Thin Film Problems in Superconductivity

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Sept 2016

Outlook:

- Thin film magnetization and transport current problems
- Mixed variational formulation
- Numerical approximation ($j$, $h$ and $e$)
- Application: magnetic traps for cold atoms
Thin high-temperature superconductor films are

- used in physical experiments;
- employed in electronic devices (fault current limiters, SQUIDs, magnetic traps for cold atoms).

Mathematical modeling is needed to understand the results of such experiments and to design these electronic devices. Usually, one wants to compute the distributions of current density, electric field, and AC losses in the film as well as the magnetic field around it.
Macroscopically, magnetization of type-II superconductors is modeled as an eddy current problem with a highly non-linear $e(j)$ relation. The most often employed relations are:

- The power law: $e = e_0 \left( \frac{j}{j_c} \right)^{p-1} \frac{j}{j_c}$; usually, $10 \leq p \leq 100$ (Rhyner 93).
- The critical-state model: the $p \to \infty$ limit of the power law (Bean 64, Kim et al. 63).

In thin film models:

$e$ - tangential-to-film component of the electric field;

$j$ - sheet current density in the film.

Analytical solutions: for the Bean model and simple geometries (thin disk, infinite strip): Mikheenko and Kuzovlev 93, Brandt et al. 93, Zhu et al. 93, Clem and Sanchez 94, ...
For a long time all numerical methods were based on formulations written for only one variable, the stream function of the sheet current density: \( \nabla \cdot j = 0 \implies j = \nabla \times g \).

- **Power law**: Brandt et al. 95-96; Vestgarden et al. 07-14, Jing, Yong and Zhou 15-16.
- **The critical-state model**: P. 98; Navau et al. 08.

Using such methods one finds:

- The scalar stream function \( g \): with high accuracy.
- Current density \( j = \nabla \times g \): the accuracy is worse but sufficient.
- The magnetic field \( h \) from \( j \) via the Biot-Savart law: good.
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**Remaining problem**: How to find \( e \)? And the local loss \( e \cdot j \)?

\( e \) is not uniquely determined by \( j \) in the critical-state model; difficult to compute accurately if the power law model is used.

The electric field can be very non-uniform, even singular.
Thin film magnetization problem

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**Solution**:
- Dual or mixed variational formulations, Barrett and P. 10-15.
Let $\Omega$ be a 2D domain, the thin film occupy $\Omega \times \{x_3 = 0\} \subset R^3$, and $b_e(t)$ be the normal to film component of a (uniform) external magnetic field.
Magnetization problem

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**Biot-Savart law:**
$$b_3(x, t) = b_e(t) + \frac{\mu_0}{4\pi} \nabla \times \int_{\Omega} \frac{j(y, t)}{|x-y|} \, dy$$

**Faraday law:**
$$\partial_t b_3(x, t) = -\nabla \times e(x, t)$$

where $x = \{x_1, x_2\} \in \Omega$,

$b_3$ is the normal to film component of the total magnetic field,
$e$ is the tangential to film component of the electric field.
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We substitute the Biot-Savart law into the Faraday law  
$$-\nabla \times e = \partial_t b_e + \frac{\mu_0}{4\pi} \nabla \times \int_{\Omega} \frac{\partial_t j(y, t)}{|x-y|} \, dy$$

and rewrite the power law relation:

$$e = e_0 \left(\frac{j}{j_c}\right)^{p-1} j \iff j = j_c \left(\frac{e}{e_0}\right)^{q-1} \frac{e}{e_0},$$

with $q = 1/p$. 

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Derivation of a variational formulation

The model:

\[-\nabla \times \mathbf{e} = \partial_t \mathbf{b}_e + \frac{\mu_0}{4\pi} \nabla \times \int_{\Omega} \frac{\partial_t \mathbf{j}(\mathbf{y}, t)}{||\mathbf{x} - \mathbf{y}||} \, d\mathbf{y}\]  \hspace{1cm} (1)

\[\mathbf{j} = j_c \left( \frac{e}{e_0} \right)^{q-1} \frac{e}{e_0}\]  \hspace{1cm} (2)
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1. Change of variables: instead of \(\{ \mathbf{e}, \mathbf{j} \}\) we use \(\{ \mathbf{v}, g \}\), where \(\mathbf{v} = (-e_2, e_1)\) is the rotated el. field and \(g\) is a stream function

\(\nabla \cdot \mathbf{j} = 0, \quad \mathbf{j}_n|_{\partial\Omega} = 0 \iff \mathbf{j} = \nabla \times g, \quad g|_{\partial\Omega} = 0.\)

(If \(\Omega\) is not simply connected, fill the holes and set \(j_c = 0\) there)

Eq. (2) becomes \(\nabla g = -j_c \left( \frac{|\mathbf{v}|}{e_0} \right)^{q-1} \frac{\mathbf{v}}{e_0}.\)
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Eq. (2) becomes \(\nabla g = -j_c \left( \frac{|\mathbf{v}|}{e_0} \right)^{q-1} \frac{\mathbf{v}}{e_0}\).

2. We multiply Eq. (1) by a test function \(\phi\) s.t. \(\phi|_{\partial \Omega} = 0\). Then

\[-(\nabla \times \mathbf{e}, \phi) = (\nabla \cdot \mathbf{v}, \phi) = -(\mathbf{v}, \nabla \phi);\]

The Green’s formula is applied to the last term in (1) too and

\(\nabla \times g \cdot \nabla \times \phi = \nabla g \cdot \nabla \phi.\)
Derivation of a variational formulation

The model:

\[-\nabla \times \mathbf{e} = \partial_t b_e + \frac{\mu_0}{4\pi} \nabla \times \int_{\Omega} \frac{\partial_t j(y, t)}{|x - y|} dy\]

\[j = j_c \left( \frac{e}{e_0} \right)^{q-1} \frac{e}{e_0}\]

and its mixed variational formulation: for any \(\phi\) s.t. \(\phi|_{\partial \Omega} = 0\)

\[a(\partial_t g, \phi) - (\mathbf{v}, \nabla \phi) = - (\partial_t b_e, \phi),\]

\[\nabla g = -j_c \left( \frac{\mathbf{v}}{e_0} \right)^{q-1} \frac{\mathbf{v}}{e_0},\]

where

\[a(\psi, \phi) = \frac{\mu_0}{4\pi} \int_{\Omega} \int_{\Omega} \nabla \psi(r) \cdot \nabla' \phi(r') \frac{d r d r'}{|r - r'|}\]
Transport current problem

The leads supplying $l_{tr}$ to the film should be taken into account. We assume the leads are semi-infinite sc strips. Far away from the film, $\mathbf{j}$ in a lead is as in an infinite strip:

$$\mathbf{j} = \{j_\eta(\zeta, t), 0\}.$$  

1. Cut the leads far enough from the film and compute $\mathbf{j}$ on the cuts by solving a 1D problem. This determines the non-homogeneous Dirichlet b.c. for the stream function.

2. Add to the external field $b_e(t)$ the field induced by the current in the cut-off semi-infinite leads:

$$\tilde{b}_e = b_e(t) + b_{z}^{in}(r, t) + b_{z}^{out}(r, t),$$

where, e.g., $b_{z}^{in}$ in strip-related coordinates $\{\eta, \zeta\}$ is

$$b_{z}^{in}(\eta, \zeta, t) = \frac{\mu_0}{4\pi} \int_{-w}^{w} \frac{j_\eta(\zeta', t)}{\zeta - \zeta'} \left[ 1 - \frac{\eta}{\sqrt{(\zeta - \zeta')^2 + \eta^2}} \right] d\zeta'$$
On each time layer $t^n = t^{n-1} + \tau^n$ we solve the problem: Find $\mathbf{v}^n$ and $g^n$ such that $g^n|_{\partial\Omega}$ satisfies the b.c. and

$$a \left( \frac{g^n - g^{n-1}}{\tau^n}, \phi \right) - (\mathbf{v}^n, \nabla \phi) = \left( \frac{\tilde{b}_e^n - \tilde{b}_e^{n-1}}{\tau^n}, \phi \right),$$

$$\nabla g^n = -j_c \left( \frac{|\mathbf{v}^n|}{e_0} \right)^{q-1} \frac{\mathbf{v}^n}{e_0},$$

for all $\phi \in H^{1/2}_{00}$ (i.e., smooth enough and zero on $\partial\Omega$).
Discretization in time and iterations

On each time layer $t^n = t^{n-1} + \tau^n$ we solve the problem:

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$$a \left( \frac{g^n - g^{n-1}}{\tau^n}, \phi \right) - (v^n, \nabla \phi) = \left( \frac{\tilde{b}_e^n - \tilde{b}_e^{n-1}}{\tau^n}, \phi \right),$$

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for all $\phi \in H^{1/2}_{00}$ (i.e., smooth enough and zero on $\partial\Omega$).

Iterations:

$$v^{n,j} = v^{n,j-1} - \frac{|v^{n,j-1}|^{q-1} v^{n,j-1} + (e_0^q / j_c) \nabla g^{n,j}}{|v^{n,j-1}|^{q-1}},$$

where $|v|_\varepsilon = \sqrt{|v|^2 + \varepsilon^2}$ and $\varepsilon$ is very small.

Over-relaxation can accelerate the convergence of these iterations.
Finite element approximation FEM1

\[ a \left( \frac{g^n - g^{n-1}}{\tau^n}, \phi \right) - (v^n, \nabla \phi) = \left( \frac{\tilde{b}_e^n - \tilde{b}_e^{n-1}}{\tau^n}, \phi \right), \]

\[ \nabla g^n = -j_c \left( \frac{|v^n|}{e_0} \right)^{q-1} \frac{v^n}{e_0} \]

1. The simplest approximation:
   - continuous p-w linear el. for \( g \) and \( \phi \);
   - vectorial p-w constant el. for \( v \).

Result: convergence for \( g \) but “mozaic” \( v \).
Useless if the electric field is needed.
Similarly for other critical state problems.
A reformulation using an additional a test function $u$:

$$a \left( \frac{g^n - g^{n-1}}{\tau^n}, \phi \right) + (\nabla \cdot \mathbf{v}^n, \phi) = \left( \frac{\tilde{b}_e^n - \tilde{b}_e^{n-1}}{\tau^n}, \phi \right),$$

$$(\nabla \cdot \mathbf{u}, g^n) = \left( \mathbf{u}, j_c \left( \frac{|\mathbf{v}^n|}{e_0} \right)^{q-1} \frac{\mathbf{v}^n}{e_0} \right)$$

2. RT approximation:
   - continuous p-w linear el. for $g$ and $\phi$;
   - div-conforming Raviart-Thomas el. for $\mathbf{v}$, $\mathbf{u}$: vectorial p-w linear with cont. normal components on edges.

Result: convergence for both $g$ and $\mathbf{v}$ for any power law. Similarly for other critical state problems.
Programming is complicated.
Finite element approximation: FEM3

\[
a \left( g^n - g^{n-1}, \phi \right) - (v^n, \nabla \phi) = \left( \tilde{b}_e^n - \tilde{b}_e^{n-1}, \phi \right),
\]

\[
\nabla g^n = -j_c \left( \frac{|v^n|}{e_0} \right)^{q-1} \frac{v^n}{e_0}
\]

3. NC approximation:

- nonconforming p-w linear el. for \( g \) and \( \phi \) (continuous in the mid-edge points);
- vectorial p-w constant el. for \( v \).

Result: convergence for both \( g \) and \( v \) for any \( p \). Similarly for other critical state problems. The programming is easier.
Dimensionless variables used in numerical simulations:

\[ x = \frac{x'}{L}, \quad t = \frac{t'}{t_0}, \quad e = \frac{e'}{e_0}, \quad j = \frac{j'}{j_c}, \]

\[ h_3 = \frac{h_3'}{j_c}, \quad g = \frac{g'}{j_cL}, \quad l_{tr} = \frac{l_{tr}'}{j_cL}, \]

where $L$ is the characteristic film size and $t_0 = \mu_0 j_c L / e_0$. 
Accuracy test 1: Magnetization of a disk

The external field grows linearly with time: \( h_e(t) = t \).

Solution for thin disk, the Bean model:

Mikheenko & Kuzovlev 93, Clem & Sanchez 94.

Numerical vs analytical results:

\[ p = 10^9, \ h_e = 0.65 \]

<table>
<thead>
<tr>
<th>el. size</th>
<th>finite element</th>
<th>( \delta(j) )</th>
<th>( \delta(e) )</th>
<th>CPU time (min)</th>
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</thead>
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<td>0.06</td>
<td>RT</td>
<td>0.89</td>
<td>3.3</td>
<td>4.1</td>
</tr>
<tr>
<td></td>
<td>NC</td>
<td>0.15</td>
<td>0.31</td>
<td>2.4</td>
</tr>
<tr>
<td>0.03</td>
<td>RT</td>
<td>0.46</td>
<td>1.3</td>
<td>125</td>
</tr>
<tr>
<td></td>
<td>NC</td>
<td>0.06</td>
<td>0.24</td>
<td>164</td>
</tr>
</tbody>
</table>

Table: Accuracy of RT and NC approximations

Thin SC films
Magnetization problem: Example 1

The electric field is strong near the boundary indentations and concave corners (Schuster et al. 1996, Vestgarden et al. 2007). In our simulation: the power law with $p = 1000$ and $h_e(t) = t$. All results (in dimensionless units) are presented for $h_e = 0.4$.

The mesh: about 9000 elements, refined near the film boundary:
Magnetization problem: Example 1

Electric field $|e|$
Magnetization problem: Example 1

Normal magnetic field level contours, computed via the Biot-Savart law

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Magnetization problem: Example 1

Current streamlines
Inhomogeneous film:
in the rectangular area $j_c = 0.5$; in the rest of the film $j_c = 1$.
Growing external field, $p = 1000$.
Results (dimensionless): for $h_e = 0.5$.
Mesh: 10.6 thousand el.
Magnetization problem: Example 2

Electric field $|e|$
Magnetization problem: Example 2

Level contours of the normal to film magnetic field

The penetration is deeper in the lower $j_c$ area.
Magnetization problem: Example 2

Current streamlines

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Thin SC films
A film with 3 holes.
The holes are filled and $j_c$ there is set to $1/500$ (in the film $j_c = 1$).

Mesh: 10.4 thousand el. Results: shown for $h_e = 0.5; \rho = 100$. 

![Graph showing the mesh and results for the problem.]
Magnetization problem: Example 3

Electric field $|e|$
Level contours of the normal to the film magnetic field
Accuracy test 2: thin strip with transport current

Growing transport current: \( l_{tr}(t) = t \).

Solution for an infinite strip, the Bean model:
Norris 70, Brandt et al. 93, Zeldov et al 94.

Numerical vs analytical results:
\( p = 10^6 \), \( \Omega = [-1, 1] \times [-1, 1] \), \( l_{tr} = 0.75 \)

Table: Accuracy of the NC approximation

<table>
<thead>
<tr>
<th>el. size</th>
<th>( \delta(j) )</th>
<th>( \delta(e) )</th>
<th>CPU time</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.02</td>
<td>1.0</td>
<td>4.7</td>
<td>17 min</td>
</tr>
<tr>
<td>0.01</td>
<td>0.5</td>
<td>3.3</td>
<td>16 h</td>
</tr>
</tbody>
</table>

The transport current problems are more difficult because the boundary cond. for \( g \) is inhomogeneous and \( b_{z}^{in} \), \( b_{z}^{out} \) are singular on the cuts. Special regularization procedure was needed for computing \( j = \nabla \times g \) (Barrett, P. and Sokolovsky 13).
In transport current problems, if the p-w linear nonconforming elements are used to approximate $g$, the directly calculated p-w constant values $j|_\sigma = \nabla \times g|_\sigma$ are scattered. A better approximation was obtained as $j|_\sigma = \nabla \times G|_\sigma$, where $G$ is the p-w linear continuous approximation of $g$ satisfying the boundary conditions at the boundary vertices and minimizing the distance

$$\sum_\sigma |\sigma| |\nabla \times (g|_\sigma - G|_\sigma)|^2 = \sum_\sigma |\sigma| |\nabla (g|_\sigma - G|_\sigma)|^2.$$ 

To find $G$ one solves the linear system

$$(\nabla G, \nabla \psi_i) = (\nabla g, \nabla \psi_i)$$

for each p-w linear continuous $\psi_i$ equal to one in the internal vertex $i$ and zero in other vertices.
Film with a hole, growing transport current $I_{tr} = t$.
Results (dimensionless units): for $I_{tr.} = 0.75$ and $h_e = 0$.
Mesh: 19,000 elements.
Modulus of the current density, $|j|$
Modulus of the electric field, $|e|$
The normal to film magnetic field, $h_3$
Meander-like film, $I_{tr.} = 0.75$. **Mesh**: 23,000 el.

Meandering films are used in fault current limiters.
Modulus of the electric field, $|e|$
An area of research where solid-state and atom physics meet.

Perez-Rios and Sanz 13:

“Magnetic trapping is a cornerstone for modern ultracold physics and its applications (e.g., quantum information processing, quantum metrology, quantum optics, or high-resolution spectroscopies).”

Cano et al. 08:

“... these traps play a fundamental role in studies of atom-surface interactions (the Casimir-Polder force), the spin decoherence of atoms near dielectric bodies, and in the usage of trapped atoms to probe local irregularities of magnetic and electric fields near conductive films.”

The main interest: properties of the Bose-Einstein condensate, the state of matter where most particles occupy the same lowest energy state and quantum effects become exhibited on a macro-scale.
Many atoms have a magnetic moment; their energy shifts in a magnetic field:

$$\Delta E = -m \cdot b$$

The magnetic moment of an atom takes on one of certain discrete values (quantized) and, placed in a strong magnetic field, becomes aligned with or against the field. If a number of atoms are placed in the same field, they are distributed over the allowed moment values for these atoms.

In a non-uniform field, those atoms whose magnetic moments are aligned with the field will have lower energies in a higher field. These atoms will tend to occupy locations with higher fields: the “high-field-seeking” atoms. Conversely, the atoms with magnetic moments aligned opposite the field will have higher energies in a higher field, these are the “low-field-seeking” atoms.
There can be no isolated maximum of $|b|$ in the free space (only at the sources of the field). Indeed, in the free space $b$ is harmonic,

$$\begin{align*}
\nabla \times b &= 0 \\
\nabla \cdot b &= 0
\end{align*} \Rightarrow 0 = \nabla \times \nabla \times b = \nabla (\nabla \cdot b) - \Delta b = -\Delta b
$$

Therefore

$$\Delta |b|^2 = 2 \sum_{i=1}^{3} (\Delta b_i \cdot b_i + |\nabla b_i|^2) = 2 \sum_{i=1}^{3} |\nabla b_i|^2 \geq 0,$$

and $|b|^2$ is a subharmonic function. An isolated minimum can be created. It is used to trap and keep the low-field-seeking ultracold atoms in a confined space.
Desired trap properties:

- The trap potential well should be much deeper than the kinetic energy of atoms: $\tilde{\mu} B_{\text{dep}} \geq 10 k_B T$, where $\tilde{\mu}$ is the atom magnetic moment, $B_{\text{dep}}$ is the difference between the max. $|b|$ level for which the iso-surface of $|b|$ is closed and the min. value of $|b|$ inside the surface; $k_B$ is the Boltzmann constant; $T$ the atom temperature.

- To avoid spin-flip transition, after which the atom escapes from the trap, $\min |b|$ should not be zero.

- Away from the minimum, the magnetic field gradient in the trap should be sufficient to prevent gravity and atom-surface interaction forces to pull atoms out of the trap.

To trap the most often used $^{87}\text{Rb}$ atoms in the $|F = 2, m_F = 2 \rangle$ state at $T = 1 \mu K$ one needs $B_{\text{dep}} \geq 0.07 \text{ G}$ and the field gradient at least 15 G/cm.
A microchip magnetic trap

Horikoshi and Nakagawa (06) used a Z-shaped gold wire to produce the magnetic field. Weak uniform bias field was applied to avoid the zero-field minimum. Bose-Einstein condensate (BEC) of $^{87}\text{Rb}$ atoms existed for about 3 s.

A similar trap based on a thin superconducting Z-shaped film:

Mukai et al. 07
Emmert et al. 09
Bernon et al. 13

BEC lifetime: 40 s - 4 min.

An advantage of a SC chip: strongly reduced electromagnetic noise near the film surface, especially, in the case of persistent currents.
The shape of atom cloud in a trap can be approximated by a closed $|\mathbf{b}|$ iso-surface corresponding to atom temperature, $k_b T / \bar{\mu}$.

$l_{tr} : 0 \rightarrow 0.7 l_c; \quad b_{1,\text{bias}} = 0.1$ (scaled by $\mu_0 j_c$)

Level surfaces: $|\mathbf{b}| = 0.045$ and $|\mathbf{b}| = 0.065$

For $\mu_0 j_c \approx 100$ G this corresponds to 4.5 and 6.5 G.

$B_{\text{dep}} \approx 4$ G, sufficient for stable trapping of $^{87}\text{Rb}$ atoms at 200 $\mu K$. 

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Thin SC films
$l_{tr} : 0 \rightarrow 0.7l_c \rightarrow 0; \ b_{1, bias} = 0.007$

**Advantage:** no noise from the current source.

Level surfaces: $|b| = 0.003$ and $|b| = 0.005$.  

Z trap, persistent current
Sierke et al. 12: persistent current induced in a square YBCO film $1 \text{mm} \times 1 \text{mm} \times 800 \text{nm}$ by two opposite pulses of the external field

(1) $b_e : 0 \rightarrow 3 \rightarrow 0$; (2) $b_e : 0 \rightarrow -1 \rightarrow 0$.

The simulated magnetic trap shape (left) resembles that of the cloud of $^{87}\text{Rb}$ atoms in this experiment (right).

$|b| = 0.08$
$|b| = 0.13$
The variational formulation of thin film problems in terms of the electric field **AND** scalar stream function makes possible accurate computation of all variables of interest, including the electric field.

The transport current problems were solved for non-trivial film geometries.

Our numerical algorithm is accurate for any power in the power law. For high powers a good approximation to the Bean model solution is obtained.

This method can be used for modeling various electronic and electrical devices based on thin superconducting films.

Thank you!
References:


