Investigation of Numerical Models for New High Temperature Superconductors

Chad Sockwell*

Co-advisors: Dr. Janet Peterson and Dr. Max Gumbiner
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 solid 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 Ginzburg Landau with inter-band coupling effects is formed to describe Magnesium Diboride.

Superconductivity and The Ginzburg Landau Model

- Superconductivity is a phenomenon where a material cooled below its critical temperature, \( T_c \) (typically close to 0 K), loses 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 a semi Meissner effect between \( H_a \) and \( H_c2 \). Type I materials exhibit this effect until a field strength of \( H_a \) is reached, then the material returns to the normal state.
- Type II materials exhibit a semi Meissner effect between \( H_a \) and \( H_c2 \).
- In 2001 a new high temperature superconductor was discovered, Magnesium Diboride or MgB2 with a \( T_c \) of 38K.
- 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.
- The Ginzburg Landau model is a mesoscopic phenomenological model that describes superconductivity and is valid for \( \Omega \rightarrow \infty \) and \( \Gamma \rightarrow \infty \).
- 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 \( \psi \) and the magnetic vector potential \( A \).
- The order parameter is proportional to the squared amplitude of the superconducting electron pair's wave functions.
- There characteristic parameters can be introduced through nondimensionalization. The coherence length \( \lambda \) and the penetration depth \( \kappa \) of the magnetic field \( A(x) \) and their ratio the Ginzburg Landau parameter \( \kappa = \frac{\kappa}{\lambda} \) 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 \( |\psi|^2 \)

Computational Methods

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

- The free-energy functional's variation in \( \psi(0), A(0) \) was found using calculus of variations, giving the weak form.
- Now the weak form was nondimensionalized using the relations from [2],[3], introducing the characteristic parameters \( \lambda, \kappa, \xi \) and \( \kappa, \lambda \).
- The system in Equations (1)-(3) is closed using a gauge transformation \( (\psi, \psi, A, \Phi) = \begin{pmatrix} \psi_1 \psi_1 \gamma \end{pmatrix} \xi \cdot \Phi, Q, Q, 0 \)\).
- The zero scalar potential gauge is chosen, yielding \( \Phi = 0 \) and boundary condition \( A \cdot n = 0 \).
- The artificial \( (\xi \cdot A \cdot \xi) \cdot A \cdot \xi \) term is added to make the system coercive, used in [4],[5].
- A set of test functions is chosen from a discrete space \( (\psi, \psi, \tilde{A}, 1) \in (\xi \cdot \kappa \cdot \gamma \cdot \xi \cdot 1) \).
- Each variable \( (\tilde{A}, \tilde{A}, \psi, \psi) \) 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, \( \psi_{n+1} = \frac{\psi_{n+1} - \psi_{n}}{\Delta t} \).
- 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 gradient stabilized or BICGSTAB solver

Modeling Magnesium Diboride (MgB2)

There are two free parameters and the two coupling constants. The external magnetic field \( H_c \) can be varied to affect the behavior of the vortices. The operating temperature \( T \) can be varied, but must remain below \( T_c \) for the sample to exhibit superconducting properties. The operating temperature also must stay within the validity of the GL model. The coupling parameters for bands in MgB2 are weak but not well understood[1]. The plots below show the evolution of \( |\psi|^2 \) and \( |\psi|^2 \) for \( \gamma = 0.1, \psi_0 = 0, \zeta = 0, T = 300K \) and \( H_c = 1e4 \).

The magnetic vortices can seen as \( |\psi|^2 \) approaches zero. The anisotropic vortices can be seen in first row, figures for \( |\psi|^2 \). A weak set of vortices can be seen in the second set of figures for \( |\psi|^2 \), induced by the inter-band coupling. The first column shows the two order parameters forming vortices 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 \( G \approx -2.556 \).

References
[1] Ratner, M. Magnetic properties and critical currents of MgB2 Superconductor Science and Technol-