Brief numerical analysis of (3+1) Ginzburg-Landau equations

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Abstract. In this contribution, we show the implementation of the Link-variable method for solve the complete set of acopled non-linear time dependent Ginzburg-Landau differential equations in a three-dimensional homogeneous and isotropic mesoscopic superconducting system. In this case, the sample is immersed in an external magnetic field at zero applied current. The effects of demagnetization are taken in count and we show the order parameter and its phase in zero field cooling and field cooling process. This numerical analysis shows good results when this solution is applied to a superconducting cubic sample.

1. Introduction

The superconducting systems has been one of the most studied topics in the last years, since its discovery. This is due to the interesting electronic, thermodynamic and magnetic properties that systems exhibit, this added to the possible technological applications that they could have in the following generations. The main properties are the Meissner-Oschenfeld effect, which describes the shielding of the applied external field, in addition to the conduction of electric currents, without Ohmic loss, for a certain critical temperature characteristic of the sample \(T_c\) \([1–4]\). However, in the last years, this branch of condensed matter has been revived quite a bit, due to the discovery of high-temperature superconductors critical in 1986 and more recently the study of multibands, multicomponents, topological, and type 1.5 superconductors, which they are part of the so-called unconventional superconductors, because they cannot be studied using the Bardeen-Cooper-Schrieffer (BCS) theory \([5–7]\).

With this, one of the theories that have had extensive applications in conventional and unconventional superconductors, is the time dependence Ginzburg-Landau (TDGL) theory, which in general are the result of the application of the second-order phase transition theory by the Gibbs functional, obtaining a system of coupled nonlinear equations for the order parameter and the potential vector is due to non-linearity and the complexity of the differential equations obtained, with which in general \((2 + 1)\) systems are studied, and even in these systems, the computational and storage cost is too great. The study of superconducting systems has been revived in recent years, thanks to the new phases discovered, such as topology \([8]\), multibands \([9–11]\), multicomponents \([12, 13]\), Mott and other effects in which the principles of the BCS theory are not applicable. With this, one of the main theories that have been used in the study...
of magnetic, electronic and thermodynamic properties is the TDGL theory [14–16]. Through
the application of TDGL, the dynamics of vortices and the main thermodynamic properties are
generally studied [14]. However, the computational cost in mesoscopic systems is very high [17],
and in (2 + 1) systems it involves long computation and storage times, in such two-dimensional
systems, the real effects on the sample are not studied, such as the demagnetization effects that
occur in three-dimensional samples, which of course has profound effects on the dynamics of
the vortices and other properties [2, 17], i.e., the real effect that the geometry of the sample
has on the main properties of the superconductor. With this, in the present work, we show
the computational implementation for a three-dimensional superconducting system, the work
is written in such a way that its implementation in Matlab, is almost immediate because we
will use the notation of the colon operator commonly used in that program. Finally, we will
present the order electronic superconducting density (order parameter and its phase) for both
field cooling (FC) and zero field cooling (ZFC) process [18].

2. Physical model

In the TDGL model, the superconducting order parameter is a complex pseudo-function
\( \psi(r,t) = \sqrt{n_s}e^{i\Phi} \), where \( n_s \), is the density of the super-electrons and \( \Phi \) its phase. So, the
time-dependent Ginzburg-Landau equations in dimensionless units for the \( \psi \) and the vector
potential \( A \), in the gauge of zero electric potential are given by [2,3,15,16].

In the Equation (1) and Equation (2), \( Re \) is the real part, \( \psi \) and \( \psi^* \) are presented in units of
\( (\alpha/\beta)^{1/2} \), distance in units of coherence length \( \xi \), time in units of \( \pi\hbar/96K_BT_c \), \( A \) in units of
\( \xi \) times the second critical field \( H_{c2} \), temperature \( T \) in units of the critical temperature \( T_c \). \( \kappa \)
is the Ginzburg-Landau parameter. We use the superconducting-dielectric boundary condition for
the order parameter and magnetic field, they are given by \( \hat{n}\cdot(-i\nabla+A)\psi|_{n}=0 \), and \( \nabla\times A = B \)
at the surface of the sample. \( \hat{n} \) is the normal vector to the surface [15,16].

\[
\frac{\partial \psi}{\partial t} = (\nabla - iA)^2 \psi + (1 - T)(1 - \psi^*\psi)\psi, \tag{1}
\]
\[
\frac{\partial A}{\partial t} = (1 - T)Re(\psi^*(-i\nabla - A)\psi) - \kappa^2 \nabla \times (\nabla \times A). \tag{2}
\]

2.1. Mathematical model

The geometry of the problem that we investigate is illustrated in Figure 1(a). The
superconducting domain covers the parallelepiped of high \( a \times a \times c \). Due to the demagnetization
effects, we need to consider a larger domain of dimensions \( L \times L \times z \). (For more details see
Ref. [17]).

Figure 1. (a) Schematic view of the geometry of the system under
investigation. (b) Projection of the numerical method.
They first we will start the initial conditions, in the matrices \( \psi(1 : Nx + 1, 1 : Ny + 1, 1 : Nz + 1) = 1.0 \) (Meissner-Ochsenfeld state), \( A_x = \text{zeros}(Nx, Ny + 1, Nz + 1) \), \( A_y = \text{zeros}(Nx + 1, Ny, Nz + 1) \) and \( A_z = \text{zeros}(Nx + 1, Ny + 1, Nz) \) (Figure 1(b)), and the the link variables (Equation (3)).

\[
U_{i,j,k}^x = \exp(-i \int_{x_0}^x A_x(\mu, y, z) d\mu); \quad U_{i,j,k}^y = \exp(i \int_{y_0}^y A(x, \eta, z) d\eta); \quad U_{i,j,k}^z = \exp(i \int_{z_0}^z A(x, y, \tau) d\tau)
\]  

(3)

2.2. Link variables (3+1) dimensions

Now we will use the Link variable method [2, 3], for establish the discrete form in this base. For notation we will use \( \psi^n(i, j, k) \) the n the time dependence and (i, j, k) the spatial domain (Equation (4) to Equation (14)); with this.

\[
\psi^n(i, j, k) = \psi^n(i, j, k) + \Delta t \left[ \frac{U^{x,n}(i, j, k)\psi^n(i + 1, j, k) - 2\psi^n(i, j, k) - U^{x,n}(i - 1, j, k)\psi^n(i - 1, j, k)}{\Delta x^2} \right. \\
+ \left. \frac{U^{y,n}(i, j, k)\psi^n(i, j + 1, k) - 2\psi^n(i, j, k) - U^{y,n}(i, j - 1, k)\psi^n(i, j - 1, k)}{\Delta y^2} \right. \\
+ \left. \frac{U^{z,n}(i, j, k)\psi^n(i, j, k + 1) - 2\psi^n(i, j, k) - U^{z,n}(i, j, k - 1)\psi^n(i, j, k - 1)}{\Delta z^2} \right. \\
+ (1 - T)(1 - \psi(i, j)\psi(i, j))\psi(i, j) \right]
\]  

(4)

Now for the numerical implementation, we will use the Matlab notation for the internal box \((i, j, k) = (x1 + 1 : x2, y1 + 1 : y2, z1 + 1 : z2)\). Now for the second TDGL equation, we will use the following change of variable.

\[
\text{Re}(\psi^*(-i \nabla - A(x, y))\psi) = \text{Re}\left[ -i \psi^*(i, j)U^{x}(i, j)\frac{\partial (U^{x}(i, j)\psi(i, j))}{\partial x} \right]
\]  

(5)

Obtaining, for every supercurrent component, Equation (6) to Equation (8).

\[
J_x = (1 - T)(\Delta x)^{-1}\Re(\psi^*(i, j, k)U^{x}(i, j, k)\psi^n(i + 1, j, k))
\]  

(6)

\[
J_y = (1 - T)(\Delta y)^{-1}\Im(\psi^*(i, j, k)U^{y}(i, j, k)\psi^n(i, j + 1, k))
\]  

(7)

\[
J_z = (1 - T)(\Delta z)^{-1}\Re(\psi^*(i, j, k)U^{z}(i, j, k)\psi^n(i, j, k + 1))
\]  

(8)

The loops for the super-currents \( J_x(i, j, k) = (1 : Nx, 2 : Ny, 2 : Nz) \), \( J_y(i, j, k) = (2 : Nx, 1 : Ny, 2 : Nz) \) and \( J_z(i, j, k) = (2 : Nx, 2 : Ny, 1 : Nz) \) and \( \Im \) is imaginary part. Now, for the last term of the second TDGL equation we take the usual definition for the rotor \( \nabla \times B = (\partial_y B_z - \partial_z B_y, \partial_z B_x - \partial_x B_z, \partial_x B_y - \partial_y B_x) \), and using the forward numerical derivate.

\[
B_x = (\Delta y)^{-1}(B_x^n(i, j, k) - B_x^n(i, j, k - 1)) - (\Delta z)^{-1}(B_z^n(i, j, k) - B_z^n(i, j, k - 1))
\]  

(9)

\[
B_y = (\Delta z)^{-1}(B_z^n(i, j, k) - B_z^n(i, j, k - 1)) - (\Delta x)^{-1}(B_x^n(i, j, k) - B_x^n(i, j, k - 1))
\]  

(10)

\[
B_z = (\Delta x)^{-1}(B_x^n(i, j, k) - B_x^n(i, j, k - 1)) - (\Delta y)^{-1}(B_y^n(i, j, k) - B_y^n(i, j, k - 1))
\]  

(11)

And finally for the second TDGL.
\[ A^{n+1}_{y}(i, j, k) = A^{n}_{y}(i, j, k) + \Delta t(1 - T)(\Delta x)^{-1}3(\psi^{n,x}(i, j, k)U^{n,x}(i, j, k)\psi^{n}(i + 1, j, k)) \\
+ \kappa^{2}\Delta t(\Delta y)^{-1}(B^{n}_{x}(i, j, k) - B^{n}_{x}(i, j, k - 1)) - \kappa^{2}\Delta t(\Delta z)^{-1}(B^{n}_{y}(i, j, k) - B^{n}_{y}(i, j, k - 1)) \]  
(12)

\[ A^{n+1}_{y}(i, j, k) = A^{n}_{y}(i, j, k) + \Delta t(1 - T)(\Delta y)^{-1}3(\psi^{n,y}(i, j, k)U^{n,y}(i, j, k)\psi^{n}(i, j + 1, k)) \\
- \kappa^{2}\Delta t(\Delta z)^{-1}(B^{n}_{x}(i, j, k) - B^{n}_{x}(i, j, k - 1)) - \kappa^{2}\Delta t(\Delta x)^{-1}(B^{n}_{y}(i, j, k) - B^{n}_{y}(i - 1, j, k)) \]  
(13)

\[ A^{n+1}_{x}(i, j, k) = A^{n}_{x}(i, j, k) + \Delta t(1 - T)(\Delta z)^{-1}3(\psi^{n,z}(i, j, k)U^{n,z}(i, j, k)\psi^{n}(i, j, k - 1)) \\
- \kappa^{2}\Delta t(\Delta x)^{-1}(B^{n}_{y}(i, j, k) - B^{n}_{y}(i, j, k - 1)) - \kappa^{2}\Delta t(\Delta y)^{-1}(B^{n}_{x}(i, j, k) - B^{n}_{x}(i - 1, j, k)) \]  
(14)

With \( A_{x}(1 : Nx, 2 : Ny, 2 : Nz) \), \( A_{y}(2 : Nx, 1 : Ny, 2 : Nz) \) and \( A_{z}(2 : Nx, 2 : Ny, 1 : Nz) \). Now for the corners of the sample, we need to study the three different axes. Using the average of the two points diagonals to it, Equation (15) to Equation (32).

For the \( y - \) axes.
\[
\psi(x, y) = 0.5(\psi(x + 1, y + 1) + \psi(x - 1, y + 1)) 
\]  
(15)

For the \( x - \) axes.
\[
\psi(x) = 0.5(\psi(x + 1, y + 1) + \psi(x - 1, y + 1)) 
\]  
(19)

For the \( z - \) axes. With this, we have the boundary condition for the external magnetic field.
\[
h_{z}(1 : Nx, 1 : Ny, 1) = H_{ext} 
\]  
(27)
\[
h_{z}(1 : Nx, 1 : Ny, Nz + 1) = H_{ext} 
\]  
(28)
\[
h_{z}(1, 1 : Ny, 2 : Nz) = H_{ext} 
\]  
(29)
\[
h_{z}(Nx, 1 : Ny, 2 : Nz) = H_{ext} 
\]  
(30)
\[
h_{z}(2 : Nx - 1, 2 : Nz) = H_{ext} 
\]  
(31)
\[
h_{z}(2 : Nx - 1, Ny, 2 : Nz) = H_{ext} 
\]  
(32)
3. Results

Now, for numerical simulations, we take $L = 40\xi$, $z = 20\xi$, $a = 10\xi$ and $c = 5\xi$, the size of the grid $\Delta x = \Delta y = \Delta z = 0.25$, the Ginzburg-Landau parameter is $\kappa = 1.0$, the time step is $\Delta t = 10^{-5}$ and the field step $\Delta H = 10^{-3}$. With this, the Figure 2(a) show the phase of the order parameter $\Delta \Phi$ and the the Figure 2(b) show the superconducting electronic density $|\psi|^2$ for $T = 0$ and indicated magnetic fields. We observe the entry of vortices symmetrically into the system. As is well know, dark and bright regions represent values of the modulus of the order parameter (as well as $\Delta \Phi/2\pi$) from 0 to 1.

![Figure 2](image)

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 $N$, then the phase changes by $2\pi N$ [19, 20]. So we can see that for $T = 0$ and $N(H = 0.9) = 0$, $N(H = 1.1) = 0$; $N(H = 1.3) = 8$; $N(H = 1.5) = 10$; $N(H = 1.7) = 14$ and $N(H = 1.9) = 15$ in the sample.

Now we see in Figure 3, we present the results for the vortex configuration in the zero field cooling process at $H = 1.1$ and indicates temperatures. In this case we appreciate non-stationary states with $N = 11$ vortices for all studied temperatures. This is a physically coherent result since the number of vortices depends on the external magnetic field. Therefore, we can observe that the symmetry of the superconducting nano-structures influences the magnetic properties of the sample. By improving the experimental process of cooling of these superconductors, the perspectives of their practical applications can be improved.

![Figure 3](image)
4. Conclusions
In this work, we show how to solve and implement numerically in cartesian coordinates, the coupled non-linear time-dependent Ginzburg Landau differential equations in a three-dimensional superconducting sample immersed in a magnetic field. The implementation of the numerical solution for the TDGL equations was written, specifically in the Matlab software. This consideration makes monitoring the paper generate a clear route for writing the program for this solution. Also, we believe that this numerical guide will help researchers interested in the field of superconductivity to implement the algorithms necessary to solve problems at a theoretical level.

5. References
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