Taking into account Abrikosov vortices in numerical solution of Ginzburg-Landau equations

P F Kartsev
National Research Nuclear University “MEPhI” (Moscow Engineering Physics Institute)
Kashirskoe shosse, 31, 115409 Moscow, Russia
E-mail: PFKartsev@mephi.ru

Abstract. The method is described to take into account the Abrikosov vortices in numerical study of superconducting quantum state in the framework of Ginzburg-Landau equations. The main idea is based on explicit extraction of the solution component related to the vortices. Such approach can be especially useful to study problems with fixed vortex positions.

1. Introduction
A correct numerical simulation of a quantum state of type-II superconductors in an external magnetic field requires taking into account physical phenomena caused by the presence of Abrikosov vortices [1, 2].

At present, to study such problems in the framework of Ginzburg-Landau (GL) theory, a standard approach is to solve the system of nonlinear partial differential equations using various numerical methods. Being very labour-intensive [3–6], this approach can be used only with the help of high-performance computing (HPC) systems. Such high demand of performance is caused, in large part, by the requirement to use the space grid fine enough to follow the fast-changing vortex characteristics. Therefore it is reasonable to combine the application of HPC with additional procedures modifying the initial mathematical problem [7] so that the vortex components of the solution are explicitly taken into consideration. In this article, such approach is presented in details.

2. Description of the procedure
In the framework of GL theory, the quantum state of a superconductor in external magnetic field is described by the system of nonlinear partial differential equations, which in the dimensionless form can be written as [5]:

\[
\left( \frac{i}{\chi} \nabla + A \right)^2 \Psi - \Psi + |\Psi|^2 \Psi = 0, \tag{1}
\]

\[
\nabla \times (\nabla \times A) + \frac{i}{2\chi} \left( \Psi^* \nabla \Psi - \Psi \nabla \Psi^* \right) + |\Psi|^2 A = 0, \tag{2}
\]

where \(\Psi\) and \(A\) are the wave function of Cooper pairs and the vector potential of the magnetic field inside the superconductor, and \(\chi\) is the dimensionless parameter of Ginzburg-Landau theory. This system of equations (1), (2) is combined with the Coulomb gauge condition for the vector potential:

\[
\nabla \cdot A = 0, \tag{3}
\]
and complemented by the boundary conditions:

\[
\left( \frac{i}{\chi} \nabla + \mathbf{A} \right) \mathbf{\Psi} \cdot \mathbf{n} = 0, \tag{4}
\]

\[
(\mathbf{\nabla} \times \mathbf{A})_t = (\mathbf{H})_t, \tag{5}
\]

where \( \mathbf{H} \) is the external magnetic field on the boundary, \( \mathbf{n} \) is a normal vector to the surface, and \( \mathbf{r} \) denotes a component tangential to the surface of the superconductor.

It is well known that generally, this system of equations can not be solved analytically and a numerical approach is required. The calculation grid should have small enough step to describe all the expected features of the solution, including those caused by the presence of Abrikosov vortices. In such case it is reasonable to split the general solution to a slowly-changing main part \( \{\mathbf{\Psi}_1(\mathbf{r}), \mathbf{A}_1(\mathbf{r})\} \) and a fast-changing component corresponding to vortices \( \{\mathbf{\Psi}_2(\mathbf{r}), \mathbf{A}_2(\mathbf{r})\} \).

A specific form of such partitioning depends on the problem under study. Specifically, to study vortex pinning or interaction between vortices one needs to fix the positions of vortices, i.e. wave function zeros, then it is preferable to use the following form:

\[
\mathbf{\Psi}(\mathbf{r}) = \mathbf{\Psi}_1(\mathbf{r}) \cdot \mathbf{\Psi}_2(\mathbf{r}), \tag{6}
\]

\[
\mathbf{A}(\mathbf{r}) = \mathbf{A}_1(\mathbf{r}) + \mathbf{A}_2(\mathbf{r}). \tag{7}
\]

Substitution of expressions (6), (7) into the initial system of equations (1) – (5) allows to obtain the modified system of GL equations for unknown functions \( \mathbf{\Psi}_1(\mathbf{r}), \mathbf{A}_1(\mathbf{r}) \). Final expressions are not shown here due to large size but their derivation is straightforward.

The vortex component \( \{\mathbf{\Psi}_2(\mathbf{r}), \mathbf{A}_2(\mathbf{r})\} \) can be composed from the known solution of simpler single-vortex problem. The solution for the single vortex centered in the point of origin in the infinite space is given by the cylindrical symmetric functions:

\[
\mathbf{\Psi}_v(\mathbf{r}) = f(\mathbf{r})e^{im\phi}, \tag{8}
\]

\[
\mathbf{A}_v(\mathbf{r}) = (-1)^m a(\mathbf{r})e^{\phi}, \tag{9}
\]

where \( m = \pm 1 \) is the sign of the vortex, and equations (1), (2) become 1D equations:

\[
-\frac{1}{\chi^2} \left( \frac{d^2f}{dr^2} + \frac{1}{r} \frac{df}{dr} - \frac{1}{r^2} f \right) - \frac{2}{\chi r} fa + a^2 f + f^3 - f = 0, \tag{10}
\]

\[
- \left( \frac{d^2a}{dr^2} + \frac{1}{r} \frac{da}{dr} \right) - \frac{1}{\chi r} f^2 + af^2 = 0. \tag{11}
\]

Boundary conditions for equations (10), (11) are

\[
f(0) = 0, \tag{12}
\]

\[
a(0) = 0, \tag{13}
\]

\[
f(+\infty) = 1, \tag{14}
\]

\[
a(+\infty) = 0. \tag{15}
\]

Numerical solution of equations (10) – (15) gives the tabulated values for \( f(\mathbf{r}) \) and \( a(\mathbf{r}) \) which are then used in equations (8), (9) to obtain the values of functions \( \mathbf{\Psi}_v(\mathbf{r} - \mathbf{r}_i) \) and \( \mathbf{A}_v(\mathbf{r} - \mathbf{r}_i) \) corresponding to the \( i \)-th vortex located in the point \( \mathbf{r}_i \). The values in the intermediate points between tabulated values can be calculated using simple linear interpolation. It does not lower the precision, however, as the possible error introduced by the interpolation is corrected back by the second component of the solution.
Figure 1. Test problem geometry: two Abrikosov vortices $\Phi_0$ and $-\Phi_0$ near to the hole of radius $R \sim \lambda$.

Finally, the values of $\Psi_2(r)$, $A_2(r)$ and their derivatives are tabulated on the grid used in the main simulation using equations (16), (17):

$$\Psi_2(r) = \prod_{i=1}^{N_v} \Psi_v \left( r - r_i \right),$$  \hspace{1cm} (16)\\
$$A_2(r) = \sum_{i=1}^{N_v} A_v \left( r - r_i \right),$$  \hspace{1cm} (17)

where $N_v$ is the number of vortices in the simulated area.

3. Test calculation
The geometry of physical system for test calculation (2D) is shown in Fig. 1: two vortices of opposite sign are placed in the plane superconductor with cylindrical hole. While the hole creates the pinning potential for each vortex, the presence of another vortex nearby is expected to affect the solution and change the system energy due to nonlinear nature of the GL equations.

To demonstrate this effect, the free energy of the system is calculated for several values of the hole radius and position offset. The simulation results for $\kappa = 20$ are shown in Figs 2 (free energy of one or two vortices near the hole) and 3 (change of free energy in the case of two vortices compared to doubled energy of single vortex). We see how the approach described in this article can be used to study the complicated multi-vortex problems. In particular, it can be used to improve the interaction model used in simulation of modern HTSC materials [1].

4. Conclusion
In this article, the procedure to take into account the Abrikosov vortices in numerical solution of the system of Ginzburg-Landau equations, is presented. The main idea of the approach consists of explicit
Figure 2. Results of test calculation: free energy of the system depending on the hole center offset $x$ in relation to positions of vortices: (a) one vortex, (b) two vortices. Y-coordinates of vortices are $\pm (R + \lambda)$.

Figure 3. Results of test calculation: free energy defect $\Delta F = 2F_1 - F_2$ caused by the cylindrical hole presence, depending on hole radius $R$.

extraction the vortex component from the general solution and respective modification of GL equations. Such reformulation of initial mathematical problem can reduce the simulation time due to coarser grid used in calculation, and is required to study the problems with fixed positions of vortices, The procedure is described in details.

As a first demonstration, the problem of two Abrikosov vortices in the vicinity of the cylindrical hole in the superconductor is studied.
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