Computational simulation of vortex matter in Type-II mesoscopic superconductors

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Abstract. In recent years, algorithms and computer simulation methodologies have developed to the stage where simulation can now play a complementary role with experiment, aiding in interpretation of experimental data. Several different approaches to the study of superconductor samples have been developed and their use demonstrated. In this work, we solve numerically the nonlinear time dependent Ginzburg Landau equations to study the vortex dynamics in a mesoscopic type II cylinder superconductor containing one rectangular hole in the presence of an external field applied perpendicular to the surfaces. We calculate the spatial distribution of the superconducting electron density and the phase of the superconducting order parameter using the numerical method based on the technique of gauge invariant variables. It is assumed that the inner hole edge is in contact with a metallic material while the outer edge is in contact with vacuum. The vortex dynamics and the magnetization curves are studied as a function of the external magnetic field.

1. Introduction
In a type-II superconductor; below some critical value $H_{c1}$, the magnetic field is expelled. Above this value a superconductor forms a lattice of vortices which carry magnetic flux through the system. Only at a higher second critical value, $H_{c2}$ superconductivity is destroyed. These responses are viewed as consequences of the vortex interaction in these systems, the energy cost of a boundary between superconducting and normal states and the thermodynamic stability of vortex excitations. In a type-II superconductor the energy cost of a boundary between the normal and the superconducting state is negative, while the interaction between vortices is repulsive. This leads to a formation of stable vortex lattices in conventional mesoscopic samples that have generated much activity in the wide scientific community. Many topologies have been studied experimentally and theoretically, such as circular and square geometry [1, 2, 3, 4], surface roughness and surface defects [5, 6]. All these superconducting structures have attracted attention as potential new components for low-temperature electronics. By solving the non-linear time dependent Ginzburg-Landau (TDGL) equations, using the Link variable technique, we calculate the magnetization and the superconducting electron density for the samples in presence of an external applied magnetic field.
2. Theoretical Formalism

Superconducting state properties are described in the Ginzburg-Landau Theory by the order parameter \( \psi \), and the potential vector \( \mathbf{A} \) (see Ref. [5, 7, 8, 9]). The TDGL equations in absence of external currents are given by:

\[
\frac{\partial \psi}{\partial t} = -\frac{1}{\eta} \left[ (i\nabla + \mathbf{A})^{2} \psi + (1 - T) \left( |\psi|^{2} - 1 \right) \psi \right] \quad (1)
\]

\[
\frac{\partial \mathbf{A}}{\partial t} = -(1 - T) \text{Re} \left[ \psi (i\nabla + \mathbf{A}) \psi \right] - \kappa^{2} \nabla \times \nabla \times \mathbf{A} \quad (2)
\]

Eqs. (1) and (2) were rescaled as follows: \( \psi \) in units of \( \psi_{\infty}(T) \), lengths in units of \( \xi(0) \), time in units of \( t_{0} \), \( H_{c} \) in units of \( H_{c2}(0) \), \( A \) in units of \( H_{c2}(0) \xi(0) \), temperatures in units of \( T_{c} \), we use \( \eta = 1 \). The dynamical equations are complemented with the appropriate boundary conditions for the order parameter \( \hat{n} \left( -i\nabla - \frac{e}{c} \mathbf{A} \right) \psi = \frac{i\psi}{\eta} \) where \( \hat{n} \) is the unity vector perpendicular to the surface of the superconductor. \( b \) is de Gennes parameter, (see Ref. [3]).

3. Numerical Method

The full discretization of the TDGL equations can be found in more detail in Ref. [9]. We used \( U\psi \) method [7] for solve the TDGL equations in a discrete grid. Complex link variables are introduced to preserve the gauge-invariant properties of the discretized equations. \( U^{x} \) and \( U^{y} \) are related to \( \mathbf{A} \) by:

\[
U^{x}(x, y, t) = \exp \left( -i \int_{x_{0}}^{x} A_{x}(\xi, y, t) d\xi \right) \Rightarrow U^{y}(x, y, t) = \exp \left( -i \int_{y_{0}}^{y} A_{y}(x, \eta, t) d\eta \right) \quad (3)
\]

The link variable method is used since a better numerical convergence is obtain in high magnetic fields [10]. The TDGL equations 1 and 2 can be written in the following form:

\[
\frac{\partial \psi}{\partial t} = \mathcal{U}_{x} \frac{\partial^{2} (U\psi)}{\partial x^{2}} + \mathcal{U}_{\eta} \frac{\partial^{2} (U\psi)}{\partial \eta^{2}} + (1 - T) \psi \left( 1 - |\psi|^{2} \right) \Leftrightarrow J_{sa} = (1 - T) \text{Im} \left[ \mathcal{U}_{x} \psi \frac{\partial (U\psi)}{\partial \alpha} \right] \quad (4)
\]

where \( \alpha = (x, \eta) \), and \( \text{Im} \) indicates the imaginary part. We used this method to obtain our results. The outline of this simulation procedure is as follows: the sample is divided in a rectangular mesh consisting of \( N_{x} \times N_{y} = 72 \) cells, with mesh spacing \( a_{x} \times a_{y} = 0.5 \) and a square defect of dimensions \( L_{x} \times L_{y} = 12 \). To derive the discrete equations let us define by \( x_{i} = (i - 1)a_{x}, \; y_{j} = (j - 1)a_{y} \), an arbitrary vertex point in the mesh and:

\[
U_{i,j}^{x} = \mathcal{U}_{i,j}^{x} U_{i+1,j}^{x} = \exp \left( -i \int_{x_{i}}^{x_{i+1}} A_{x}(\xi, y_{j}) d\xi \right) \Rightarrow U_{i,j}^{y} = \exp \left( -i \int_{y_{j}}^{y_{j+1}} A_{y}(x_{i}, \eta) d\eta \right)
\]

\[
L_{i,j} = U_{i,j}^{x} U_{i+1,j}^{y} \tilde{U}_{i,j+1}^{y} = \exp (-ia_{x}a_{y}H_{c})
\]

Then the discretized version of the TDGL equations maintaining second order accuracy in space are given by:

\[
\frac{\partial \psi_{i,j}}{\partial t} = U_{i,j}^{x} \psi_{i,j} - 2\psi_{i,j} + U_{i-1,j}^{x} \psi_{i-1,j} + \frac{U_{i,j+1}^{y} - \psi_{i,j} - 2\psi_{i,j} + U_{i,j-1}^{y} \psi_{i,j-1}}{\eta} \quad (1 - T) \psi_{i,j} (\tilde{\psi}_{i,j} \psi_{i,j} - 1) \psi_{i,j}
\]

\[
\frac{\partial U_{i,j}^{x}}{\partial t} = -i(1 - T)U_{i,j}^{x} \text{Im} \left( \tilde{\psi}_{i,j} U_{i,j}^{x} \psi_{i+1,j} \right) - \frac{\kappa^{2}}{a_{x}^{2}} U_{i,j}^{x} \left( \tilde{L}_{i,j-1} L_{i,j} - 1 \right)
\]

\[
\frac{\partial U_{i,j}^{y}}{\partial t} = -i(1 - T)U_{i,j}^{y} \text{Im} \left( \tilde{\psi}_{i,j} U_{i,j}^{y} \psi_{i,j+1} \right) - \frac{\kappa^{2}}{a_{y}^{2}} U_{i,j}^{y} \left( \tilde{L}_{i,j} L_{i-1,j} - 1 \right)
\]
4. Results and Discussion

The parameters used in our numerical simulations were: $\kappa = 5.0$, $T = 0.53, b = 2.0$ simulating a metallic defect, the applied magnetic field was ramped in steps of $\Delta H = 10^{-4}$. Figures 1 show the magnetization as a function of increasing applied magnetic field for a superconducting square with a centered defect. From these figures, we can see that the first surface barrier field is independent of the metallic quality of the defects, but third critical thermodynamic fields are dependent. The growth of the magnetization with $b$ means that the less the metallic boundary is the more diamagnetic the material is. This effect can be even more enhanced if the interface is a superconductor of higher $T_c$, ($b < 0$), see (Ref ??). In the Figures 2 and 3 we shown the contour plot of the order parameter and its phase $\Theta$ and the magnetic induction for several vorticities. Following the panels from the left to the right, in this order, we can see initially the sample with eight defect increasing the magnetic field sixteen vortices sit in the sample, eight in the hole and the other eight in the superconductor region. Although they are not visible in the contour plot of the magnitude of order parameter, there is a change in the phase around the hole equal to $\Delta \Theta = 16\pi$. Values of the phase close to zero are given by dark gray regions and close to $2\pi$ by light gray regions. The phase allows to determine the number of vortices in a given region, by counting the phase variation in a closed path around this region. If the vorticity in this region is $L$, then the phase changes by $2\pi L$. At a higher magnetic field forty vortices nucleate the sample, twelve at the defect position and twenty eight in the superconducting sample. In conclusion we investigated theoretically the spatial distribution of the vortices in a square mesoscopic superconductor with one metallic square hole. The presence of this hole affects the vortex entry. If the hole is filled with any metallic material the number of vortices into the hole increases, the first critical field $H_{c1}$ remains constant while the third thermodynamic field decrease with the decrease of the value of $b$.

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Figure 2. (Color online) Contour plot of the order parameter for a square with dimension $36\xi(T) \times 36\xi(T)$ and one centered metallic defect with dimension $10\xi(T) \times 10\xi(T)$, simulated by $b = 2.0\xi(T)$. Dark and bright regions represent values of the modulus of the order parameter from 0 to 1.

Figure 3. (Color online) Contour plot of the magnetic induction for a square with dimension $36\xi(T) \times 36\xi(T)$ and one centered metallic defect with dimension $10\xi(T) \times 10\xi(T)$, simulated by $b = 2.0\xi(T)$. Dark and bright regions represent values of the modulus of the order parameter ((as well its phase as $\Delta\Theta/2\pi$, from 0 to 1). From 0 to 1)

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