Numerical results for two order parameter superconductors

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Theoretical multiple order parameter superconductors have been treated in a number of papers Babaev [1] [2]. These papers deal primarily with the thermodynamics of vortex liquid transitions. In this paper I use the Ginzburg-Landau phenomenological theory [3] to numerically model multi-order parameter condensates and make qualitative predictions about the behavior of theoretical materials.

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I. FORMALISM

A. The GL Free Energy

The N color GL free energy functional is

\[ F = \sum_{\nu} \left( \alpha_{\nu} |\psi_{\nu}|^2 + \frac{1}{2} \beta_{\nu} |\psi_{\nu}|^4 \right) \]

\[ + \sum_{\nu} \left( \frac{1}{4m_{\nu}} \left( -i\hbar \nabla - 2e\vec{A} \right) |\psi_{\nu}|^2 \right) \]

\[ + \frac{1}{2} \sum_{\nu \neq \mu} \left( \gamma_{\nu\mu} |\psi_{\nu}|^2 |\psi_{\mu}|^2 + \sigma_{\nu\mu} \psi_{\nu}^* \psi_{\mu} \psi_{\mu}^* \right) \]

\[ + \frac{B^2}{2\mu_0} \]  

(1)

where the first sum is the pairing potential, the second sum is the kinetic energy, the third sum is the two lowest order cross terms, and the last term is the magnetic energy. In singlet multi band superconductors such as MgB$_2$, the Josephson term controlled by $\sigma$ couples the phase of the order parameters which effectively breaks the two order parameter degree of freedom. The Josephson term is eliminated in the liquid metallic hydrogen case (and triplet superconductors?). The charge on the carriers is assumed to be the same as an electron. For positive charges this equation is valid up an hermitian conjugate as long as the Josephson term is zero.

B. The GL equations

Applying Euler-Lagrange to the GL free energy produces a set of coupled non-linear differential equations. Minimizing with respect to the vector potential $\vec{A}$ produces the vector equation

\[ E_{\vec{A}} = \sum_{\nu} \left( \frac{i e \hbar}{2m} \left( \psi_{\nu}^* \nabla \psi_{\nu} - \psi_{\nu} \nabla \psi_{\nu}^* \right) + \frac{2e}{m} |\psi_{\nu}|^2 \vec{A} \right) \]

\[ - \frac{\nabla^2 \vec{A}}{\mu_0} + \frac{\nabla (\nabla \cdot \vec{A})}{\mu_0} = 0. \]

(2)

Minimizing with respect to $\psi_{\nu}^*$ produces the complex equations

\[ E_{\psi_{\nu}^*} = \alpha_{\nu} \psi_{\nu} + \beta_{\nu} |\psi_{\nu}|^2 \psi_{\nu}^* \]

\[ + \frac{1}{4m} \left( i\hbar \nabla + 2e\vec{A} \right)^2 \psi_{\nu} \]

\[ + \sum_{\mu} \left( \gamma_{\nu\mu} |\psi_{\mu}|^2 \psi_{\nu} + \sigma_{\nu\mu} \psi_{\nu}^* \psi_{\mu} \psi_{\mu}^* \right) = 0. \]

(3)

From this point on, I will only consider 2 order parameters to simplify the analysis. In order for a superconducting state to form, at least one $\alpha$ must be less than 0. For stability, all $\beta$ must be greater than 0. The cross term $\gamma$ must be less than $\sqrt{\beta_1 \beta_2}$ for stability. There is no stability requirement on $\sigma$ since the Josephson term is second order in $\psi$.

The coherence length is given by

\[ \xi = \frac{\hbar}{\sqrt{2m}|\alpha|}. \]

(4)

The penetration depth for an isolated vortex of one order parameter is given by

\[ \lambda = \sqrt{\frac{m}{2e^2 \mu_0}} \frac{1}{|\psi|} \approx \sqrt{\frac{m}{2e^2 \mu_0}} \frac{\beta}{|\alpha|} \]

(5)

where the approximate is included because $\psi$ also depends on also on the cross coupling terms.

C. Numerical Solutions

The GL equations are non-linear coupled PDE and as such are not solvable analytically. I use an iterative Newton’s method with an approximate Jacobean to solve the GL equations on a 2D. The grid represents a 3D material that is isotropic in the $Z$ direction. The method has the limitation of only being valid for small $|\vec{A}|$. The simulations are limited to systems with two order parameters.
II. RESULTS

For a two order parameter superconductor, there are 4 possible vortex flavors. For condensate type A there will be a type A vortex ($V_a$) and a type A anti-vortex ($-V_A$), and the same pair for condensate type B. The vortex number of each type in a region is conserved and can be determined by the line integral

$$N_a = \int \nabla \arg(\psi) \cdot dl.$$  \hspace{1cm} (6)

The vortex $V_a$ will repel another vortex of type $V_a$ and will attract and mutually annihilate a vortex of type $-V_A$. $V_a$ and $V_b$ will attract while $V_a$ and $-V_b$ repel.

The fact that $V_a$ and $V_b$ attract is counter intuitive since overlapping increases the magnetic energy. The reason for the attraction appears to be the kinetic energy. Consider a gauge where $A = 0$ and there are initially no supercurrents. Now add a vortex of type B. This vortex causes the $A$ field to go as $1/r$ where $r$ is the distance to the center of the vortex. Since type A can have no closed loops of current without also having a vortex, its phase will be unchanged. The kinetic energy of $\psi_A$ will have a contribution that goes as $|A|^2|\psi_A|^2$.

A. Fractional Flux

A vortex in a single order parameter superconductor will always have one flux quantum ($\Phi_0$). In a two order parameter superconductor, this flux quantum is shared between a $V_a$ and $V_b$ vortex. Normally the two vortices will overlap spatially to produce a single flux quantum. Theory predicts that a vortex liquid state may exist where thermal excitations overcome the $V_a$ $V_b$ attraction. Each $V_a$ vortex will carry a constant amount of flux given by

$$\Phi_a = \frac{n_a}{n_a + n_b} \Phi_0$$  \hspace{1cm} (7)

so to some degree, the flux is still quantized. (This relation was experimentally determined.)

B. Forced Separation

A positive value of the $\gamma$ parameter has the property of lowering the energy of an isolated vortex. The $\gamma$ induced repulsion is short range and therefore leaves the pair still bound but at a small separation. Figure 1 shows the bound vortex pair. The possibility also exists for bound triples and vortex clustering.

C. Bound Pair

$V_a$ and $-V_b$ vortices will repel each other. A negative value of $\gamma$ will produce a local attraction which produces a bound state of $V_a$ and $-V_b$ vortices. These bound states are local minimum only. Once the separation between the vortices gets greater than some minimum distance, the vortices will repel.

D. Josephson term

A non-zero Josephson term adds phase frustration to the model when the momentum for each type of order parameter does not match. The energy associated with a separated pair of vortices will grow with the square of the distance between them. This can be understood by noting there will be a line going from one vortex to the other vortex where frustration is greatest and that the spatial width of the frustration energy distribution will be proportional to the separation.

The sign of $\sigma$ does not matter for my simulations since it just picks a preferred relative zero or $\pi$ phase difference between order parameters. I suspect however that tunneling experiments would detect the difference in a real material.
E. Liquid Metallic H

I am not able to simulate large enough systems to study the vortex liquid states predicted by Babaev et al [1]. I did notice that the electron vortices are more mobile than the proton vortices due to the differences in masses. It may be possible to separate them using a current to induce vortex motion at temperatures lower than the vortex liquid melting point.