Investigation into Numerical Models of New High Temperature Superconductors

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Overview

What is Superconductivity?

- A hallmark property of superconductivity is zero electrical resistance when a metal is supercooled.
- This property persists below a critical temperature T_c.
- This phenomena was first discovered by Onnes in 1911.

$$\rho = \frac{1}{\sigma} = 0 \tag{1}$$

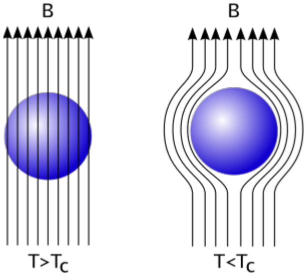
$$\sigma = \frac{1}{\rho} \longrightarrow \infty \tag{2}$$

where ρ is the resistivity and σ is the conductivity.

- What are other properties of superconductors?

The Meissner Effect

- The Meissner Effect occurs when a superconductoring material is supercooled in a external magnetic field.
- The field induces super currents on the surface of the material that keep the material from penetrating the sample
- This persist until the field reaches a critical strength $\mathbf{H}_c$
- This is known as the the thermodynamic critical field



- Do all superconducting materials react in the same manner?

Type I and Type II superconductors

- Type I superconductors loose all superconducting properties once $\mathbf{H} > \mathbf{H}_c$
- Type II superconductors experience a mixed-state where the sample is penetrated by magnetic flux vortices
- This behavior is exhibited for Type II superconductors beyond a field strength of $\mathbf{H} > \mathbf{H}_{c,1}$
- Once a second critical field strength is reached, $\mathbf{H} > \mathbf{H}_{c,2}$, superconductivity is destroyed
- Thus Type II superconductors have two critical fields and below $\mathbf{H}_{c,1}$ the full Meissner effect is exhibited

Applied Currents

- An current can can be carried very efficiently in a superconductor.
- The superconducting properties are destroyed once the a critical current density $\mathbf{J}_c$ is reached.
- The applied current induces a field, found by $\mathbf{J}_a = \nabla \times \mathbf{H}_a$.
- In Type II superconductors this spatially dependent field produces vortices and move them across the sample.

Applied Currents in Type II Superconductors

- The movement of vortices will eventually create large normal site and destroy superconductivity.
- The situation is more complicated when an external field $\mathbf{H}_e$ is involved.
- To prevent this, the vortices can be pinned by a pinning force F_p

$$F_p = \mathbf{J}_a \times \mathbf{H}_e \tag{3}$$

- Typically this force is provided by some impurity or imperfection in the material, that give a preferential position for the vortex.

High Temperature Superconductors

- Most materials do not exhibit superconducting properties until they are cooled very close to 0K.
- More recently superconductors with higher critical temperature were discovered
- Once such material is Magnesium Diboride (MgB_2), discovered in 2001, a type II material with $T_c = 39K$
- However this material comes with some odd properties not associated with low temperature superconductors such as anisotropy in the upper critical magnetic field $H_{c,2}$ and an upward curvature in the field as a function of temperature.

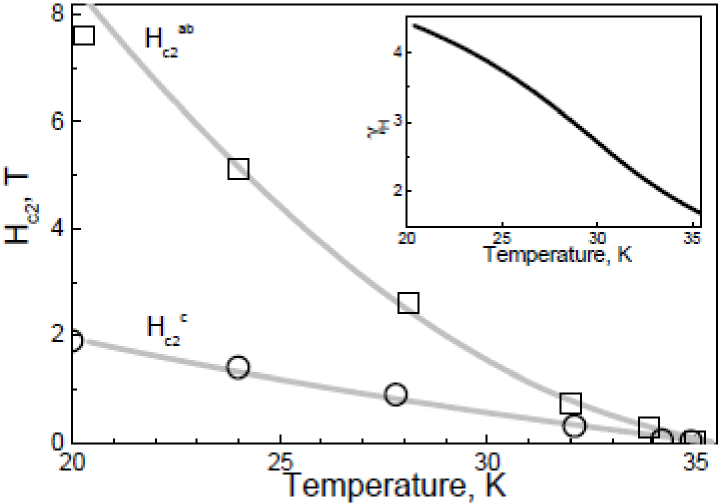


Image from V. H. Dao, M. E. Zhitomirsky: Anisotropy of the upper critical field in MgB2.

Modeling Vortex Dynamics and Applied current

- Can we model the vortex dynamics in a superconductor with an applied current?
- Can we use the model to make predictions or investigate how to enhance certain properties?

Ginzburg and Landau

- Ginzburg and Landau derived a free energy functional describing a superconductor in magnetic field (1950)
- Gor'kov proved this to be a limiting case of the microscopic BCS theory in 1959
- In the model, a complex order parameter ψ describes the density of superconducting electrons by $|\psi|^2 = n_s$. ψ and the magnetic vector potential $\mathbf{A}$ are the variables of interest.

The free energy functional

$$G = F_n + \int_\Omega \alpha(T)|\psi|^2 + \frac{1}{2}\beta(T)|\psi|^4 + \frac{1}{2m^*}|(-i\hbar\nabla - \frac{e^*}{c}\mathbf{A})\psi|^2 + \frac{|\mathbf{h} - \mathbf{H}_e|^2}{8\pi}\, d\Omega \tag{4}$$

- $\alpha < 0$ when the sample is in the superconducting state and $\beta > 0$
- F_n is the free energy in the normal state, the α and β terms are the energy from the phase transition
- The next terms is the kinetic energy of the superconducting electrons using the gauge invariant derivate
- The last term is the energy associated from the induced and external magnetic fields, with $\mathbf{h} = \nabla \times \mathbf{A}$

- Using calculus of variations, the Euler-Lagrange equations of the free energy functional can be found.

$$\lim_{\epsilon \to 0} \frac{G(\psi + \epsilon\tilde{\psi}) - G(\psi)}{\epsilon} = 0 \tag{5}$$

$$\lim_{\epsilon \to 0} \frac{G(\mathbf{A} + \epsilon\tilde{\mathbf{A}}) - G(\psi)}{\epsilon} = 0 \tag{6}$$

The Ginzburg Landau Equations

- The Euler-Lagrange equations of the free energy functional are the Ginzburg Landau Equations.
- Let Ω be a square superconducting sample in the x,y plane and let $\partial\Omega$ be its boundary.

$$\alpha(T)\psi + \beta(T)|\psi|^2\psi + \frac{1}{2m^*}(-i\hbar\nabla - \frac{e^*\mathbf{A}}{c})^2\psi = 0, \quad in \;\; \Omega \tag{7}$$

$$\frac{1}{4\pi}\nabla \times (\nabla \times \mathbf{A} - \mathbf{H}) = \frac{-ie^*\hbar}{2m^*}(\psi^*\nabla\psi - \psi\nabla\psi^*) - \frac{e^{2*}}{m^*c}|\psi|^2\mathbf{A} = \mathbf{J}_s, \quad in \;\; \Omega \tag{8}$$

with boundary conditions for an insulating boundary:

$$\begin{aligned} (-i\hbar\nabla - \frac{e^*}{c}\mathbf{A})\psi \cdot \mathbf{n} = 0, \quad on \;\; \partial\Omega \\ (\nabla \times \mathbf{A} - \mathbf{H}_e) \times \mathbf{n} = 0, \quad on \;\; \partial\Omega \end{aligned} \tag{9}$$

Normal Metal-Superconducting Boundary Conditions

- For normal metal superconducting interfaces, some of the superconducting electrons leak into the normal metal, through the Josephson effect.
- This effect can be captured by including the following term in the free energy functional

$$\int_{\partial\Omega} \zeta|\psi|^2 \tag{10}$$

- This generates the S-N boundary condition

$$(-i\hbar\nabla - \frac{e^*}{c}\mathbf{A})\psi \cdot \mathbf{n} = i\hbar\zeta\psi \quad on \quad \partial\Omega \tag{11}$$

Time dependence

- To include the time dependence in the Ginzburg Landau equations, lets rearrange the free energy as,

$$G = F_s + \int_{\Omega} \frac{|\mathbf{h} - \mathbf{H}_e|^2}{8\pi} \, d\Omega \tag{12}$$

- The variation in the free energy with respect can be set equal to a small disturbance in the equilibrium of the sample. The inclusion of Φ, the electrical potential, is to ensure the gauge invariance.

$$\Gamma(\frac{\partial \psi}{\partial t} + \frac{ie^*}{\hbar}\Phi\psi) = -\frac{\delta G}{\delta \psi *} \tag{13}$$

Time dependence (Continued)

- To include the time dependence in vector potential equation, let J_n and J_s be the normal current and super current densities respectively,

$$\mathbf{J}_n = \sigma_n \mathbf{E} = -\sigma_n(\frac{1}{c}\frac{\partial \mathbf{A}}{\partial t} + \nabla\Phi)$$
$$\mathbf{J}_s = -c\frac{\partial F_s}{\partial A} = -(\frac{ie^*\hbar}{2m^*}(\psi^*\nabla\psi - \psi\nabla\psi^*) + \frac{e^{*2}}{m^*c}|\psi^2|\mathbf{A}) \quad (14)$$

- The total current in the superconducting sample is,

$$\mathbf{J} = \mathbf{J}_n + \mathbf{J}_s = \sigma_n(-\frac{1}{c}\frac{\partial A}{\partial t} - \nabla\phi) - c\frac{\partial F_s}{\partial A} \quad (15)$$

Temperature Dependence

- Using the BCS theory, the Temperature dependence can be separated from the material dependent constants $\alpha(T)$ and $\beta(T)$ when $T \approx T_c$

$$\begin{aligned} \alpha(T) &\approx -\alpha(0)(1 - \frac{T}{T_c}) = \alpha(1 - \frac{T}{T_c}) \\ \beta(T) &\approx \frac{7\zeta(3)\nu(0)}{8\pi^2 T_c^2} = \beta \end{aligned} \tag{16}$$

- What is $T \approx T_c$?

The Time Dependent Ginzburg Landau Equations

- Combing the time and temperature dependencies

$$\Gamma(\frac{\partial \psi}{\partial t}+\frac{ie}{\hbar}\Phi\psi)+\alpha(1-\frac{T}{T_c})\psi+\beta|\psi|^2\psi+\frac{1}{2m^*}(-i\hbar\nabla-\frac{e^*\mathbf{A}}{c})^2\psi=0, \quad in \ \ \Omega \tag{17}$$

$$\frac{1}{4\pi}\nabla \times (\nabla \times \mathbf{A} - \mathbf{H}) =$$

$$\sigma_n(-\frac{1}{c}\frac{\partial A}{\partial t} - \nabla\Phi) + \frac{-ie^*\hbar}{2m^*}(\psi^*\nabla\psi - \psi\nabla\psi^*) - \frac{e^{*2}}{m^*c}|\psi|^2\mathbf{A}, \quad in \ \ \Omega \tag{18}$$

with initial and boundary conditions:

$$\begin{aligned} (-i\hbar\nabla - \frac{e_s}{c}\mathbf{A})\psi \cdot \mathbf{n} = 0, \quad on \ \ \partial\Omega \ \ and \ \ \forall t \\ (\nabla \times \mathbf{A} - H_e) \times \mathbf{n} = 0, \quad on \ \ \partial\Omega \ \ and \ \ \forall t \\ \psi(x,0) = \psi_0(x), \quad on\Omega \\ \mathbf{A}(x,0) = \mathbf{A}_0(x), \quad on\Omega \end{aligned} \tag{19}$$

The Time Dependent Ginzburg Landau Equations(continued)

- The TDGL equations can be used to model vortex dynamics.
- First we must discuss important parameters and gauge the system.
- The penetration depth λ is material specific and is shown in the Meissner effect.

$$\Delta \mathbf{H} = \frac{1}{\lambda^2}\mathbf{H} \tag{20}$$

- The coherence length ξ is the characteristic length of change of ψ
- The Ginzburg Landau parameter is the ratio $\kappa = \frac{\lambda}{\xi}$

$$\lambda(T) = \sqrt{-\frac{m^*\beta c^2}{4\pi\alpha(T)e^{2*}}} \quad \xi(T) = \sqrt{-\frac{\hbar^2}{2m^*\alpha(T)}} \tag{21}$$

- $\kappa < \frac{1}{\sqrt{2}}$ for Type I and $\kappa > \frac{1}{\sqrt{2}}$ for Type II
- The value of ψ deep inside a superconducting sample is known as the solution in the bulk, ψ_∞, found by solving,

$$\alpha(T)\psi + \frac{1}{2}\beta(T)|\psi|^2\psi = 0 \tag{22}$$

$$\psi_\infty = \sqrt{\frac{-\alpha}{\beta}} \tag{23}$$

- The thermodynamic critical can defined in terms of free energy densities.

$$f_s - f_n = \frac{-H_c^2}{8\pi} = \frac{-\alpha^2}{\beta} \tag{24}$$

Gauging the system

- Since we have three variable ψ,$\mathbf{A}$,Φ, and two equations, the system needs to be closed
- This can be done by using the zero potential gauge

$$\frac{\partial \chi}{\partial t} = \Phi = 0 \tag{25}$$

- with initial conditions (at $t = 0$),

$$\begin{aligned} \Delta \chi &= -\nabla \cdot \mathbf{A} \quad on \quad \Omega \\ \nabla \chi \cdot \mathbf{n} &= -\mathbf{A} \cdot \mathbf{n} \quad on \quad \partial \Omega \end{aligned} \tag{26}$$

Non-Dimensionalization

- To introduce the characteristic length λ, and ξ, as well as rescale the system the TDGL equations are non-dimensionalized.
- Using the following non dimensionalized variables (with bars)

$$
\begin{aligned}
x &= x_0 \bar{x}, \qquad t = \bar{t}\frac{(-\alpha)}{\Gamma \hbar} \\
H_c &= \sqrt{\frac{8\pi\alpha^2}{\beta}}, \quad \mathbf{A} = H_c x_0 \bar{\mathbf{A}} \\
\mathbf{H} &= \sqrt{2} H_c \bar{\mathbf{H}} \qquad \psi = \sqrt{\frac{-\alpha}{\beta}}\bar{\psi} \\
\lambda &= \sqrt{-\frac{c^2 m^* \beta}{4\pi e^{*2}\alpha}}, \qquad \xi = \sqrt{-\frac{\hbar^2}{2m^*\alpha}} \\
\sigma_n &= \frac{\Gamma c^2}{2\pi\hbar}\bar{\sigma}, \qquad \Phi = \frac{-\alpha}{\Gamma}\bar{\Phi}
\end{aligned}
\tag{27}
$$

ND TDGL

- The non-dimenionalized TDGL equations in the zero potential gauge equations are suitable for numerical calculations

$$(\frac{\partial \psi}{\partial t}) + (|\psi|^2 - (1 - \frac{T}{T_c})\psi + (-i\frac{\xi}{x_0}\nabla - \frac{x_0}{\lambda}\mathbf{A})^2\psi = 0 \tag{28}$$

$$\sigma(\frac{1}{\lambda^2}\frac{\partial \mathbf{A}}{\partial t}) + \nabla \times \nabla \times \mathbf{A} + \frac{i}{2\kappa}(\psi\nabla\psi^* - \psi^*\nabla\psi) + \frac{1}{\lambda^2}|\psi|^2\mathbf{A} = \nabla \times \mathbf{H}_e \tag{29}$$

$$\begin{gathered} \nabla\psi \cdot \mathbf{n} = 0, \quad on \quad \partial\Omega \quad and \quad \forall t \\ (\nabla \times \mathbf{A} - H_e) \times \mathbf{n} = 0, \quad on \quad \partial\Omega \quad and \quad \forall t \\ \mathbf{A} \cdot \mathbf{n} = 0, \quad on \quad \partial\Omega \quad and \quad \forall t \\ \nabla \cdot \mathbf{A}(\mathbf{x}, 0) = 0 \quad \Omega \\ \psi(x, 0) = \psi_0(x), \Omega \\ \mathbf{A}(x, 0) = \mathbf{A}_0(x), \Omega \end{gathered} \tag{30}$$

Finite Element Method

- The finite element method is used to approximate solutions of partial differential equations such as the TDGL equations
- The partial differential equations must be put in the weak form.
- This is done by multiplying by a test function from a vector space V and integrating by parts over the spatial domain.
- Boundary conditions on the solution are enforced on the test space V, while the ones on the derivate are naturally included.
- Then the problem is stated as find a solution in the space V that solve the weak form all test functions in the space V

Finite Element Method (Continued)

- The method is implemented numerically by discretizing the domain Ω in to element.
- The vector space V is also discretized into basis functions defined in a piecewise manner on the elements.
- A system of equations is formed and solved to give a continuous solution over the domain.
- The detail of the specific finite element implementation can be seen in the thesis

Verification

- The finite element codes were written and verified for problems with exact solutions
- This was extended to multi-variable, non-linear, and time dependent problems to prepare for the TDGL.

Time discretizations

- The backward Euler method (first order convergence) was used to approximate the time derivative

$$\frac{\partial \psi}{\partial t}\Big|_{t=tn} \approx \frac{\psi(t_n) - \psi(t_{n-1})}{\Delta t} \tag{31}$$

- The forward Euler method is not used because it offer no advantage. Higher order implicit methods will give greater accuracy but come at a cost.

The Weak Form

- The weak problem is stated as seek a solution $\psi \in V$ and $\mathbf{A} \in \mathbf{Z}$ and test against all $\tilde{\psi} \in V$ and $\tilde{\mathbf{A}} \in \tilde{\mathbf{Z}}$ in Ω

$$(\frac{\partial \psi}{\partial t}, \tilde{\psi}) + ([|\psi|^2 - \tau)\psi], \tilde{\psi}) + (-i\frac{\xi}{x_0}\nabla\psi - \frac{x_0}{\lambda}\mathbf{A}\psi, -i\frac{\xi}{x_0}\nabla\tilde{\psi} - \frac{x_0}{\lambda}\mathbf{A}\tilde{\psi}) = 0 \tag{32}$$

$$\sigma(\frac{1}{\lambda^2}\frac{\partial \mathbf{A}}{\partial t}, \tilde{\mathbf{A}}) + (\nabla \times \mathbf{A}, \nabla \times \tilde{\mathbf{A}}) + \epsilon(\nabla \cdot \mathbf{A}, \nabla \cdot \tilde{\mathbf{A}})$$

$$+(\frac{i}{2\kappa}[\psi\nabla\psi^* - \psi^*\nabla\psi], \tilde{\mathbf{A}}) + (\frac{1}{\lambda^2}|\psi|^2\mathbf{A}, \tilde{\mathbf{A}}) = (\mathbf{H}_e, \nabla \times \tilde{\mathbf{A}}) \tag{33}$$

$$\tau = (1 - \frac{T}{T_c})$$

- with initial conditions

$$\begin{aligned} \nabla \cdot \mathbf{A}(\mathbf{x}, 0) &= 0 \quad \Omega \\ \psi(x, 0) &= \psi_0(x), \Omega \\ \mathbf{A}(x, 0) &= \mathbf{A}_0(x), \Omega \end{aligned} \tag{34}$$

Weak Form (continued)

- The inner product $(\cdot, \cdot)$ is defined as,

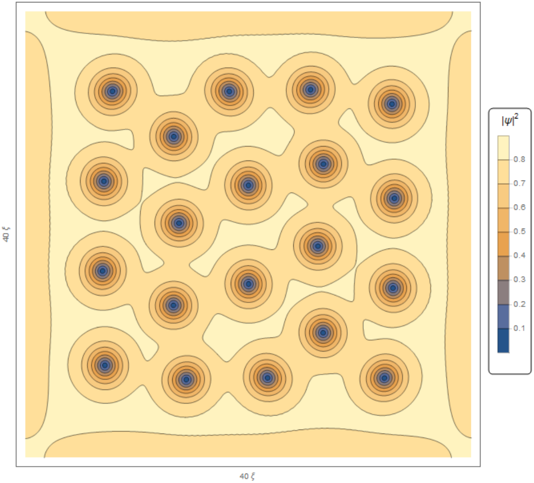
$$(f, g) = \int_{\Omega} f^* \cdot g \; d\Omega \tag{35}$$

- The penalty term, $\epsilon(\nabla \cdot \mathbf{A}, \nabla \cdot \tilde{\mathbf{A}})$ is used to help convergence and is proved to give the correct steady state by Du.

An FEM approximation

- Using FEM we can approximate the solutions of the TDGL equations and show evolution of vortex dynamics as well as the steady state.
- Consider a Type II superconductor with the following parameters
- In Figure 3.1 is an example of the order parameter ψ for $\lambda = 60nm$, $\xi = 5nm$, $(1 - \frac{T}{T_c}) = 0.7$, $\frac{T}{T_c}$=0.3, $\mathbf{H}_e = 1.5 = 1.5\sqrt{2}\mathbf{H}_c$. Ω is $20nm \times 20nm$.

Steady State Order Parameter Plot and Movie



Anisotropy

- Some superconductors such as MgB_2 have anisotropic effects, such as the anisotropy in $\mathbf{H}_{c,2}$
- The directional dependent effects can be captured using the effective mass GL model.
- In this model the effective mass $m*$ is replaced by an anisotropic mass tensor.

$$\mathbf{M} = \begin{pmatrix} m_x & 0 \\ 0 & m_y \end{pmatrix} \tag{36}$$

- This gives a characteristic length in each direction ξ_x, λ_x,ξ_y and λ_y

$$\gamma = \frac{m_x}{m_y} = (\frac{\lambda_x}{\lambda_y})^2 = (\frac{\xi_y}{\xi_x})^2 = \frac{\mathbf{H}_c}{\mathbf{H}_{a,b}} \tag{37}$$

The Effective Mass Model

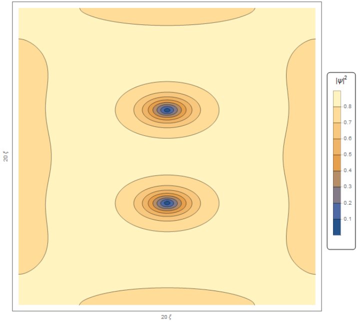
$$(\frac{\partial\psi}{\partial t}) + (|\psi|^2 - \tau)\psi + (-i\frac{\xi_x}{x_0}\frac{\partial}{\partial x} - \frac{x_0}{\lambda_x}A_x)^2\psi + \gamma(-i\frac{\xi_x}{x_0}\frac{\partial}{\partial y} - \frac{x_0}{\lambda_x}A_y)^2\psi = 0 \tag{38}$$

$$\begin{aligned} &\sigma(\frac{1}{\lambda_x^2}\frac{\partial \mathbf{A}}{\partial t}) + \nabla\times\nabla\times\mathbf{A} + \{\frac{i}{2\kappa}(\psi\frac{\partial}{\partial x}\psi^* - \psi^*\frac{\partial}{\partial x}\psi) + \frac{x_0^2}{\lambda_x^2}|\psi|^2 A_x\} + \\ &\gamma\{\frac{i}{2\kappa}(\psi\frac{\partial}{\partial y}\psi^* - \psi^*\frac{\partial}{\partial y}\psi) + \frac{x_0^2}{\lambda_x^2}|\psi|^2 A_y\} = \nabla\times\mathbf{H}_e \end{aligned} \tag{39}$$

$$\begin{aligned} \nabla\psi\cdot\mathbf{n} &= 0, \quad on \quad \partial\Omega \quad and \quad \forall t \\ (\nabla\times\mathbf{A} - H_e)\times\mathbf{n} &= 0, \quad on \quad \partial\Omega \quad and \quad \forall t \\ \mathbf{A}\cdot\mathbf{n} &= 0, \quad on \quad \partial\Omega \quad and \quad \forall t \\ \nabla\cdot\mathbf{A}(\mathbf{x},0) &= 0 \quad \Omega \\ \psi(x,0) &= \psi_0(x), \Omega \\ \mathbf{A}(x,0) &= \mathbf{A}_0(x), \Omega \end{aligned} \tag{40}$$

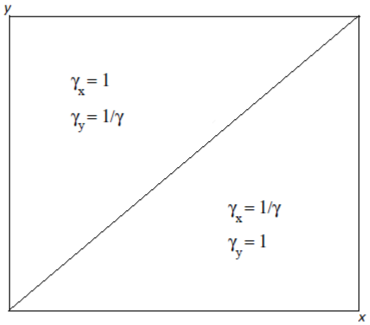
The Effective Mass Model (continued)

- The effects are most pronounce in the vortices, contracting by $\frac{l_x}{l_y} = \sqrt{\frac{m_x}{m_y}}$
- Consider a Type II superconductor on a $10nm \times 10nm$. The parameters are $\lambda = 60nm$, $\xi = 5nm$, $(1 - \frac{T}{T_c}) = 0.7$, $\frac{T}{T_c}$=0.3, $\mathbf{H}_e = 1.5 = 1.5\sqrt{2}\mathbf{H}_c$, $\gamma = \frac{1}{4}$.



Grain boundaries

- Some anisotropic materials have domain walls where the crystal structure is reoriented
- These are known as grain boundaries, and the anisotropy is changed as the boundary is crossed
- This can be captured by using two functions $\gamma_x(x, y)$ and $\gamma_y(x, y)$, where the anisotropy is flipped across the boundary



The Two Band Model

- Multi-band superconductivity was used to describe the upward curvature of $\mathbf{H}_{c,2}$ by Dao, Zhitomirsky and others
- The Two band model uses a second order parameter ψ_2 to represent the second band.
- The bands are coupled through Josephson effect like terms (η), inter-gradient coupling (η_1), and through the magnetic vector potential equation.
- The bands have different characteristics and critical temperatures $T_{c,1}$ and $T_{c,2}$, both below the materials critical temperature T_c.
- The coupling between the bands gives superconducting effects above both bands critical temperatures.

ND TB-TDGL

$$
\begin{aligned}
&(\frac{\partial\psi_1}{\partial t} + i\Phi\psi_1) + (|\psi_1|^2 - \tau_1)\psi_1 + (-i\frac{\xi_1}{x_0}\nabla - \frac{x_o}{\lambda_1}\mathbf{A})^2\psi_1 \\
&+\eta\psi_2 + \eta_1\frac{\xi_1}{\nu\xi_2}(-i\frac{\xi_2}{x_0}\nabla - \nu\frac{x_o}{\lambda_2}\mathbf{A})^2\psi_2 = 0 \\
&\Gamma(\frac{\partial\psi_2}{\partial t} + i\Phi\psi_2) + (|\psi_2|^2 - \tau_2)\psi_2 + (-i\frac{\xi_1}{x_0}\nabla - \nu\frac{x_o}{\lambda_1}\mathbf{A})^2\psi_2 \\
&+\eta\psi_1 + \eta_1\nu\frac{\xi_2}{\xi_1}(-i\frac{\xi_1}{x_0}\nabla - \frac{x_o}{\lambda_1}\mathbf{A})^2\psi_1 = 0 \\
&\nu = (\frac{\lambda_2\xi_1}{\lambda_1\xi_2})
\end{aligned} \tag{41}
$$

ND TB-TDGL (Continued)

$$\nabla \times (\nabla \times \mathbf{A} - \mathbf{H}) = \sigma(-\frac{x_o^2}{\lambda_1^2}\frac{\partial A}{\partial t} - \frac{1}{\kappa_1}\nabla\Phi) + i\frac{1}{2\kappa_1}(\psi_1\nabla\psi_1^* - \psi_1^*\nabla\psi_1)$$
$$-\frac{x_0^2}{\lambda_1}|\psi_1|^2\mathbf{A} + i\frac{1}{2\kappa_2\nu}(\psi_2\nabla\psi_2^* - \psi_2^*\nabla\psi_2) - \frac{x_0^2}{\lambda_2}|\psi_2|^2\mathbf{A}$$
$$+i\eta_1\frac{\xi_1}{2\lambda_2}(\psi_2\nabla\psi_1^* - \psi_2^*\nabla\psi_1 + \psi_1\nabla\psi_2^* - \psi_1^*\nabla\psi_2)$$
$$-\eta_1\frac{x_0^2}{\lambda_1\lambda_2}\mathbf{A}(\psi_1\psi_2^* + \psi_2\psi_1^*) \tag{42}$$

ND TB-TDGL (Continued)

and non-dimensionalized boundary and initial conditions,

$$
\begin{aligned}
((-i\frac{\xi_1}{x_0}\nabla - \frac{x_o}{\lambda_1}\mathbf{A})\psi_1 + \eta_1\frac{1}{\nu}(-i\frac{\xi_1}{x_0}\nabla - \nu\frac{x_o}{\lambda_1}\mathbf{A})\psi_2)\cdot\mathbf{n} &= i\zeta_1\frac{\xi_1}{x_0}\psi_1 \quad on \quad \partial\Omega \times (\\
((-i\frac{\xi_1}{x_0}\nabla - \nu\frac{x_o}{\lambda_1}\mathbf{A})\psi_2 + \eta_1\nu(-i\frac{\xi_1}{x_0}\nabla - \frac{x_o}{\lambda_1}\mathbf{A})\psi_1)\cdot\mathbf{n} &= i\zeta_2\frac{\xi_2}{x_0}\psi_2 \quad on \quad \partial\Omega \times (\\
(\nabla \times \mathbf{A}) \times \mathbf{n} &= \mathbf{H}_e \times \mathbf{n} \quad on \quad \partial\Omega \times (0, t')\\
\psi_1(x, y, 0) &= \psi_{1,0}(x, y) \quad on \quad \Omega\\
\psi_2(x, y, 0) &= \psi_{2,0}(x, y) \quad on \quad \Omega\\
\mathbf{A}(x, y, 0) &= A_0(x, y) \quad on \quad \Omega
\end{aligned}
\tag{43}
$$

The non-dimensionalizations are

$$
\begin{gathered}
x = x_0\bar{x}, \qquad t = \bar{t}\frac{(-\alpha)}{\Gamma_1\hbar} \\
H_c = \sqrt{\frac{8\pi\alpha_1^2}{\beta_1}}, \quad \mathbf{A} = H_c x_0 \bar{\mathbf{A}} \\
\Phi = \frac{\hbar(-\alpha_1)}{2\Gamma_1 e^*}\bar{\Phi}, \quad \Gamma = \frac{\Gamma_1(-\alpha_1)}{\Gamma_2(-\alpha_2)} \\
\kappa_i = \sqrt{\frac{c^2 m_i^* \beta_i}{2\pi e^{*2}\hbar^2}} \quad \nu = \frac{\lambda_2\xi_2}{\lambda_1\xi_1} = \sqrt{\frac{\alpha_1^2\beta_2}{\alpha_2^2\beta_1}} \\
\eta = \eta\sqrt{\frac{\beta_1\alpha_2}{\beta_2\alpha_1}}\frac{1}{\alpha_1} \quad \eta_1 = \epsilon_1 2\sqrt{m_1^* m_2^*} \\
\sigma = \frac{\sigma_n m_1^* \beta_!}{\Gamma_1 e^{*2}}
\end{gathered}
\tag{44}
$$

Applied current

- The TB-TDGL can be put in the current gauge to include an applied current in the sample

$$\mathbf{J}_a = -\frac{\sigma}{\kappa_1}\nabla\Phi \leftrightarrow \Phi_a = -\frac{\kappa_1}{\sigma}J_a y \tag{45}$$

$$\mathbf{J}_a = \nabla \times \mathbf{H}_{app} \leftrightarrow \mathbf{H}_{app} = -J_a(x - \frac{x_0}{2})\hat{z} \tag{46}$$

- Assuming the applied current in in the y direction and the S-N interface is used
- The first relation is used in the ψ equations, and the second is used the in **A** equation.

Modeling Magnesium Diboride

- MgB_2 is a layered, two-band, type II material, with $T_c = 39$ and containing a strong anisotropy in it's upper critical field
- Superconducting bands are the anisotropic σ band and the isotropic π band
- It also posses clean grain boundaries where the anisotropy is changed but does not impede applied current
- This allows for the practical use of MgB_2 for carrying current.
- Using our previous model we can make a model to capture all these properties.

The Parameters

Table 4.1

$\xi_\sigma(0) = 13nm$	$\lambda_\sigma(0) = 47.81nm$	$\kappa_\sigma = 3.68$
$\xi_\pi(0) = 51nm$	$\lambda_\pi(0) = 33.6nm$	$\kappa_\pi = 0.66$
T_c=39K	$T_{c,\sigma}$=35.6K	$T_{c,\pi}$=11.8K
$\gamma_\sigma = 4.55$	$\gamma_\pi = 1$	T=31K

Table : These are the parameters for a clean sample MgB_2.

The Anisotropic 2B-TDGL w/ Applied Current and a Grain Boundary (Weak Form)

$$\int_\Omega \frac{\partial \psi_1}{\partial t}\tilde{\psi} - i\frac{\kappa_1}{\sigma}J_a y sin(\omega t)\psi_1\tilde{\psi} + (|\psi_1|^2 - \tau_1)\psi_1\tilde{\psi} + \mathbf{D}_1\psi_1 \cdot \boldsymbol{\gamma} \cdot \mathbf{D}_1\tilde{\psi}_1 + \eta\psi_2\tilde{\psi}$$

$$+\eta_1\frac{\xi_1}{\nu\xi_2}\mathbf{D}_2\psi_2 \cdot \boldsymbol{\gamma} \cdot \mathbf{D}_2\tilde{\psi}\, d\Omega = -\int_{\partial\Omega}\zeta_1\frac{\xi_1^2}{x_0}\psi_1\tilde{\psi}\, dS \tag{47}$$

$$\int_\Omega \Gamma\frac{\partial \psi_2}{\partial t}\tilde{\psi} - i\frac{\kappa_1}{\sigma}J_a y sin(\omega t)\psi_1\tilde{\psi}_2 + (|\psi_2|^2 - \tau_2)\psi_2\tilde{\psi} + \mathbf{D}_2\psi_2 \cdot \mathbf{D}_2\tilde{\psi} + \eta\psi_1\tilde{\psi}$$

$$+\eta_1\frac{\xi_2}{\xi_1}\mathbf{D}_1\psi_1 \cdot \boldsymbol{\gamma} \cdot \mathbf{D}_1\tilde{\psi}\, d\Omega = -\int_{\partial\Omega}\zeta_2\frac{\xi_2^2}{x_0}\psi_2\tilde{\psi}\, dS \tag{48}$$

$$\boldsymbol{\gamma} = \begin{pmatrix} \frac{1}{\gamma_x(x,y)} & 0 \\ 0 & \frac{1}{\gamma_y(x,y)} \end{pmatrix} \quad \mathbf{D}_1 = (-i\tfrac{\xi_1}{x_0}\nabla - \tfrac{x_0}{\lambda_1}\mathbf{A}),\ \mathbf{D}_2 = (-i\tfrac{\xi_2}{x_0}\nabla - \nu\tfrac{x_0}{\lambda_2}\mathbf{A})$$

Continued

$$
\begin{aligned}
\int_\Omega \sigma \frac{x_o^2}{\lambda_1^2} \frac{\partial \mathbf{A}}{\partial t} \tilde{\mathbf{A}} + \epsilon(\nabla \cdot \mathbf{A}) \cdot (\nabla \cdot \tilde{\mathbf{A}}) + (\nabla \times \mathbf{A}) \cdot (\nabla \times \tilde{\mathbf{A}}) + \\
\mathscr{R}\{i \frac{1}{\kappa_1} (\gamma \cdot \nabla \psi_1) \cdot \psi_1 \cdot \tilde{\mathbf{A}}\} + \frac{x_0^2}{\lambda_1^2} |\psi_1|^2 \gamma \cdot \mathbf{A} \cdot \tilde{\mathbf{A}} \\
+ \mathscr{R}\{i \frac{1}{\nu \kappa_1} (\nabla \psi_2) \cdot \psi_2 \tilde{\mathbf{A}}\} + \frac{x_0^2}{\lambda_2^2} |\psi_2|^2 \mathbf{A} \cdot \tilde{\mathbf{A}} \\
+ \eta_1 \gamma \cdot (\mathscr{R}\{i \frac{\xi_1}{\lambda_2} (\cdot \nabla \psi_1) \cdot \psi_2 \tilde{\mathbf{A}}\} + \mathscr{R}\{i \frac{\xi_1}{\lambda_2} (\cdot \nabla \psi_2) \cdot \psi_1 \tilde{\mathbf{A}}\}) \\
+ \eta_1 \frac{x_0}{\lambda_1 \lambda_2} \gamma \cdot \{(\psi_1 \psi_2^* + \psi_2 \psi_1^*) \mathbf{A} \cdot \tilde{\mathbf{A}}\} \; d\Omega \\
= \int_\Omega (\mathbf{H}_e - J_a sin(\omega t)(x - \frac{x_0}{2} \hat{(}z)) \cdot (\nabla \times \tilde{\mathbf{A}}) \; d\Omega
\end{aligned}
\tag{49}
$$

Investigating the effect of η on the critical temperature

- We can use this model for numerical studies to investigate the effect of the order parameter
- The non dimensionlized values can used and the results can tell experimentalist how to tune dimensionalized parameters
- Effects seen in the study may lead to improvement in the material if possible
- We also verify things that are know experimentally

Critical Current Vs Applied field for MgB_2 at various T

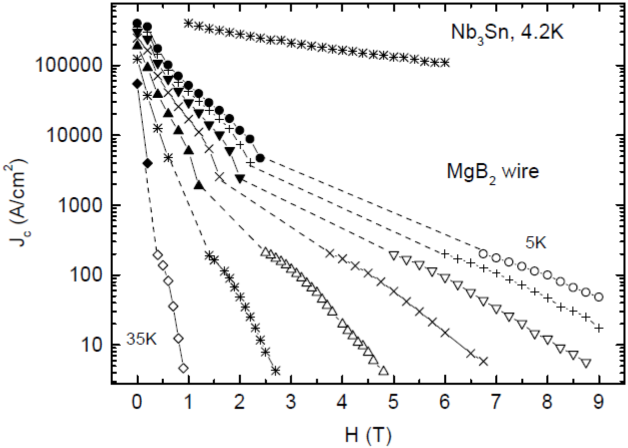


Image from An Overview of the Basic Physical Propertiesof MgB2 P.C. Canfield, S.L. Budko, D.K. Finnemore

Numerical studies

- For example1 $J_a = 20$ to see if this value exceed the critical current. The sample contains a grain boundary across the diagonal ($x = y$ line) where the anisotropy flips from the y direction to the x directions. Here $\eta = 0.8$ (strong coupling), $\mathbf{H}_e = 1.6$ (moderate), $\zeta_{1,2} = 0.1$, and ω=0.025. This same is approximately $15\xi_1 \times 15\xi_1$ or $200nm \times 200nm$.
- For example 2 $J_a = 7$, the superconductivity is improved,$|\psi_i|_{max} \leq \sqrt{4max\{\eta, \nu^2\eta\} + max\{\tau_1, \tau_2\}}$
- For example 3 $J_a = 2.0$ and $\eta = 0.2$, the superconductivity is not completely destroyed but it is severely diminished
- For example 4 $J_a = 2.0$ and $\eta = 0.2$ but $\mathbf{H}_e = 0$ and $\eta_1 = 0.2$. This shows a vortex anti vortex pair annihilating
- For example 5 we have $J_a = 2.0$ and $\eta = 0.2$ but $\mathbf{H}_e = 0$, and see as the previous figure predicts, the superconductivity is improved in a lower field.

The End