Investigation of Numerical Models for New High Temperature Superconductors

Chad Sockwell*

Co-advisors:
Dr. Janet Peterson and Dr. Max Gunzburger
Florida State University

Abstract Recent discoveries of new high temperature superconductors initiated investigations to harness these new material's properties. Unfortunately, many new high temperature superconductors come with odd properties such as multi-band interactions and anisotropic behavior, as is the case for Magnesium Diboride. In this research, Ginzburg Landau model variants are modified to try and simulate these materials more realistically at a mesoscopic scale. In particular an Anisotropic Two-Band Time dependent Gnzburg Landau with inter-band coupling effects is formed to describe Magnesium Diboride.

Superconductivity and The Ginzburg Landau Model

- Superconductivity is a phenomena where a material cooled below its critical temperature, T_c (typically close to 0 K), looses all electrical resistance.
- Another feature of superconductivity is perfect diamagnetism in the presence of an applied magnetic field. This is also known as the Meissner Effect. Type I and Type II materials exhibit this effect differently
- Type I materials exhibit this effect until a field strength of H_{c1} is reached, then the material returns to the normal state.
- Type II materials exhibit a semi Meissner effect between H_{c1} and an upper critical field H_{c2}.
- In 2001 a new high temperature superconductor was discovered, Magnesium Diboride or MgB_2, with a T_c of 39K
- This new material also comes with a variety of new properties such as two superconducting bands, anisotropies in the critical magnetic field H_c, modified length scales, and inter-band interactions from the two superconducting bands[1]
- The Ginzburg Landau model is a mesoscopic phenomenological model that describes superconductivity and is valid for $0.6\,T_c < T < T_c$
- The model was derived by Ginzburg and Landau by applying Landau's theory of Second Order Phase Transitions to superconductors.
- The variables of interest are the order parameter $|\psi|^2$ and the magnetic vector potential $\mathbf{A}$.
- The order parameter is proportional to the squared amplitude of the superconducting electron pairs' wave functions.
- There characteristic parameters can be introduced through nondimensionalization. The coherence length of the order parameter $\xi(T)$, the penetration depth of th magnetic field $\lambda(T)$, and their ratio the Ginzburg Landau parameter $\kappa = \frac{\lambda}{\xi}$, which characterizes a material as a Type I or II material.

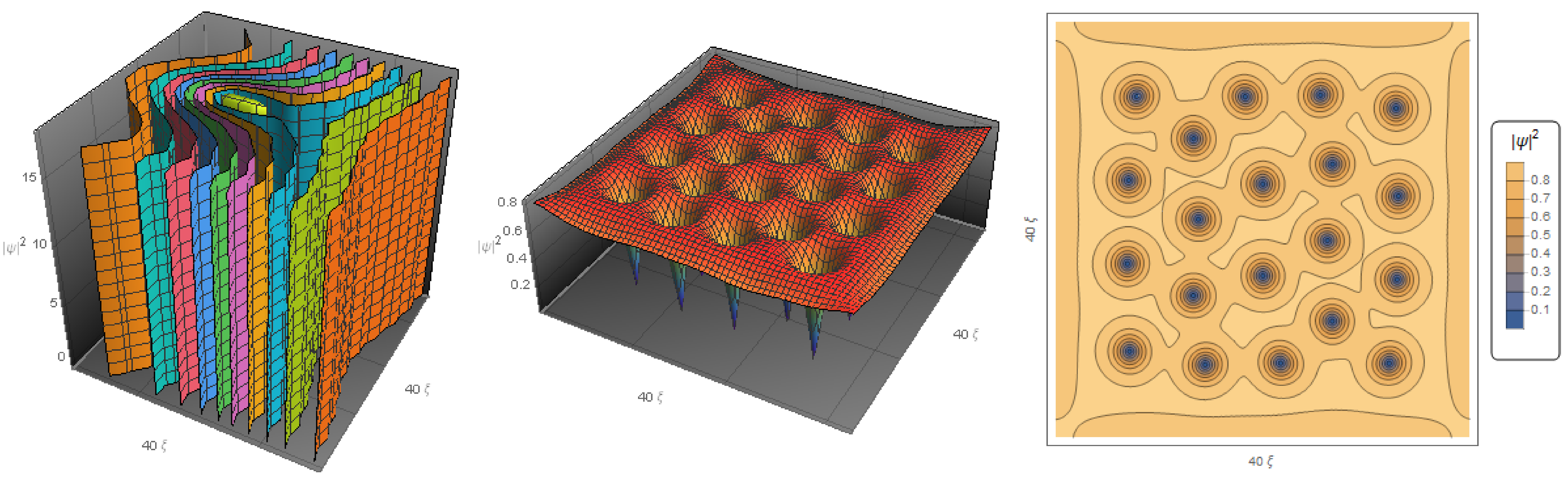


Figure 1: (left) A 3D Example of $|\psi|^2$. (Center and right) A 2D example of $|\psi|^2$.

Anisotropic Two Band Time-Dependent Ginzburg Landau Model with Interband Coupling Effects

Several modifications can be made to Ginzburg Landau model to describe unconventional high temperature superconductors. In the case of a clean sample of MgB_2, a second order parameter equation is added, the anisotropy of the upper critical magnetic field H_{c2} is captured using an anisotropic effective mass tensor $\boldsymbol{\gamma}$, and interband coupling terms (η, η_1) are added for interactions between the superconducting bands. The system is considered isothermal throughout the evolution.The following set of equations can be derived from the models found in[2],[3]for (x,y,t)$\in \Omega \times (0, t_{max})$. This model is known as the Anisotropic TB-TDGL model for short.

$$\int_\Omega \frac{\partial \psi_1}{\partial t}\tilde{\psi} + (|\psi_1|^2 - \tau_1)\psi_1\tilde{\psi} + \mathbf{D}_1\psi_1 \cdot \mathbf{D}_1\tilde{\psi}_1 + \eta\psi_2\tilde{\psi} + \eta_1\frac{\xi_1}{\nu\xi_2}\mathbf{D}_2\psi_2 \cdot \mathbf{D}_2\tilde{\psi}\, d\Omega = -\int_{\partial\Omega} \zeta_1 \frac{\xi_1^2}{x_0}\psi_1\tilde{\psi}\, d(\partial\Omega) \quad (1)$$

$$\int_\Omega \Gamma_e\frac{\partial \psi_2}{\partial t}\tilde{\psi} + (|\psi_2|^2 - \tau_2)\psi_2\tilde{\psi} + \mathbf{D}_2\psi_2 \cdot \mathbf{D}_2\tilde{\psi} + \eta\psi_1\tilde{\psi} + \eta_1\frac{\xi_2}{\xi_1}\mathbf{D}_1\psi_1 \cdot \mathbf{D}_1\tilde{\psi}\, d\Omega = -\int_{\partial\Omega} \zeta_2 \frac{\xi_2^2}{x_0}\psi_2\tilde{\psi}\, d(\partial\Omega) \quad (2)$$

$$\begin{aligned}\int_\Omega \sigma_e \frac{x_o^2}{\lambda_1^2}\frac{\partial \mathbf{A}}{\partial t}\tilde{\mathbf{A}} + (\nabla\cdot\mathbf{A})\cdot(\nabla\cdot\tilde{\mathbf{A}}) + (\nabla\times\mathbf{A})\cdot(\nabla\times\tilde{\mathbf{A}}) + \mathscr{R}\{i\frac{1}{\kappa_1}(\boldsymbol{\gamma}_1\cdot\nabla\psi_1)\cdot\psi_1\cdot\tilde{\mathbf{A}}\} + \frac{x_0^2}{\lambda_1^2}|\psi_1|^2\mathbf{A}\cdot\tilde{\mathbf{A}} \\ + \mathscr{R}\{i\frac{1}{\nu\kappa_1}(\boldsymbol{\gamma}_2\cdot\nabla\psi_2)\cdot\psi_2\tilde{\mathbf{A}}\} + \frac{x_0^2}{\lambda_2^2}|\psi_2|^2\mathbf{A}\cdot\tilde{\mathbf{A}} + \eta_1(\mathscr{R}\{i\frac{\xi_1}{\lambda_2}(\boldsymbol{\gamma}_1\cdot\nabla\psi_1)\cdot\psi_2\tilde{\mathbf{A}}\} + \mathscr{R}\{i\frac{\xi_1}{\lambda_2}(\boldsymbol{\gamma}_2\cdot\nabla\psi_2)\cdot\psi_1\tilde{\mathbf{A}}\}) \\ + \eta_1\frac{x_0}{\lambda_1\lambda_2}\{(\psi_1\psi_2^* + \psi_2\psi_1^*)\mathbf{A}\cdot\tilde{\mathbf{A}}\}\, d\Omega = \int_\Omega \mathbf{H}_e\cdot(\nabla\times\tilde{\mathbf{A}})\, d\Omega\end{aligned} \quad (3)$$

With

$$\boldsymbol{\gamma}_i = \begin{pmatrix} \frac{1}{\gamma_{i,x}} & 0 \\ 0 & \frac{1}{\gamma_{i,y}} \end{pmatrix}, \quad \tau_i = 1 - \frac{T}{T_{c,i}}, \quad \nu = (\frac{\lambda_2(0)\xi_1(0)}{\lambda_1(0)\xi_2(0)}),\ \mathbf{D}_1 = \boldsymbol{\gamma}_1\cdot(-i\frac{\xi_1}{x_0}\nabla - \frac{x_0}{\lambda_1}\mathbf{A}),\ \mathbf{D}_2 = \boldsymbol{\gamma}_2\cdot(-i\frac{\xi_2}{x_0}\nabla - \nu\frac{x_0}{\lambda_2}\mathbf{A})$$

and boundary conditions on $\partial\Omega \times (0, t_{max})$ and initial conditions on Ω:

$$[(-i\frac{\xi_1}{x_0}\boldsymbol{\gamma}_1\cdot\nabla\psi_1) + \frac{\eta_1}{\nu}(-i\frac{\xi_2}{x_0}\boldsymbol{\gamma}_2\cdot\nabla\psi_2)]\cdot\mathbf{n} = i\zeta_1\frac{x_1}{x_0}\psi_1\ , \quad (\nabla\times\mathbf{A}\times\mathbf{n}) = \mathbf{H}_e\times\mathbf{n}$$

$$[(-i\frac{\xi_2}{x_0}\boldsymbol{\gamma}_2\cdot\nabla\psi_2) + \frac{\eta_1}{\nu}(-i\frac{\xi_1}{x_0}\boldsymbol{\gamma}_1\cdot\nabla\psi_1)]\cdot\mathbf{n} = i\zeta_2\frac{x_1}{x_0}\psi_2\ , \quad (\mathbf{A}\cdot\mathbf{n}) = 0$$

$$\psi_1(x,y,0) = \psi_{10}(x,y),\ \psi_2(x,y,0) = \psi_{20}(x,y),\ \mathbf{A}(x,y,0) = \mathbf{A}_0(x,y)$$

*Undergraduate double majoring in Computational Science and Physics. Double B.A. expected in Fall 2015.

Computational Methods

Finite element approximations were used to solve the model given by Equations (1)-(3). The steps below are methods used to obtained and solve the model given by Equations (1)-(3), from the modified Free energy functional from [2],[3].

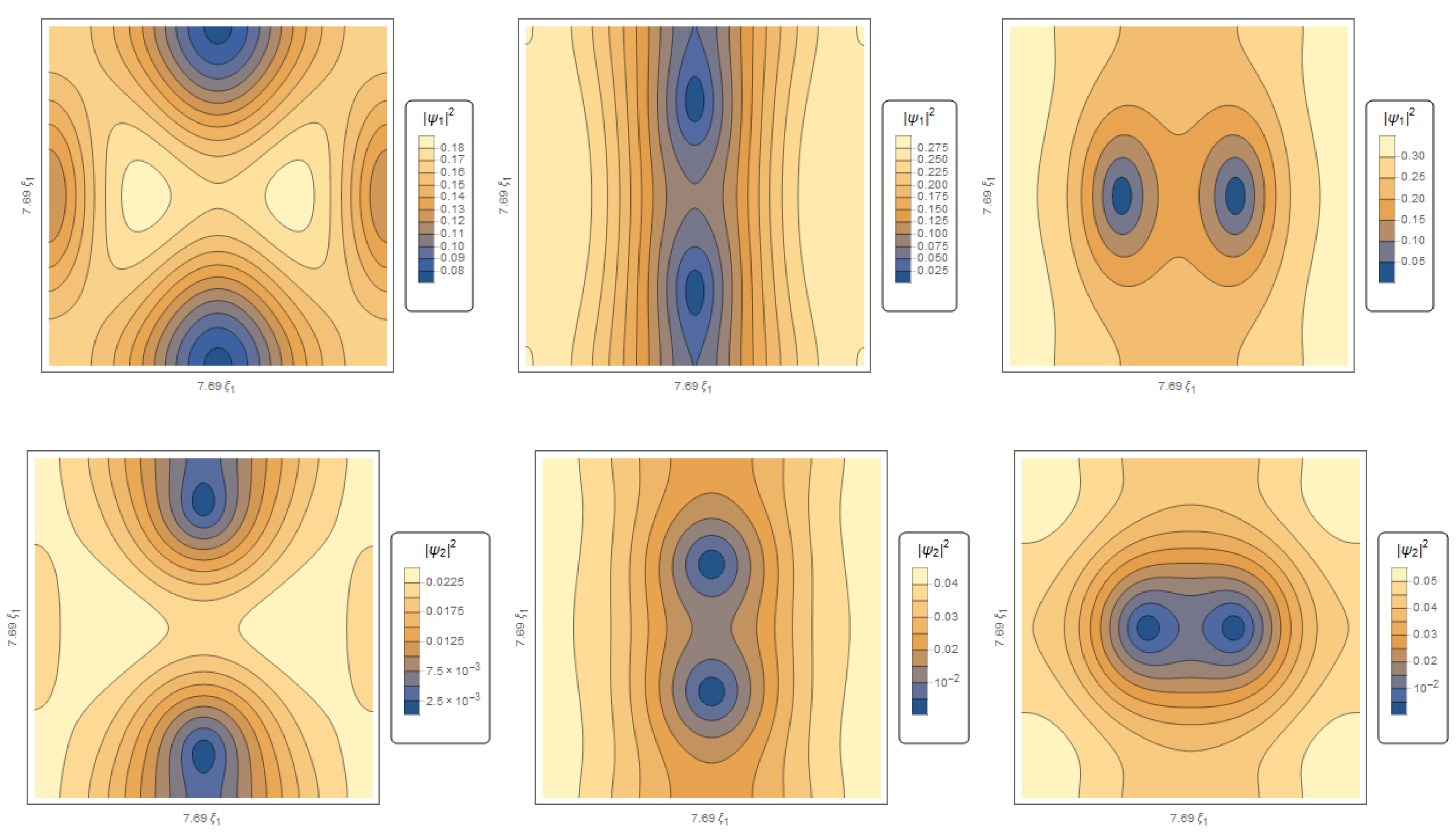
- The free energy functional's variation in $(\psi_1, \psi_2, \mathbf{A})$ was found using calculus of variations, giving the weak form.
- Next the weak form was nondimensionalized using the relations from [2],[3], introducing the characteristic parameters λ, ξ, and κ
- The system in Equations (1)-(3) is closed using a gauge transformation $(\psi_1, \psi_2, \mathbf{A}, \Phi) = G_\chi(\Lambda_1, \Lambda_2, \mathbf{Q}, \Theta)$
- The zero scalar potential gauge is chosen, yielding $\Phi = 0$ and boundary condition $\mathbf{A}\cdot\mathbf{n} = 0$
- The artificial $(\nabla\cdot\mathbf{A}, \nabla\cdot\tilde{\mathbf{A}})$ term is added to make the system coercive, used in [3],[4]
- A set of test functions is chosen from a discrete space, $(\tilde{\psi}_1^h, \tilde{\psi}_2^h, \tilde{\mathbf{A}}^h) \in (\mathcal{V}^h \times \mathcal{V}^h \times \mathbf{V}^h) \subset \mathbb{P}^2$
- Each variable , $(\psi_1^h, \psi_2^h, \mathbf{A}^h)$, is approximated as linear combination of test functions, by expanding them in the discrete space
- The time domain is discretized using the Backward Euler method, $\frac{\partial u}{\partial t}|_{t=tn} \approx \frac{u^n - u^{n-1}}{\Delta t}$
- The resulting system is non linear and must be made into a Newton system before solving.
- The Newton system is then solved at every time step using A Biconjugate conjugate gradient stabilized or BICGSTAB solver

Modeling Magnesium Diboride (MgB_2)

The finite element approximations of the Anisotropic TB-TDGL model can used to describe and make predictions about new high temperature superconductors. One choice is a clean sample of MgB_2. This material shows two band and anisotropic superconducting properties [1].One band possesses highly anisotropic σ energy gap structure. The second band has a nearly isotropic π energy gap structure. This creates an interesting situation where one band has Type II (σ) properties and the other possess Type I properties(π). The vortex dynamics in MgB_2 can studied using the finite element approximations. Physical results such as vortex pinning forces, critical currents, and the Gibbs free energy can obtained from the model and compared to experimental results. The parameters given in the table below were used to model MgB_2,[1][5].

$\xi_\sigma(0)$	$\lambda_\sigma(0)$	κ_σ	$\xi_\pi(0)$	$\lambda_\pi(0)$	κ_π	T_c	$T_{c,\sigma}$	$T_{c,\pi}$	$\gamma_{\sigma,x}$	$\gamma_{\sigma,y}$	$\gamma_{\pi,x,y}$	$\mu_0 H_{c2}^{\parallel}$	$\mu_0 H_{c2}^{\perp}$
13nm	47.81nm	0.66	51nm	33.6nm	3.68	39K	35.6K	11.8K	4.55	1	1	3.2T	14.5T

There are two free parameters and the two coupling constants. The external magnetic field $\mathbf{H}_e$ can be varied to affect the behavior of the vortices. The operating temperature T can be varied, but must remain under T_c for the sample to exhibit superconducting properties. The operating temperature also must stay with in the validity of the GL model. The coupling parameters for bands in MgB_2 are weak but not well known[1]. The plots below show the evolution of $|\psi_1|^2$ and $|\psi_2|^2$ for $\eta = 0.1$, $\eta_1 = 0$, $\zeta = 0$, T=30K,and $\mathbf{H}_e$=1.6. The magnetic vortices can seen as $|\psi_{1,2}|^2$, approaches zero. The anisotropic vortices can be seen in first row figures for $|\psi_1|^2$. A weak set of vortices can be seen in the second set of figures for $|\psi_2|^2$, induced by the inter-band coupling. The first columns shows the two order parameters forming vortices's in the sample. The next column shows the vortices approaching the center of the sample at a later time. The last column shows the two order parameters in the steady state with a Gibbs free energy of $G = -2.556$.



References

[1] Eisterer, M *Magnetic properties and critical currents of MgB 2*,Superconductor Science and Technology, 20(12): R47, 2007

[2] Deang, Jennifer*A Study of Inhomogeneities and Anisotropies in Superconductors via Ginzburg-Landau type models*, Virginia Polytechnic Institute, Dissertation, 1997

[3] Chan, Wan-Kan, *Analysis and approximation of a two-band Ginzburg-Landau model of superconductivity*, 2007, ProQuest

[4] Du, Q. and Gunzburger, M. and Peterson, J., *Analysis and Approximation of the Ginzburg Landau Model of Superconductivity*, SIAM Review, 34(1):54-81, 1992.

[5] Moshchalkov, Victor and Menghini, Mariela and Nishio, T. and Chen, Q. H. and Silhanek, A. V. and Dao, V. H. and Chibotaru, L. F. and Zhigadlo, N. D. and Karpinski, J. , *Type-1.5 Superconductivity*, Phys. Rev. Lett., 2009 @articlePhysRevLett.102.117001,