# Energetics of Half-Quantum Vortices

Kevin Roberts

UIUC

October 3, 2012

Excerpt from the Proceedings of the 2012 COMSOL Conference in Boston

Kevin Roberts (UIUC)

Energetics of Half-Quantum Vortices

October 3, 2012 2 / 24

3

3 D ( 3 D )

# Outline

### Introduction

Experimental Results

### 3) Theory

4 Use of COMSOL Multiphysics

### 5 Results



3

# What is a quantum vortex?

• Magnetic fields of sufficient magnitude produce normal (N) regions in superconductors (SC)-the intermediate state.

< ロ > < 同 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ >

# What is a quantum vortex?

• Magnetic fields of sufficient magnitude produce normal (N) regions in superconductors (SC)-the intermediate state.



Proceedings of the Royal Society A248 464. The Royal Society

 In Type I superconductors the surface energy between SC and N regions is postive, and the intermediate state consists of macroscopic SC and N regions.

A B F A B F

# What is a quantum vortex?



H. F. Hess et al., *Phys. Rev. Lett.*, **62**, 214 (1989)

- In Type II superconductors, the surface energy is negative, and the system seeks to increase the surface area.
- There is a quantum limit to how finely the regions can proliferate and how little flux is allowed penetrate the sample. These penetrating quanta of flux (h/2e) form a hexagonal Abrikosov lattice.

- 4 同 6 4 日 6 4 日 6

# What is a half-quantum vortex? Why do I care?

- A vortex with a magnetic flux of h/4e, of course.
- Indicative of p-wave Cooper pairing. The electrons are bound in a spin-triplet state.
- HQVs have non-trivial topological properties enabling interesting quantum mechanics-possibly quantum computation.
- COMSOL provides us with a tool to solve the complicated non-linear equations derived from Ginzburg-Landau theory.

# Outline

### Introduction

### 2 Experimental Results

#### 3 Theory



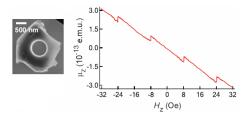
#### 5 Results



3

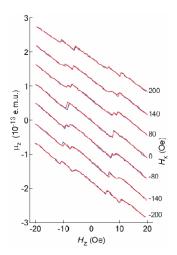
# HQVs in SRO

- Properties of SRO suggest p-wave pairing. What about HQVs?
- A HQV's free energy diverges logarithmically with system size so one needs micron size samples to detect.
- Jang, Budakian, et al manufactured mesoscopic rings of SRO and measured the magnetic moment using magnetic cantilever techniques[1].



[1] J. Jang, et al, Observation of half-height magnetization steps in Sr<sub>2</sub>RuO<sub>4</sub>, Science, 331, 6014 (2011) (2011)

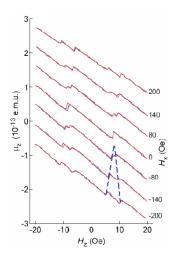
# Stability Wedge



 Results show an increased stabilization of the half-flux state with increasing in-plane magnetic field.

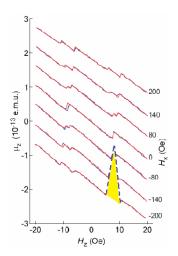
October 3, 2012 9 / 24

# Stability Wedge



- Results show an increased stabilization of the half-flux state with increasing in-plane magnetic field.
- Stability region grows linearly with in-plane field creating a "stability wedge".

# Stability Wedge



- Results show an increased stabilization of the half-flux state with increasing in-plane magnetic field.
- Stability region grows linearly with in-plane field creating a "stability wedge".

# Outline



#### Experimental Results

### 3 Theory



#### 5 Results



3

## Model Free Energy

• Superconductivity in SRO described by ESP state with spin-up and spin-down condensates.

3

## Model Free Energy

- Superconductivity in SRO described by ESP state with spin-up and spin-down condensates.
- Use GL theory with two order parameters and appropriate couplings.

## Model Free Energy

- Superconductivity in SRO described by ESP state with spin-up and spin-down condensates.
- Use GL theory with two order parameters and appropriate couplings.
- We use the model free energy

$$\begin{split} F &= \int d^3 r \left\{ \sum_{i=\uparrow,\downarrow} \left[ -|\psi_i|^2 + \frac{1}{2} |\psi_i|^4 + \left| \left( \frac{\nabla}{\kappa} - i\mathbf{A} \right) \psi_i \right|^2 \right] \right. \\ &+ 2\beta \mathbf{J}_{\uparrow} \cdot \mathbf{J}_{\downarrow} + \mu_{HI} \cdot \mathbf{B} + (\mathbf{B} - \mathbf{B}_{ext})^2 \right\} \\ \end{split}$$
where  $\mathbf{J}_i &= \operatorname{Re} \left\{ \psi_i^* \left( \frac{\nabla}{\kappa} - i\mathbf{A} \right) \psi_i / 2i \right\}. \end{split}$ 

# Model Free Energy

- Superconductivity in SRO described by ESP state with spin-up and spin-down condensates.
- Use GL theory with two order parameters and appropriate couplings.
- We use the model free energy

$$F = \int d^3r \left\{ \sum_{i=\uparrow,\downarrow} \left[ -|\psi_i|^2 + \frac{1}{2} |\psi_i|^4 + \left| \left( \frac{\nabla}{\kappa} - i\mathbf{A} \right) \psi_i \right|^2 \right] \right. \\ \left. + 2\beta \mathbf{J}_{\uparrow} \cdot \mathbf{J}_{\downarrow} + \boldsymbol{\mu}_{HI} \cdot \mathbf{B} + (\mathbf{B} - \mathbf{B}_{ext})^2 \right\}$$

where  $\mathbf{J}_i = \operatorname{Re} \left\{ \psi_i^* \left( \frac{\nabla}{\kappa} - i \mathbf{A} \right) \psi_i / 2i \right\}.$ 

• Half flux state exists when the total winding number  $n_{\uparrow} + n_{\downarrow}$  is odd.

くほと くほと くほと

### Kinematic Spin Polarization

• If we make the correspondences  $|\psi|^2 = \rho$  and  $\mathbf{v}_s = \nabla \theta / \kappa - \mathbf{A}$  the GL equations for a single order parameter are

$$\rho \mathbf{v}_s^2 + \rho(\rho - 1) = 0$$

ignoring gradients in the density and second order derivatives.

くほと くほと くほと

### Kinematic Spin Polarization

• If we make the correspondences  $|\psi|^2 = \rho$  and  $\mathbf{v}_s = \nabla \theta / \kappa - \mathbf{A}$  the GL equations for a single order parameter are

$$\rho \mathbf{v}_s^2 + \rho(\rho - 1) = 0$$

ignoring gradients in the density and second order derivatives.

• This is a sort of Bernoulli equation. If  $\mathbf{v}_s^2$  increases,  $\rho$  decreases.

### Kinematic Spin Polarization

• If we make the correspondences  $|\psi|^2 = \rho$  and  $\mathbf{v}_s = \nabla \theta / \kappa - \mathbf{A}$  the GL equations for a single order parameter are

$$\rho \mathbf{v}_s^2 + \rho(\rho - 1) = 0$$

ignoring gradients in the density and second order derivatives.

- This is a sort of Bernoulli equation. If  $\mathbf{v}_s^2$  increases,  $\rho$  decreases.
- Victor Vakaryuk and Tony Leggett showed that a difference in densities occurs in the HQV since the fluid velocities are different[2].

## Kinematic Spin Polarization

• If we make the correspondences  $|\psi|^2 = \rho$  and  $\mathbf{v}_s = \nabla \theta / \kappa - \mathbf{A}$  the GL equations for a single order parameter are

$$\rho \mathbf{v}_s^2 + \rho(\rho - 1) = 0$$

ignoring gradients in the density and second order derivatives.

- This is a sort of Bernoulli equation. If  $\mathbf{v}_s^2$  increases,  $\rho$  decreases.
- Victor Vakaryuk and Tony Leggett showed that a difference in densities occurs in the HQV since the fluid velocities are different[2].
- A difference in densities is interpreted as a spin polarization lying in the ab-plane which can be used to lower the half flux state's free energy via the term

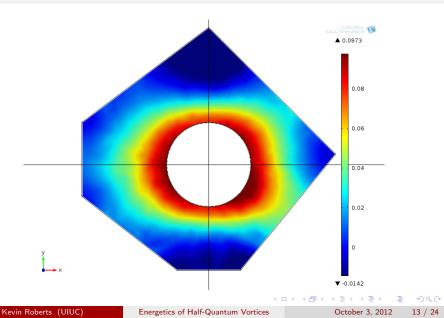
$$oldsymbol{\mu}_{HI}\cdot {f B}=\mu\left(|\psi_{\uparrow}|^2-|\psi_{\downarrow}|^2
ight)B_{ab}$$

[2] Vakaryuk, Leggett, Phys. Rev. Lett., 103, 057003 (2009)

Kevin Roberts (UIUC)

Energetics of Half-Quantum Vortices

# $\Delta |\psi|^2$ in the HQV



# Outline



- Experimental Results
- 3 Theory



#### Results

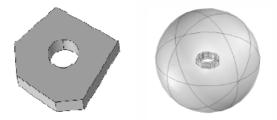


3

(人間) トイヨト イヨト

# Simulation Geometry

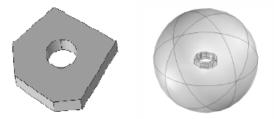
- I drew a ring geometry which was similar to those that were used in the experiment.
- The ring was placed in a surrounding spherical volume.



Kevin Roberts (UIUC)

# Simulation Geometry

- I drew a ring geometry which was similar to those that were used in the experiment.
- The ring was placed in a surrounding spherical volume.



 Modeling the free space around the ring is important to properly calculate the increase in free energy due to the diamagnetism of the sample because one does not know a priori what the field is at the edge of the sample.

Kevin Roberts (UIUC) Energetics of Half-Quantum Vortices

# Free Energy $\rightarrow$ GL equations

 The equations and boundary conditions were derived by varying the free energy with respect to the field variables ψ<sub>↑</sub>, ψ<sub>↓</sub> and A.

くほと くほと くほと

# Free Energy $\rightarrow$ GL equations

- The equations and boundary conditions were derived by varying the free energy with respect to the field variables ψ<sub>↑</sub>, ψ<sub>↓</sub> and A.
- By setting the time derivative of the field equal to minus the free energy's functional derivative, the system was allowed to relax from chosen initial conditions to a stable equilibrium

$$\frac{\partial \psi_{\uparrow}}{\partial t} = -\frac{\delta F}{\delta \psi_{\uparrow}^*}, \quad \frac{\partial \psi_{\downarrow}}{\partial t} = -\frac{\delta F}{\delta \psi_{\downarrow}^*}, \quad \frac{\partial \mathbf{A}}{\partial t} = -\frac{\delta F}{\delta \mathbf{A}}$$

イロト イポト イヨト イヨト

# Free Energy $\rightarrow$ GL equations

- The equations and boundary conditions were derived by varying the free energy with respect to the field variables ψ<sub>↑</sub>, ψ<sub>↓</sub> and A.
- By setting the time derivative of the field equal to minus the free energy's functional derivative, the system was allowed to relax from chosen initial conditions to a stable equilibrium

$$\frac{\partial \psi_{\uparrow}}{\partial t} = -\frac{\delta F}{\delta \psi_{\uparrow}^*}, \quad \frac{\partial \psi_{\downarrow}}{\partial t} = -\frac{\delta F}{\delta \psi_{\downarrow}^*}, \quad \frac{\partial \mathbf{A}}{\partial t} = -\frac{\delta F}{\delta \mathbf{A}}$$

• The resulting equations are daunting.

- 4 同 6 4 日 6 4 日 6

## Equations

Do you want to solve these analytically? Here are the equations

• 
$$\frac{\partial \psi_i}{\partial t} - \nabla \cdot \left(\frac{1}{\kappa^2} \nabla \psi_i - \frac{i}{\kappa} \psi_i \mathbf{A} - \frac{\beta}{i\kappa} \psi_i \mathbf{J}_j\right) = (|\psi_i|^2 - A^2 + 2\beta \mathbf{J}_j \cdot \mathbf{A}) \psi_i - \left(\frac{i}{\kappa} \mathbf{A} + \frac{\beta}{i\kappa} \mathbf{J}_j\right) \cdot \nabla \psi_j$$
  
•  $\frac{\partial \mathbf{A}}{\partial t} - \nabla^2 \mathbf{A} = \mathbf{J}_{\uparrow} + \mathbf{J}_{\downarrow} + \beta \left(|\psi_{\uparrow}|^2 \mathbf{J}_{\downarrow} + |\psi_{\downarrow}|^2 \mathbf{J}_{\uparrow}\right)$   
•  $\mathbf{J}_i = \operatorname{Re} \left\{ \psi_i^* \left(\frac{\nabla}{\kappa} - i\mathbf{A}\right) \psi_i / 2i \right\}$ 

and boundary conditions

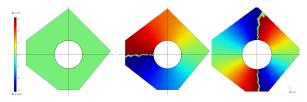
• 
$$\hat{\mathbf{n}} \cdot \left(\frac{1}{\kappa^2} \nabla \psi_i - \frac{i}{\kappa} \psi_i \mathbf{A} - \frac{\beta}{i\kappa} \psi_i \mathbf{J}_j\right) = 0$$
  
•  $\hat{\mathbf{n}} \times (\mathbf{B} - \mathbf{B}_{ext}) = 0$ 

3

(人間) トイヨト イヨト

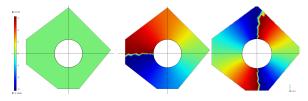
# Initial Conditions

- The vector potential was set on the edge of the sphere, fixing the amount of flux through the system.
- The initial conditions for the OPs were set to fix the winding numbers.



# **Initial Conditions**

- The vector potential was set on the edge of the sphere, fixing the amount of flux through the system.
- The initial conditions for the OPs were set to fix the winding numbers.



- The winding number/flux state of the OP is topolgically protected. COMSOL will find an equilibrium state **given that winding number**, even if another winding number is more stable.
  - $\rightarrow$  Calculate free energies for all states and compare.

#### Results

## Outline

- Introduction
- 2 Experimental Results
- 3 Theory
- 4 Use of COMSOL Multiphysics
- 5 Results

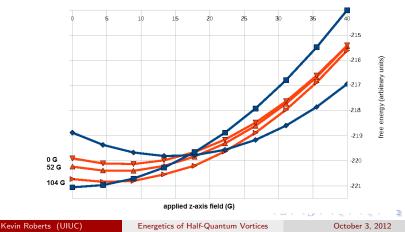


3

#### Results

## Free Energy Curves

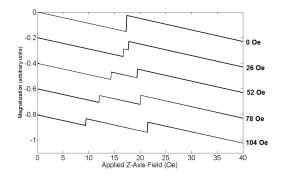
- After solving the GL equations for the particular flux state and magnetic field, the free energy could be calculated by performing the appropriate integral.
- Produce free energy diagrams of integer and half flux states.



20 / 24

## Magnetization Curves

• One can then calculate  $-\frac{\partial F}{\partial B_{z,ext}}$  to produce magnetization curves.



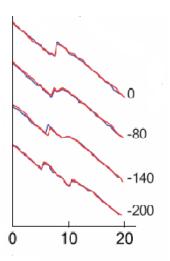
October 3, 2012 21

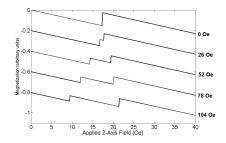
< 3 >

21 / 24

Results

# Magnetization Curves





< 回 ト < 三 ト < 三 ト

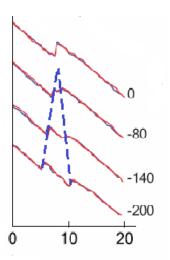
Kevin Roberts (UIUC)

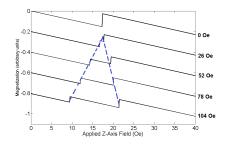
October 3, 2012 22 / 24

æ

Results

# Magnetization Curves





< □ > < □ > < □ >

October 3, 2012 22 / 24

# Outline



- Experimental Results
- 3 Theory
- 4 Use of COMSOL Multiphysics

#### Results



3

- COMSOL shows that the GL model can qualitatively and quantitativly reproduce the experimental data.
- Drawing a general phase diagram in (β, μ) space isn't possible. The energetics depends on the geometry so there is a phase diagram for every ring.
- Acquiring accurate values of β and μ are difficult since we don't know exactly what portions of the ring are superconducting. Unconventional superconductivity is very sensitive to crystal defects and damage during construction is inevitable.