}$$

As $R \longrightarrow +\infty$, we have

$$G = m_1 R + O(\log R) \tag{4.43}$$

where m_1 is a constant which can be determined from the functions f_0, W and Z.

In summary, we have obtained the following inner solution for H in the core of the j-th vortex:

$$H = \epsilon(-n_j \log R + C^*) + \epsilon^2 n_j m_1 \dot{\xi}_j \cdot X + \ldots \tag{4.44}$$

Outer solution revisited:

Coming back to the outer solution, we let $r_j = |x - \xi_j(t)|$. From (4.23) we have

$$h_1(x) \longrightarrow -n_j \log r_j, \quad \text{as } r_j \longrightarrow 0. \tag{4.45}$$

The solution of (4.12) and (4.45) is given by

$$h_1(x) = -2\pi \sum_{j=1}^{N} n_j K_0(|x - \xi_j(t)|) \tag{4.46}$$

Here $K_0(r)$ is the modified Bessel function.

The asymptotic behavior of $K_0(r)$ is given by:

$$K_0(r) \sim \begin{cases} \frac{1}{2\pi}\ell n r, & r \longrightarrow 0 \\ -\frac{1}{2\pi}(\frac{\pi}{2r})^{1/2} e^{-r}, & r \longrightarrow +\infty \end{cases} \tag{4.47}$$

For $r_j \ll 1$, we have locally:

$$H_1(x) = -n_j \log r_j + C_1 - \left(\sum_{i \neq j} n_i \nabla K_0(|\xi_j - \xi_i|)\right) \cdot (x - \xi_j(t)) + O(r_j^2) \tag{4.48}$$

where $C_1 = \sum_{i \neq j} K_0(|\xi_j - \xi_i|)$.

Matching:

Write (4.44) as

$$H = \epsilon(-n_j \log r_j + n_j \log \epsilon + C^* + n_j m_1 \dot{\xi}_j \cdot (x - \xi_j(t))) + \dots \tag{4.49}$$

Matching of (4.48) and (4.49) gives:

$$C^* = C_1 - n_j \log \epsilon \tag{4.50}$$

$$n_j m_1 \dot{\xi}_j = \sum_{i \neq j} n_i \nabla K_0(|\xi_j - \xi_i|) \tag{4.51}$$

Ideally we should have included an order $\epsilon \log \epsilon$ term in the inner expansion. But this is only a matter of formality.

(4.51) is the equation we are looking for. We can rewrite it as

$$m_1 \dot{\xi}_j = -\nabla_{\xi_j} \mathcal{H}(\xi_1, \dots \xi_N) \tag{4.52}$$

where

$$\mathcal{H}(\xi_1, \dots \xi_N) = \sum_{i \neq j} n_i n_j K_0(|\xi_i - \xi_j|) \tag{4.53}$$

An immediate consequence is that the interaction between a pair of vortices is repulsive if their indices have the same sign, and attractive if their indices have different sign.

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Numerical Experiments on the Ginzburg-Landau Equations

*Man Kam Kwong**

Abstract. We report on some numerical experiments done on the Ginzburg-Landau equations of the theory of superconductivity. The equations under periodic boundary conditions are solved numerically by using a nonstandard discretization and the sweeping algorithm. The programs, written in Matlab and Fortran, work in an interactive mode and include graphics display.

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1. Introduction

In this article we report on experiments we did on solving the Ginzburg-Landau (GL) equations on a Sun Sparc II workstation. Our contributions consist of a careful formulation of the discrete form of the equations, a choice of a suitable gauge transformation to simplify the equations, a new "sweeping" algorithm, and a practical implementation of the solution procedure that includes run-time graphics display. More details will be given in a forthcoming paper [9].

The GL equations arise in the theory of superconductivity. For a recent survey of previous work done on the equations, see the articles [3] by Chapman, Howison, and Ockendon and [5] by Du, Gunzburger, and Peterson.

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Theoretical physicists have long been able to extract useful information from the GL equations by constructing their solutions "analytically," based on series approximations, or by ignoring certain unimportant variations in the solutions. One of the triumphs of this approach was the prediction by Abrikosov [1] that certain superconductors, classified as Type II, admit vortices of supercurrent, a fact confirmed by experiments only ten years later. Numerical solution of the full equations, especially for the simulation of vortices, has been successful only in recent years. The different approaches include simulated annealing (Doria et al.[4]), the relaxation method (Adler and Piran [2], Wang and Hu [13]), optimization (Garner et al. [7]), and finite elements (Du, Gunzburger, and Peterson [5,6]).

Although simulated annealing, being a Monte Carlo method, consumes many computing cycles, it carries a better assurance for finding the global minimizer of the energy functional. All other approaches yield local critical points which, although they are solutions to the GL equations, may not be the physically meaningful global minimizer. The relaxation method is simple in theory, but time-consuming because small time steps are required to avoid instability of the numerical scheme. Wang and Hu applied it only to the case of a single vortex. More recent work by Maekawa, Kato, and Enomoto [12] employs the same technique to treat the time-dependent GL equations. The optimization approach makes use of state-of-the-art optimization and linear algebra techniques in advanced scientific computing and is the choice for designing large-scale production codes. The finite elements method is important because it is applicable to arbitrary geometry and admits higher-order refinements, while the other methods are limited to first-order finite difference approximations.

Our work falls between the optimization and the finite element approaches. Our code runs on a Sparc II with reasonable speed; it can be easily parallelized to work faster on larger computers. It gives the user more control over the experiment. For instance, parameters can be altered interactively and the experiment repeated without having to recompile the program; The results are displayed graphically for the user to monitor the progress. These capabilities are made possible by using the Matlab package, which provides a powerful programming environment. The code is able to employ finer grids to give smoother solutions than those achievable in [6]. Unlike the optimization approach, our method can be and has actually been successfully modified to solve the time-dependent GL equations.

2. The Discrete GL Model

We discuss only the two-dimensional case in this paper; the generalization to the full three-dimensional case is straightforward. The superconducting material is in the form of a thin film occupying a domain in R^2. When placed in a magnetic field, with the direction of the field perpendicular to the film, Type-II superconductors form vortices of superconducting current. Close to regular hexagonal arrangements of these vortices have been observed experimentally. Distortions can be attributed to impurities and defects in the material. A typical numerical result is shown in Figure 1. In the periodic GL model, it is assumed that, at least deep into the interior of the domain when boundary effects are negligible, the magnetic state of a pure and homogeneous material varies doubly periodically: one can carve out a core region Ω such that the state of the entire superconductor, except for a thin boundary layer, can be accurately reproduced by extending that of Ω periodically. Traditionally (see, for example, [4]), Ω is chosen to be a rectangle, such as that shown on the left in Figure 1. In order to reproduce a regular hexagonal lattice, the aspect ratio of the rectangle has to be $1 : \sqrt{3}$.

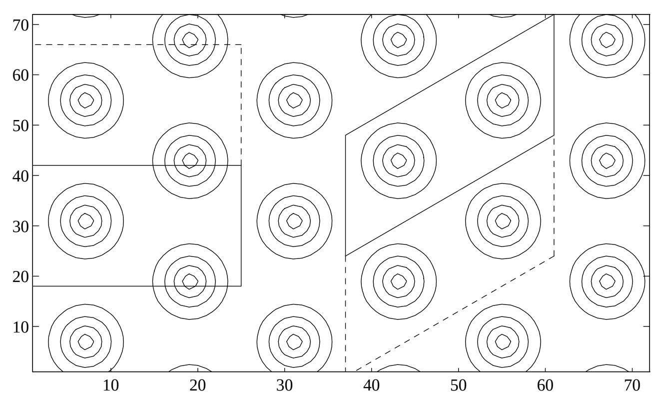

Figure 1. Core regions

Du, Gunzburger, and Peterson [6] suggested the more general parallelogram region, such as that shown on the right of Figure 1. For a hexagonal lattice, the acute angle of the parallelogram is $60°$. The two special choices shown here in Figure 1 are actually equivalent. To see this, we can dissect the parallelogram into two triangles as shown in Figure 2, and translate the upper one to form a rectangle that is congruent to the rectangular region.

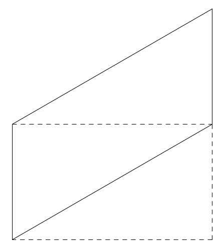

Figure 2. Equivalence of two special core regions

According to Ginzburg and Landau [8], the magnetic state of the material is completely determined by two functions, a complex-valued scalar function ψ and a (two-dimensional in our two-dimensional version) vector potential $\mathbf{A} = (A, B)$. The fundamental postulate is that for equilibrium these functions seek to minimize an energy functional, which, in dimensionless units, has the form

$$\mathcal{G}(\psi, \mathbf{A}) = \int_\Omega \left(\frac{|\psi|^4}{2} - |\psi|^2 + |(\nabla - i\mathbf{A})\psi|^2 + \kappa^2 |\nabla \times \mathbf{A}|^2 \right) d\mathbf{x}, \qquad (2.1)$$

where κ is a constant characteristic of the metal. The superconductor is classified as Type II if $\kappa > 1/\sqrt{2}$, and as Type I otherwise.

The functional is invariant under the so-called gauge transformations. Let χ be any real-valued function on Ω. Then the transformed pair $(\overline{\psi}, \overline{\mathbf{A}})$

$$\overline{\psi} = \psi e^{i\chi}, \quad \overline{\mathbf{A}} = \mathbf{A} + \nabla\chi, \qquad (2.2)$$

yields the same energy as that of $(\psi, \mathbf{A})$. Indeed, $(\psi, \mathbf{A})$ and $(\overline{\psi}, \overline{\mathbf{A}})$ are considered as equivalent representatives of the same magnetic state of the material.

This gauge invariance has more than one consequence. First, there is not only one single minimizer to the free energy, but an entire class of gauge equivalent solutions. Second, the assumption that the magnetic state varies periodically does not imply that $(\psi, \mathbf{A})$ varies periodically, but only that they are gauge equivalent on opposite edges of Ω. These facts gives rise to complications in the formulation of the boundary value problem, but they can also be used to our advantage. We can confine our search to solutions that have special properties. The technique has traditionally been called "fixing a gauge." For instance, the London gauge requires that $\nabla \cdot \mathbf{A} = 0$, and Wang and Hu note that B can be chosen independent of y. An excellent discussion of gauge fixing can be found in Du, Gunzburger, and Peterson [5]. In [9], we show the existence of a gauge stronger than that of Wang and Hu and compatible with a simplified set of "quasi-periodic" boundary conditions. To summarize:

A is fully periodic and is constant along the top edge,
B and ψ are periodic with respect to the top and bottom edges,
B is independent of y and has a jump of h on the vertical edges, and
ψ has a phase change e^{ihy} on the vertical edges.

Here $h = 2\pi n/L_y$ is a constant determined by the number of vortices n in Ω and the length L_y of the vertical edge of Ω. In turn, h determines the external magnetic field. The fact that B is independent of y significantly reduces the total number of unknowns to be solved. Another advantage of this choice of gauge is that the ensuing differential equations for A and B are "decoupled" in the sense that a cross-term involving B is absent in the equation for A and vice versa. This makes it simple to solve for A and B in each iterative step.

Gauge field theorists do not use standard finite difference methods on the continuous form of the energy functional for numerical purposes. With such methods, the discretized form of the gauge transform no longer preserves the energy, as a result of truncation errors. Field theorists have adopted the following modifications (see, for example, [2]). Suppose that Ω is discretized as usual with a uniform rectangular grid, with grid spacings of h_x and h_y. The order parameter ψ takes values at each of the grid points. The x-component A of $\mathbf{A}$ takes values on the bond (line) joining a grid point with its right-hand neighbor, while B takes values on the bond joining a grid point with its upper neighbor. To simplify the formulas, we define

$$U = \mathrm{e}^{iAh_x} \quad \text{and} \quad V = \mathrm{e}^{iBh_y}. \tag{2.3}$$

The free energy is then approximated by the discrete functional

$$\begin{aligned} \mathcal{G}_d = \sum_{\text{grid}} \Bigg(& \frac{|\psi|^4}{2} - |\psi|^2 + \left| \frac{\psi^{\rightarrow} - U\psi}{h_x} \right|^2 + \left| \frac{\psi^{\uparrow} - V\psi}{h_y} \right|^2 \\ & + \kappa^2 \left| \frac{A^{\uparrow} - A}{h_y} \right|^2 + \kappa^2 \left| \frac{B^{\rightarrow} - B}{h_x} \right|^2 \Bigg) h_x h_y . \end{aligned} \tag{2.4}$$

The arrow direction indicates the appropriate neighbors (boundary grid points have neighbors that are outside of Ω, but these can be interpreted as the appropriate value on grid points lying on the the opposite edge, modified according to the given boundary conditions). The conventional justification for this formula is that after an expansion in Taylor series, (2.1) and (2.4) agree up to first-order terms. Invariance is restored under a discrete gauge transformation:

$$\overline{\psi} = \psi \mathrm{e}^{i\chi}, \quad \overline{A} = A + \frac{\chi^{\rightarrow} - \chi}{h_x}, \quad \overline{B} = B + \frac{\chi^{\uparrow} - \chi}{h_y}. \tag{2.5}$$

In [9] we give a new interpretation to the discrete functional, clarify what "A and B are defined on the bonds" means, and show that the approximation offered by (2.4) is, in fact, of a higher order than is traditionally believed.

There is another disadvantage of working directly with the discretized form of (2.2). The order parameter ψ is a highly oscillatory function, as a result of large variations of its phase. A moderately fine spatial grid, as is allowable in practice, is usually not adequate to resolve ψ in regions of high oscillation. In such cases, the finite difference $(\psi^{\rightarrow} - \psi)/h_x$ can be a very poor approximation for the derivative $\partial\psi/\partial x$. On the other hand, in (2.4) it is the difference between $\psi^{\rightarrow}$ and $U\psi$ that is being computed. As pointed out in [9], we are actually approximating the derivative $\partial(\psi e^{i\int A})/\partial x$ by means of a central difference. The product function $U\psi$ oscillates much less than ψ itself. We have, therefore, chosen (2.4) as the starting point of our numerical method.

The Euler equations corresponding to the minimization of (2.4) are then

$$\frac{U^{\leftarrow}\psi^{\leftarrow} - 2\psi + U^{*}\psi^{\rightarrow}}{h_x^2} + \frac{V^{\downarrow}\psi^{\downarrow} - 2\psi + V^{*}\psi^{\uparrow}}{h_y^2} + (1 - |\psi|^2)\psi = 0, \tag{2.6}$$

$$\frac{A^{\uparrow} - 2A + A^{\downarrow}}{h_y^2} + \frac{\Im\left(\psi^{\rightarrow}\psi^{*}U^{*}\right)}{h_x} = 0, \tag{2.7}$$

and

$$\frac{B^{\leftarrow} - 2B + B^{\rightarrow}}{h_x^2} + \frac{1}{N_y}\sum_{\text{column}} \frac{\Im\left(\psi^{\uparrow}\psi^{*}V^{*}\right)}{h_y} = 0, \tag{2.8}$$

where $\Im(.)$ denotes the imaginary part of a complex number, and N_y is the number of rows in the grid. Although (2.6) is probably known to everyone who uses the discrete functional, it has not been mentioned in the literature. Note the simplicity of the linear operator on ψ represented by the first two terms (as compared to the corresponding Euler equation obtained from (2.1)); it is a generalized discrete Laplace operator, having variable coefficients instead of the familiar $\{1, -2, 1\}$. Each of (2.6) and (2.7) stands for as many equations as there are grid points, while (2.8) stands for only N_x equations. Note also that there would be an extra term involving B in (2.7) and one involving A in (2.8), if we had not used our special gauge.

To conclude the section, we summarize the numerical problem we are tackling:

> Given a rectangular region Ω of suitable size ($L_x \times L_y$), a grid (with $N_x \times N_y$ points), and the number of vortices in Ω (n which is usually 2, 4, or 8), we wish to find the $2N_x \times N_y + N_x$ unknown values: ψ (at each grid point), A (on each bond), and B (on each column of bonds) that satisfy the GL equations (2.6)–(2.7) and the appropriate boundary conditions.

3. The Solution — the Sweeping Algorithm

We describe in this section how the solution to the problem is computed by using an iterative scheme. The system of equations (2.6)–(2.8) are quasi-linear and can be rewritten in the operator form:

$$\mathcal{L}\psi = (|\psi|^2 - 1)\psi = F(\psi), \tag{3.1}$$

$$\mathcal{M}A = f(\psi, A), \tag{3.2}$$

$$\mathcal{N}B = g(\psi, B). \tag{3.3}$$

After inverting the linear operators, we obtain the following iterative formulas:

$$\psi_{n+1} = \mathcal{L}^{-1}F(\psi_n), \quad A_{n+1} = \mathcal{M}^{-1}f(\psi_n, A_n), \quad B_{n+1} = \mathcal{N}^{-1}g(\psi_n, B_n). \tag{3.4}$$

For our initial triple (ψ_0, A_0, B_0), we take ψ_0 to be random, A_0 to be 0, and B_0 to be linear and increasing from $-h/2$ to $h/2$. The formulas (3.4) are used recursively to form the sequence of approximations (ψ_n, A_n, B_n) until they converge.

In our actual program, we employed some additional techniques to gain faster convergence. Rather than using (3.4), we solve (3.1)–(3.3) by using a quasi-Newton method. A damping factor is introduced to achieve stability. Also instead of taking (ψ_n, A_n, B_n) to be the starting point for the next iteration, a line search in the direction of this triple is performed to obtain a better starting point with lower energy.

Equation (3.3) is a cyclic tridiagonal linear system and can easily be solved by the linear algebra package Matlab. Although (3.2) comprises more equations than (3.3), once the right-hand side is known (computed from the results from the previous iterative step), the equations for each column of grid bonds are decoupled from those of another column. Thus, there are N_x systems of cyclic tridiagonal linear systems, each of which can be solved in exactly the same way as for (3.3).

The more interesting and difficult job is to invert $\mathcal{L}$, a five-point stencil that is a linear combination of the values of ψ at each grid point and its four neighbors: left, right, down, and up. The general form of a five-point stencil is

$$S[z] = Cz + Lz^{\leftarrow} + Rz^{\rightarrow} + Dz^{\downarrow} + Uz^{\uparrow}, \tag{3.5}$$

where C, L, D, and U are coefficients that can vary from one grid point to another. A nonhomogeneous stencil equation is

$$S[z] = b, \tag{3.6}$$

where b is given at each grid point.

The classical method for solving (3.6) is to treat it as a sparse linear system of order equal to the total number of grid points. Efficient use of existing sparse matrix solvers can then be used. The technique, however, is not simple for many who are not familiar with the subject area. In [10], we proposed an intuitively more straightforward method, the sweeping algorithm, for inverting certain regular five-point stencils including, $\mathcal{L}$. The method is related to the shooting method for solving boundary value problems of ordinary differential equations. Regular forms of the method are not hard to implement, and Matlab programs have been successfully written and reported in [11]. These Matlab programs are adequate for the purpose of our experiments on solving the GL equations.

One of the basic ideas of the sweeping algorithm is that once the values of the variable z is known on two columns (or rows) of grid points, its values on an adjacent column (row) can be computed from (3.6), provided that none of the stencil coefficients vanishes. For instance, take the column to the right of the two known columns. Each grid point is a right-hand neighbor of some grid point on the second column. Hence, from (3.6),

$$z^{\rightarrow} = \frac{b - (Cz + Lz^{\leftarrow} + Dz^{\downarrow} + Uz^{\uparrow})}{R}. \tag{3.7}$$

Continuing in this way, we can compute the values of z on every column, and can solved (3.6). The difficulty, of course, is to figure out the values on the two initial columns.

Our idea is to start with a wild guess, find out how much error we have made, and then fine-tune the initial guess to obtain the correct answer. Since one wild guess is just as good (or as bad) as another, we pick the simplest one, namely, that $z = 0$ on the two initial columns. We then compute z on the remaining columns. After we have finished with the computation, we will have used $N_x - 2$ columns of the stencil equations. There are two more columns of equations that have not been used; they are not likely to be satisfied, however, since our initial guess is rather haphazard. The discrepancy (from satisfying these remaining equations) is a vector E of order $2N_y$ and serves as a measure of how much we have missed the target and also as our guide for making corrections in the steps to come.

We next sweep the homogeneous stencil for a unit variation in each of the grid points on the two initial columns. The ensuing discrepancy in the last two columns of equations tells us what difference will be introduced by tuning each of the initial grid points. All this information is thee gathered to form a rectifying matrix $\mathcal{R}$. The knowledge of E and $\mathcal{R}$ will inform us how to choose the values of z on the initial columns correctly.

This simple procedure works remarkably well for grids of moderate sizes. For large grid sizes, some sophisticated modifications are needed to avoid instability (the rapid growth of z after repeated application of (3.7)). Two methods, multi-stage and partial sweepings, together with their implementations are described in detail in [10] and [11].

Besides its simplicity, the sweeping algorithm has other advantages. The complete information for constructing the inverse of the five-point stencil is stored in the relatively small inverse of the $2N_y \times 2N_y$ matrix $\mathcal{R}$. There is also great potential for exploiting parallelism in the algorithm, but further work needs to be done along this line.

To conclude this section, we make some remarks concerning local minimizers of the GL equations. Although many people are apt to claim that, in their computation, they never see a critical point that is not the global minimizer, our experience seems to indicate the opposite. As the results in the next section show, the vortices appear at different heights in the core region. However, if one starts with a symmetric initial guess, then, at least in theory, the nonannealing methods should lead to a symmetric solution with the two vortices located at the same height. One can argue that such a solution is normally "unstable," so that any small perturbation (such as those arising from rounding errors), is enough to shift the unstable solution to a stable one. Yet some numerical methods for solving nonlinear equations, such as Newton's method, do not distinguish between stable and unstable solutions. Indeed, in our experience, this is what will happen if we use a quasi-Newton's method on (3.1) too early in the process. Our use of a random initial ψ_0 is an attempt to maximize the chance of starting near the correct solution. Also, our experiments indicate that, for regions containing many vortices, there can be numerous locally stable configurations distinct from the global minimizer.

4. Numerical Experiments

The main programs are written in Matlab to take advantage of its interactive features. In order to achieve greater speed, those commands connected with the sweeping algorithm have been recoded in Fortran by A. J. Lindeman and the compiled object file have been dynamically linked to Matlab through the "mex" facility. Lindeman, who also helped with most of the experiments mentioned in this section, is a participant in the summer 1992 Student Research Participation Program at Argonne National Laboratory, and is currently a physics graduate student at Purdue University

A typical run of an experiment is as follows. One sets, either interactively or by using a Matlab script file, the various parameters of the problem: the size of the domain L_x and L_y, the number of vortices n, the superconductor constant κ, the number of grid points N_x and N_y, the tolerance used to terminate the iteration, etc. The user needs to issue only two commands to get the experiment going. The first is a subroutine `setup` to set up the grid, to pick the initial state as a starting point for iteration, and to compute the various quantities needed to impose the quasi-periodic boundary conditions. The command `setup` calls an other subroutine `rr` automatically to compute the coefficients of the five-point stencil equation (3.4) and the rectifying matrices for the sweeping algorithm. This command is needed only at the beginning of the experiment. The second command, `rn`, performs the iteration process. It calls two subroutines, `onep` and `oneAB`, automatically and repeatedly to accomplish each iteration step until the desired accuracy is reached. After each step, various information, such as the maximum value of ψ_n, and the free energy are printed on the screen. A contour plot of $|\psi_n|$ is also displayed, for the user to monitor the progress.

In our experiments, we obtained plots of $|\psi|^2$ for various domain sizes. Two of these are shown below. Both are computed with $\kappa = 5$. The contour heights in the graphs are (0.05,0.1,0.15,0.20) and (0.1,0.3,0.5,0.7,0.9), respectively.

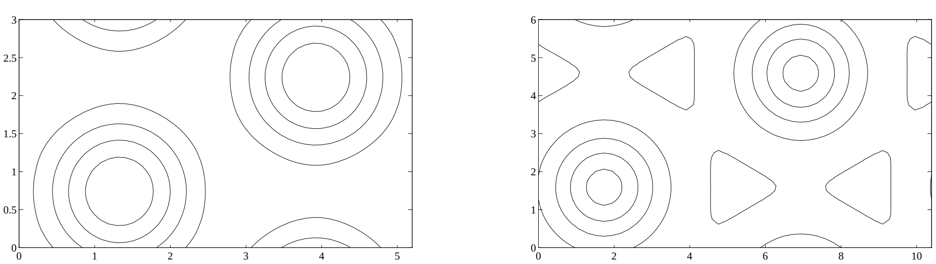

Figure 3. Two sample contour plots of $|\psi|^2$

We have investigated whether a parallelogram core region with angle 60°, corresponding to a strict hexagonal lattice, gives the best vortex configuration, with the lowest energy. To this end, we used core regions of the same area ($= 3 \times 3\sqrt{3}$) but different aspect ratios, and computed the least energy solutions for each. At first we discovered, to our surprise, that 60° is not the optimal angle. A plot of the energy (minus 16.2295 against the aspect ratio of the core region (width/height) is shown below. We used a grid size of 24×24 and $\kappa = 5$.

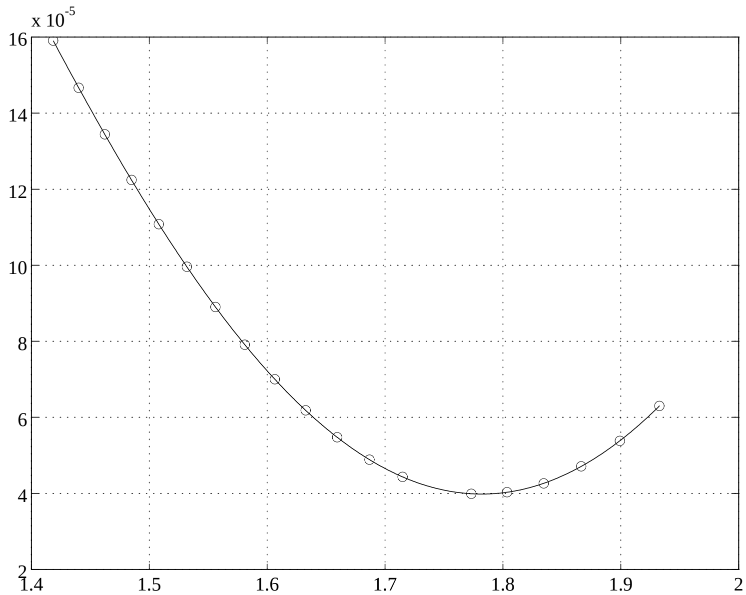

Figure 4. Energy against aspect ratio of core region

More experimentation revealed that this was due to discretization error. Increasing the grid size shifts the optimal angle towards 60°, and indeed an extrapolation with $N_x, N_y \to \infty$ shows the optimal angle to be 60°, within approximation error.

We have experimented with the phenomenon of pinning. A pinning site is caused by some defect in the superconducting material. It has a high resistivity to currents and so tends to pin down the center of a vortex. We modeled a pinning center by adding a penalty term $\gamma|\psi(\mathbf{x})|^2$ to the energy functional, where γ is a large positive constant and $\mathbf{x}$ is the location of the defect. This extra term alters the stencil coefficient C at the grid point corresponding to the pinning site. Our method successfully simulated the phenomena by giving a solution that nearly vanishes at the site.

Finally, we were also able to detect numerically the upper critical field. An increase in the external magnetic field corresponds to a more tightly packed vortex lattice, or a smaller core region. We solved the GL equations over core regions of different sizes and discovered that the maximum of ψ falls as the area decreases. Below the bifurcation point, $L_y = 2.68929$, which corresponds to an upper critical field of $H_{c2} = 1.00316868$, the trivial solution, $\psi \equiv 0$, takes over as the global minimizer. A plot of $\max|\psi|$ against the external field H is given below.

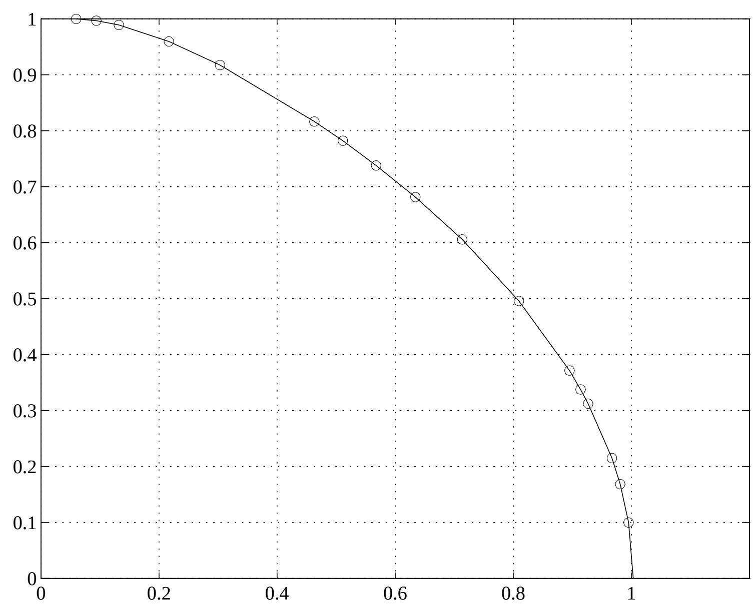

Figure 5. $\max|\psi|$ against external field

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