Efficient solution of 3D Ginzburg-Landau problem
for mesoscopic superconductors

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Abstract. The recently proposed approach for the solution of Ginzburg-Landau (GL) problem
for 2D samples of arbitrary shape is, in this article, extended over 3D samples having the shape
of (i) a prism with arbitrary base and (ii) a solid of revolution with arbitrary profile. Starting
from the set of Laplace operator eigenfunctions of a 2D object, we construct an approximation to
or the exact eigenfunctions of the Laplace operator of a 3D structure by applying an extrusion or
revolution to these solutions. This set of functions is used as the basis to construct the solutions
of the linearized GL equation. These solutions are then used as basis for the non-linear GL
equation much like the famous LCAO method. To solve the non-linear equation, we used the
Newton-Raphson method starting from the solution of the linear equation, i.e., the nucleation
distribution of superconducting condensate. The vector potential approximations typically used
in 2D cases, i.e., considering it as corresponding to applied constant field, are in the 3D case
harder to justify. For that reason, we use a locally corrected Nystrom method to solve the
second Ginzburg-Landau equation. The complete solution of GL problem is then achieved by
solving self-consistently both equations.

1. Introduction
Many theoretical studies were made in the past on the distribution of the superconducting order
parameter in mesoscopic samples. Most of them were done for very thin (infinitely thin) or
very thick (infinitely thick) prisms samples (reducing the problem always to a 2D problem)
nevertheless some exceptions can be found where the full 3D case was treated [1]. In the very
thick samples, it is normally assumed that there is no variation of the order parameter along
the direction of the applied field. In these studies, the vortex distributions in the sample were
calculated and, notably, new vortex types induced by the geometry were found, such as the giant
vortices [2] and anti-vortices [3]. These studies where mainly based on the Ginzburg-Landau
(GL) theory, but recently also microscopic theory based on Bogoliubov de Gennes, and Usadel
equations are starting to be employed[4]. The GL equations have been proven to be sufficient for
calculation of vortex distributions, as they showed remarkable agreement with the experimental
results [5] and also with the already referred microscopic theories.

In the past, the 2D gauge method has proven to be very accurate, i.e. the vortex phase
diagrams were constructed for many shape samples and predictions of the geometrically induced
anti-vortices have been made for some geometries. These methods have also proven to be
experimentally correct by predicting vortex patterns on samples measured by scanning tunneling
microscopy [5]. Recently an improvement to the method allowed to solve the GL equations in
generic 2D geometries. The aim of the present article is to describe a method that brings the
qualities of the previously developed 2D semi-analytical gauge method to the three-dimensional
space. This way, allowing the study of vortex arrangements constrained by 2D boundaries enclosing a 3D superconducting sample.

2. Method
We report here a method to obtain the solutions of the GL system

\[ \frac{1}{2m}(-i\hbar \vec{\nabla} - \frac{2e}{c} \vec{A})\Psi + \alpha \Psi + \frac{1}{2} \beta |\Psi|^2 \Psi = 0 \] (1)

\[ \vec{\nabla} \times \vec{\nabla} \times \vec{A} = i(\Psi \vec{\nabla} \Psi^* + \Psi^* \vec{\nabla} \Psi) - |\Psi|^2 \vec{A} \] (2)

( where \( \Psi, \vec{A}, m \) and \( i \) are the order parameter wave function, the vector potential, the mass of the carriers and the imaginary constant, respectively ) supplemented by the boundary condition ( b.c. )

\[ (-i\hbar \vec{\nabla} - \frac{2e}{c} \vec{A})^2 \Psi_n |_{n.b.} = 0, \] (3)

( n.b. means that the equation is projected on the unit vector normal to the boundary ) applied to two possible types of two-dimensional boundaries, first prisms with arbitrary base and second solids of revolution with an arbitrary profile. In the following, we will refer to these GL problems [Eq. (1) and Eq. (2)] as first and second GL problem, respectively.

To solve the GL system, we start by solving the first GL equation with the magnetic field equal to the applied magnetic field \( \vec{A}_0 \) and then solve the second GL equation with the order parameter equal to the solution of the first equation. Then, we continue to solve both equations self-consistently.

To solve the first GL equation, we first fixed the gauge of the vector potential in order to simplify the GL b.c. to the Neumann b.c., \( \vec{\nabla}|_{n.b.} \Psi = 0 \), we will call this gauge “superconducting gauge”. To fix this gauge, we must satisfy the condition \( \vec{A}|_{n.b.} = 0 \) on the boundary (the boundary in the present case is an embedded two-dimensional surface in a three-dimensional space) and for that we must find gauge function \( S(\vec{r}) \) that fulfills the condition (superconducting gauge):  

\[ \vec{\nabla}|_{n.b.} S = -\vec{A}|_{n.b.} \] (4)

\[ \vec{A} = \vec{A} + \vec{\nabla} S. \] (5)

This condition is still insufficient to fully define \( S(\vec{r}) \), so we can add one more condition,

\[ \Delta S = 0, \] (6)

that conveniently will simplify the solution of the second GL equation, by setting the vector potential on the Coulomb gauge. \( \vec{\nabla} \cdot \vec{A} = 0 \). The Eq. (6) with the b.c. given by Eq. (4), defines a Poisson problem with arbitrary Neumann b.c. We used a finite element method with second order basis functions [6] to solve this general problem. Then by using Eq. (5) we can get the vector potential in the new gauge.

Secondly, we created a set of basis functions to discretize the first GL equation. This functions must satisfy the Neumann b.c. We present a solution for finding this basis functions for two cases: (i) prism with an arbitrary base and (ii) figure of revolution with arbitrary profile. In both cases, we have a 2D shape that then is, for (i), extruded and, for (ii), revolved, to construct a 3D shape. We will find a basis of functions that satisfy the superconducting b.c. (i.e. Eq. (3)) in two-dimensions for the 2D shape. This procedure is schematically described in the Fig.1.

In some geometries (circle, triangle, square, and more) where the eigenfunctions of the 2D Laplace operator are known, we used the eigenfunctions, \( \Phi_{l,j}^{2D} \), as basis functions to the 2D shape. For a more general case, we created a conformal mapping from the a circle (an auxiliary geometry) to the 2D shape. Then, we got the eigenvectors of the Laplace equation in the circle
Figure 1. Scheme for the construction of the basis functions for the first GL equation in 3D samples with the help of Laplace operator eigenfunctions for the circle geometry. We find the eigenfunctions $\tilde{\Phi}_{l,j}^{2D}$ for the circle, map them into a 2D shape, and create finally new functions from the mapped ones suitable for the 3D shape (see text for details).

geometry($\Phi_{l,j}^{2D}$) and mapped them into the 2D shape. We normalized these mapped functions to obtain the basis functions, $\Phi_{l,j}^{2D}$, where the $l$ and $j$ are the quantum numbers for the radial and angular motions, respectively. A more detailed description of this procedure is given in the previous publication [5].

The basis functions, $\Phi_{l,j}^{2D}(x, y)$, will now become a building block for the 3D basis functions. For (i) the 3D basis will be given by

$$\Phi_{l,j,n}^{3D}(x, y, z) = \Phi_{l,j}^{2D}(x, y) e^{-i(2\pi n)z/h}$$

and for (ii) by

$$\Phi_{l,j,n}^{3D}(r, \phi, z) = \Phi_{l,j}^{2D}(r, \phi) e^{-i(2\pi n)\phi/h}.$$  

where the radial component $r$ only covers one side of the 2D figure, that is symmetric around the revolution axis. With these bases, we can discretize the linearized GL equation

$$\frac{1}{2m} (-i\hbar \vec{\nabla} - 2e\vec{A})^2 \Psi = \alpha \Psi.$$  

that will become a matrix system. This is an eigenvalue equation where the lowest eigenvalue and its correspondent eigenfunction are the nucleation value for $\alpha$ and the distribution of the order parameter at nucleation. The eigenvalues and eigenfunctions of this equation are used to discretize Eq. (1). Finally, the Newton-Raphson method is used to find the solution to the nonlinear equation using as initial value the lowest eigenfunction.

Now we will present the solution for the second GL equation. A dimensionless version of this equation in the Coulomb gauge is

$$\Delta \vec{A} = \kappa^{-2} (i(\Psi \vec{\nabla} \Psi^* - \Psi^* \vec{\nabla} \Psi) - |\Psi|^2 \vec{A}).$$

We can reformulate the differential equation into an volumetric integral equation and also add to this equation the term of the vector potential ($\vec{A}_0$) corresponding to the external applied magnetic field

$$\vec{A} = \int \kappa^{-2} \frac{i(\Psi_G \vec{\nabla} \Psi_G^* - \Psi_G^* \vec{\nabla} \Psi_G) - |\Psi_G|^2 \vec{A}}{|r_i^j - r_j^i|} dV + \vec{A}_0.$$  

We note that the applied vector potential \( \vec{A}_0 \) must be in the same gauge (the Coulomb gauge) as the vector potential \( \vec{A} \). Also the order parameter must correspond to the gauge, which we can achieve using the previously calculated gauge function \( S(\vec{r}) \), i.e. \( \Psi = e^{iS} \). This new equation is a Fredholm equation of second kind. We have used the locally corrected Nystrom method \([7]\) to discretize the kernel of this equation in the points \( r_i \) and in the patches with Lagrange nodal basis functions \([6]\) \( N_i \) defined on \( r_i \), as it is made in the finite element method. The kernel of the equation becomes

\[
[K]_{j,k} = \begin{cases} 
\frac{1}{|\vec{r}_i - \vec{r}_j|} & \text{if } r_i \text{ is far from } r_j \\
\int N_j(r') |r_i - r'| d\vec{r}' & \text{if } r_i \text{ is close to } r_j.
\end{cases} \tag{13}
\]

Then Eq. (12) is converted into a linear system

\[
[M][\vec{A}] = [\vec{F}] \tag{14}
\]

\[
[M]_{j,k} = 1 - [K]_{j,k} |\Psi(r_k)|^2
\]

\[
[F]_j = \sum_k \left( [K]_{j,k} i(\Psi(r_k)^* \vec{\nabla}\Psi(r_k) - \Psi(r_k)^* \vec{\nabla}\Psi(r_k)) + |\Psi(r_k)|^2 \vec{\nabla}S(r_k) \right) + \vec{A}_0(r_j)
\]

\[
[A]_j = \vec{A}(r_j)
\]

We can solve this system by traditional methods like LU decomposition and get a new value for \( \vec{A} \). We can then insert the solution back in the first GL equation and solve it again, thus solving the problem iteratively.

### 3. Conclusions

We presented a method to solve the GL system for the three-dimensional space. The method permits solving the first GL equation in a way that extends the accuracy and speed of the previous semi-analytical methods proposed to solve the first GL equation in two-dimensional space. For the second equation, we used a promising method borrowed from the electromagnetic problems with open boundaries. Examples showing the accuracy and efficiency of the method will be given in subsequent publications.

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