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Pseudospectral method for the quantum state determination of the superconductor in the nonuniform magnetic field

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Abstract. In this work, we present the numerical approach to determine the quantum state of a superconductor using the Ginzburg-Landau equations by means of a pseudospectral method. Its convergence is demonstrated by simulation of a test problem. All the analytics is given with details.

1. Introduction

A standard approach to find the quantum state of a superconductor placed in a nonuniform magnetic field, is to apply the Ginzburg-Landau (GL) equations which can be solved numerically [1, 2, 3, 4]. In a dimensionless form, GL equations are written as [1]:

$$\left(\frac{\mathrm{i}}{\varkappa}\boldsymbol{\nabla}+\mathbf{A}\right)^2\Psi-\Psi+|\Psi|^2\Psi=0, \tag{1}$$

$$\boldsymbol{\nabla}\times(\boldsymbol{\nabla}\times\mathbf{A})+\frac{\mathrm{i}}{2\varkappa}(\Psi^*\boldsymbol{\nabla}\Psi-\Psi\boldsymbol{\nabla}\Psi^*)+|\Psi|^2\mathbf{A}=\mathbf{0}, \tag{2}$$

where Ψ is the wave function of the Cooper pair condensate, $\mathbf{A}$ is the vector potential of magnetic field inside the superconductor, and $\varkappa$ is the dimensionless Ginzburg-Landau parameter.

The system of equations (1) and (2) is complemented by the gauge for vector potential (we choose the Coulomb gauge):

$$\boldsymbol{\nabla}\cdot\mathbf{A}=0, \tag{3}$$

and boundary conditions:

$$\left(\frac{\mathrm{i}}{\varkappa}\boldsymbol{\nabla}+\mathbf{A}\right)\Psi\cdot\boldsymbol{n}=0, \tag{4}$$

$$(\boldsymbol{\nabla}\times\mathbf{A})_\tau=(\mathbf{H})_\tau, \tag{5}$$

where $\mathbf{H}$ is the external magnetic field on the boundary, $\boldsymbol{n}$ is a normal vector to the surface, and τ denotes a component tangential to the surface.

The case of nonuniform external field is the most interesting from the practical point of view but makes the computation very labor-intensive. More effective way should involve representing the approximate solution in the form appropriate to simplify the mathematical formulation of the problem.

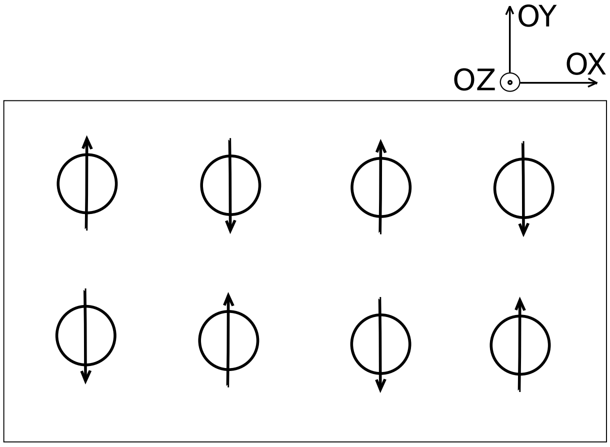

Figure 1. Geometry of the problem under consideration.

In this report, we present the numerical approach to solve the GL equations using a pseudospectral method.

We analyze the case of highly-nonuniform external field present in the localized area of superconductor, so that far enough from the source, its influence on the superconducting state is negligible. As a model problem, we consider a superconducting film in the field of periodic array of magnetic particles placed in alternating way, as shown in figure 1. Alternation is needed to guarantee that no macroscopic current is flowing through the system. As a result, the external magnetic field and the state of the film are made periodic.

With periodic boundary conditions applied, the solution is represented by the series of plane waves:

$$\Psi(x,y,z) = \sum_{k_x,k_y} \psi_{k_x,k_y}(z)\mathrm{e}^{\mathrm{i}(k_x x + k_y y)} \equiv \sum_{\boldsymbol{k}} \psi_{\boldsymbol{k}} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}, \tag{6}$$

$$\mathbf{A}(x,y,z) = \sum_{k_x,k_y} \boldsymbol{a}_{k_x,k_y}(z)\mathrm{e}^{\mathrm{i}(k_x x + k_y y)} \equiv \sum_{\boldsymbol{k}} \boldsymbol{a}_{\boldsymbol{k}} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}, \tag{7}$$

where $\boldsymbol{r} = \{x,y\}$, $k_\alpha = \frac{2\pi}{L_\alpha} l_\alpha$, $\alpha = x,y$, and $l_\alpha = l_{\min},\ldots,l_{\max}$. The range of the summation is limited by practical considerations.

Such form of the solution allows us to convert the 3D(x,y,z) problem into 1D(z) and take advantage of Fourier transform.

2. Main theory

Substituting equations (6) and (7) into initial system (1)–(5) and collecting similar terms, we get for the wave function:

$$\begin{aligned} -\frac{1}{\varkappa^2}\left(\frac{\mathrm{d}^2\psi_{\boldsymbol{k}}}{\mathrm{d}z^2} - \boldsymbol{k}^2\psi_{\boldsymbol{k}}\right) - \psi_{\boldsymbol{k}} + \\ + \frac{2\mathrm{i}}{\varkappa}\sum_{\boldsymbol{p}}\left(\left(a_{\boldsymbol{p}}^{(x)}(k_x - p_x) + a_{\boldsymbol{p}}^{(y)}(k_y - p_y)\right)\mathrm{i}\psi_{\boldsymbol{k}-\boldsymbol{p}} + a_{\boldsymbol{p}}^{(z)}\frac{\mathrm{d}\psi_{\boldsymbol{k}-\boldsymbol{p}}}{\mathrm{d}z}\right) + \\ + \sum_{\boldsymbol{p},\boldsymbol{q}}\left((\boldsymbol{a}_{\boldsymbol{p}}\cdot\boldsymbol{a}_{\boldsymbol{q}})\psi_{\boldsymbol{k}-\boldsymbol{p}-\boldsymbol{q}} + \psi_{\boldsymbol{p}}\psi_{\boldsymbol{q}}^*\psi_{\boldsymbol{k}-\boldsymbol{p}+\boldsymbol{q}}\right) = 0, \end{aligned} \tag{8}$$

for three components of vector potential:

$$\boldsymbol{k}^2 a_{\boldsymbol{k}}^{(x)} - \frac{\mathrm{d}^2 a_{\boldsymbol{k}}^{(x)}}{\mathrm{d}z^2} - \frac{1}{2\varkappa}\sum_{\boldsymbol{p}}(k_x + 2p_x)\psi_{\boldsymbol{p}}^*\psi_{\boldsymbol{k}+\boldsymbol{p}} + \sum_{\boldsymbol{p},\boldsymbol{q}} a_{\boldsymbol{p}}^{(x)}\psi_{\boldsymbol{q}}\psi_{\boldsymbol{p}+\boldsymbol{q}-\boldsymbol{k}}^* = 0, \tag{9}$$

$$\boldsymbol{k}^2 a_{\boldsymbol{k}}^{(y)} - \frac{\mathrm{d}^2 a_{\boldsymbol{k}}^{(y)}}{\mathrm{d}z^2} - \frac{1}{2\varkappa}\sum_{\boldsymbol{p}} (k_y + 2p_y)\psi_{\boldsymbol{p}}^*\psi_{\boldsymbol{k}+\boldsymbol{p}} + \sum_{\boldsymbol{p},\boldsymbol{q}} a_{\boldsymbol{p}}^{(y)}\psi_{\boldsymbol{q}}\psi_{\boldsymbol{p}+\boldsymbol{q}-\boldsymbol{k}}^* = 0, \tag{10}$$

$$\boldsymbol{k}^2 a_{\boldsymbol{k}}^{(z)} - \frac{\mathrm{d}^2 a_{\boldsymbol{k}}^{(z)}}{\mathrm{d}z^2} + \frac{\mathrm{i}}{2\varkappa}\sum_{\boldsymbol{p}} \left(\psi_{\boldsymbol{p}}^*\frac{\mathrm{d}\psi_{\boldsymbol{k}+\boldsymbol{p}}}{\mathrm{d}z} - \psi_{\boldsymbol{k}+\boldsymbol{p}}\frac{\mathrm{d}\psi_{\boldsymbol{p}}^*}{\mathrm{d}z}\right) + \sum_{\boldsymbol{p},\boldsymbol{q}} a_{\boldsymbol{p}}^{(z)}\psi_{\boldsymbol{q}}\psi_{\boldsymbol{p}+\boldsymbol{q}-\boldsymbol{k}}^* = 0, \tag{11}$$

for boundary conditions:

$$\left(\frac{\mathrm{i}}{\varkappa}\left\{\mathrm{i}k_x\psi_{\boldsymbol{k}}, \mathrm{i}k_y\psi_{\boldsymbol{k}}, \frac{\mathrm{d}\psi_{\boldsymbol{k}}}{\mathrm{d}z}\right\} + \sum_{\boldsymbol{p}} \boldsymbol{a}_{\boldsymbol{p}}\psi_{\boldsymbol{k}-\boldsymbol{p}}\right)\cdot\boldsymbol{n} = 0, \tag{12}$$

$$\left\{\mathrm{i}k_y a_{\boldsymbol{k}}^{(z)} - \frac{\mathrm{d}a_{\boldsymbol{k}}^{(y)}}{\mathrm{d}z}, \frac{\mathrm{d}a_{\boldsymbol{k}}^{(x)}}{\mathrm{d}z} - \mathrm{i}k_x a_{\boldsymbol{k}}^{(z)}, \mathrm{i}k_x a_{\boldsymbol{k}}^{(y)} - \mathrm{i}k_y a_{\boldsymbol{k}}^{(x)}\right\}_\tau = (\boldsymbol{h}_{\boldsymbol{k}})_\tau, \tag{13}$$

and for the gauge:

$$\mathrm{i}k_x a_{\boldsymbol{k}}^{(x)} + \mathrm{i}k_y a_{\boldsymbol{k}}^{(y)} + \frac{\mathrm{d}a_{\boldsymbol{k}}^{(z)}}{\mathrm{d}z} = 0. \tag{14}$$

Note multiple summations in the nonlinear terms of equations (8)–(12). Direct numerical calculation of these sums is very time-consuming. More effective way is based on the Convolution Theorem [5] allowing to calculate the discrete convolution using two successive Fourier transforms:

$$(f*g)_{\boldsymbol{k}} = \sum_{\boldsymbol{p}} f_{\boldsymbol{p}} g_{\boldsymbol{k}-\boldsymbol{p}} = \frac{1}{V}\sum_{\boldsymbol{r}} \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}} F_{\boldsymbol{r}} G_{\boldsymbol{r}}, \tag{15a}$$

$$(f*g*h)_{\boldsymbol{k}} = \frac{1}{V}\sum_{\boldsymbol{r}} \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}} F_{\boldsymbol{r}} G_{\boldsymbol{r}} H_{\boldsymbol{r}}. \tag{15b}$$

Here $F_{\boldsymbol{r}}$ is the Fourier transform of $f_{\boldsymbol{k}}$ calculated in the $\boldsymbol{k}$-range extended by factor of 2 (the factor depends on the number of functions in the convolution), with function values $f_{\boldsymbol{k}}$ outside initial range $K_{\min} \le k_\alpha \le K_{\max}$ manually set to zero (this is the so-called 'zero-padding' known in digital signal processing [5]).

Applying (15a) and (15b) to nonlinear terms in equations (8)–(11), we obtain:

$$\begin{aligned}\sum_{\boldsymbol{p}} \left(\left(a_{\boldsymbol{p}}^{(x)}(k_x - p_x) + a_{\boldsymbol{p}}^{(y)}(k_y - p_y)\right)\mathrm{i}\psi_{\boldsymbol{k}-\boldsymbol{p}} + a_{\boldsymbol{p}}^{(z)}\frac{\mathrm{d}\psi_{\boldsymbol{k}-\boldsymbol{p}}}{\mathrm{d}z}\right) = \\ = \frac{1}{V}\sum_{\boldsymbol{r}}\left(\left(k_x a_{\boldsymbol{r}}^{(x)} + k_y a_{\boldsymbol{r}}^{(y)} - \left(p_x a^{(x)}\right)_{\boldsymbol{r}} - \left(p_y a^{(y)}\right)_{\boldsymbol{r}}\right)\mathrm{i}\psi_{\boldsymbol{r}} + a_{\boldsymbol{r}}^{(z)}\left(\frac{\mathrm{d}\psi}{\mathrm{d}z}\right)_{\boldsymbol{r}}\right)\mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}},\end{aligned} \tag{16}$$

$$\sum_{\boldsymbol{p},\boldsymbol{q}} \left((\boldsymbol{a}_{\boldsymbol{p}}\cdot\boldsymbol{a}_{\boldsymbol{q}})\psi_{\boldsymbol{k}-\boldsymbol{p}-\boldsymbol{q}} + \psi_{\boldsymbol{p}}\psi_{\boldsymbol{q}}^*\psi_{\boldsymbol{k}-\boldsymbol{p}+\boldsymbol{q}}\right) = \frac{1}{V}\sum_{\boldsymbol{r}}\left(\boldsymbol{a}_{\boldsymbol{r}}^2 + |\psi_{\boldsymbol{r}}|^2\right)\psi_{\boldsymbol{r}}\mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}, \tag{17}$$

$$\sum_{\boldsymbol{p}} (k_x + 2p_x)\psi_{\boldsymbol{p}}^*\psi_{\boldsymbol{k}+\boldsymbol{p}} = \frac{1}{V}\sum_{\boldsymbol{r}}\left(k_x|\psi_{\boldsymbol{r}}|^2 + 2\left(p_x\psi^*\right)_{\boldsymbol{r}}\psi_{\boldsymbol{r}}\right)\mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}, \tag{18}$$

$$\sum_{\boldsymbol{p}} (k_y + 2p_y)\psi_{\boldsymbol{p}}^*\psi_{\boldsymbol{k}+\boldsymbol{p}} = \frac{1}{V}\sum_{\boldsymbol{r}}\left(k_y|\psi_{\boldsymbol{r}}|^2 + 2\left(p_y\psi^*\right)_{\boldsymbol{r}}\psi_{\boldsymbol{r}}\right)\mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}, \tag{19}$$

$$\sum_{\boldsymbol{p},\boldsymbol{q}} a_{\boldsymbol{p}}^{(x)}\psi_{\boldsymbol{q}}\psi_{\boldsymbol{p}+\boldsymbol{q}-\boldsymbol{k}}^* = \frac{1}{V}\sum_{\boldsymbol{r}} a_{\boldsymbol{r}}^{(x)}|\psi_{\boldsymbol{r}}|^2\mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}, \tag{20}$$

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$$\sum_{\boldsymbol{p},\boldsymbol{q}} a^{(y)}_{\boldsymbol{p}} \psi_{\boldsymbol{q}} \psi^*_{\boldsymbol{p}+\boldsymbol{q}-\boldsymbol{k}} = \frac{1}{V} \sum_{\boldsymbol{r}} a^{(y)}_{\boldsymbol{r}} |\psi_{\boldsymbol{r}}|^2 \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}, \tag{21}$$

$$\sum_{\boldsymbol{p},\boldsymbol{q}} a^{(z)}_{\boldsymbol{p}} \psi_{\boldsymbol{q}} \psi^*_{\boldsymbol{p}+\boldsymbol{q}-\boldsymbol{k}} = \frac{1}{V} \sum_{\boldsymbol{r}} a^{(z)}_{\boldsymbol{r}} |\psi_{\boldsymbol{r}}|^2 \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}, \tag{22}$$

$$\sum_{\boldsymbol{p}} \left(\psi^*_{\boldsymbol{p}} \frac{\mathrm{d}\psi_{\boldsymbol{k}+\boldsymbol{p}}}{\mathrm{dz}} - \psi_{\boldsymbol{k}+\boldsymbol{p}} \frac{\mathrm{d}\psi^*_{\boldsymbol{p}}}{\mathrm{dz}} \right) = \frac{1}{V} \sum_{\boldsymbol{r}} \left(\psi^*_{\boldsymbol{r}} \left(\frac{\mathrm{d}\psi}{\mathrm{dz}} \right)_{\boldsymbol{r}} - \psi_{\boldsymbol{r}} \left(\frac{\mathrm{d}\psi^*}{\mathrm{dz}} \right)_{\boldsymbol{r}} \right) \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}. \tag{23}$$

Finally, we have the system of equations for Fourier-transformed wave function $\psi_{\boldsymbol{k}}(z)$ and vector potential $\boldsymbol{a}_{\boldsymbol{k}}(z)$, consisting of algebraic expressions for these components, and additional Fourier transforms in extended $\boldsymbol{k}$-range with appropriate zero-padding.

3. Test realization

For the problem shown in figure 1, the boundary conditions (12) and (13) are written as:

$$\frac{\mathrm{i}}{\varkappa} \frac{\mathrm{d}\psi_{\boldsymbol{k}}}{\mathrm{dz}} + \sum_{\boldsymbol{p}} a^{(z)}_{\boldsymbol{p}} \psi_{\boldsymbol{k}-\boldsymbol{p}} = 0, \tag{24}$$

$$\frac{\mathrm{d}a^{(x)}_{\boldsymbol{k}}}{\mathrm{dz}} = \mathrm{i}k_x a^{(z)}_{\boldsymbol{k}} + h^{(y)}_{\boldsymbol{k}}, \tag{25}$$

$$\frac{\mathrm{d}a^{(y)}_{\boldsymbol{k}}}{\mathrm{dz}} = \mathrm{i}k_y a^{(z)}_{\boldsymbol{k}} - h^{(x)}_{\boldsymbol{k}}. \tag{26}$$

In our realization, the GL equations and boundary conditions are approximated by first-order finite differences. On the first boundary ($z = 0$), the corresponding equations are the following:

$$\frac{\mathrm{i}}{\varkappa} \frac{[\psi_{\boldsymbol{k}}]^u_1 - [\psi_{\boldsymbol{k}}]^u_0}{\Delta z} + \sum_{\boldsymbol{p}} \left[a^{(z)}_{\boldsymbol{p}}\right]^u_0 [\psi_{\boldsymbol{k}-\boldsymbol{p}}]^u_0 = 0, \tag{27}$$

$$\frac{\left[a^{(x)}_{\boldsymbol{k}}\right]^u_1 - \left[a^{(x)}_{\boldsymbol{k}}\right]^u_0}{\Delta z} = \mathrm{i}k_x \left[a^{(z)}_{\boldsymbol{k}}\right]^u_0 + \left[h^{(y)}_{\boldsymbol{k}}\right]^u_0, \tag{28}$$

$$\frac{\left[a^{(y)}_{\boldsymbol{k}}\right]^u_1 - \left[a^{(y)}_{\boldsymbol{k}}\right]^u_0}{\Delta z} = \mathrm{i}k_y \left[a^{(z)}_{\boldsymbol{k}}\right]^u_0 - \left[h^{(x)}_{\boldsymbol{k}}\right]^u_0, \tag{29}$$

$$\mathrm{i}k_x \left[a^{(x)}_{\boldsymbol{k}}\right]^u_0 + \mathrm{i}k_y \left[a^{(y)}_{\boldsymbol{k}}\right]^u_0 + \frac{\left[a^{(z)}_{\boldsymbol{k}}\right]^u_1 - \left[a^{(z)}_{\boldsymbol{k}}\right]^u_0}{\Delta z} = 0, \tag{30}$$

while on the second boundary ($z = z_d$):

$$\frac{\mathrm{i}}{\varkappa} \frac{[\psi_{\boldsymbol{k}}]^u_d - [\psi_{\boldsymbol{k}}]^u_{d-1}}{\Delta z} + \sum_{\boldsymbol{p}} \left[a^{(z)}_{\boldsymbol{p}}\right]^u_d [\psi_{\boldsymbol{k}-\boldsymbol{p}}]^u_d = 0, \tag{31}$$

$$\frac{\left[a^{(x)}_{\boldsymbol{k}}\right]^u_d - \left[a^{(x)}_{\boldsymbol{k}}\right]^u_{d-1}}{\Delta z} = \mathrm{i}k_x \left[a^{(z)}_{\boldsymbol{k}}\right]^u_d + \left[h^{(y)}_{\boldsymbol{k}}\right]^u_d, \tag{32}$$

$$\frac{\left[a^{(y)}_{\boldsymbol{k}}\right]^u_d - \left[a^{(y)}_{\boldsymbol{k}}\right]^u_{d-1}}{\Delta z} = \mathrm{i}k_y \left[a^{(z)}_{\boldsymbol{k}}\right]^u_d - \left[h^{(x)}_{\boldsymbol{k}}\right]^u_d, \tag{33}$$

$$\mathrm{i}k_x \left[a_{\boldsymbol{k}}^{(x)}\right]_d^u + \mathrm{i}k_y \left[a_{\boldsymbol{k}}^{(y)}\right]_d^u + \frac{\left[a_{\boldsymbol{k}}^{(z)}\right]_d^u - \left[a_{\boldsymbol{k}}^{(z)}\right]_{d-1}^u}{\Delta z} = 0, \tag{34}$$

where $[\cdots]_v^u$ denote the values of $\psi_{\boldsymbol{k}}$ and $\boldsymbol{a_k}$ at the nodes of the calculation mesh with coordinates (u,v) of time and z-axis, respectively.

We see that the equations for the vector potential components are independent of the wave function and linear, thus they can be solved analytically. The values of the wave function, in their turn, can be calculated using the procedure similar to calculation of nonlinear terms of GL equations. It should be noted that the order of approximation can be increased using the method of fictitious areas.

Our realization is based on the pseudoviscosity method [1]. Time steps are made with explicit Euler method, the space is discretized with uniform mesh with step Δz. To test the stability and convergence of the suggested approach, we simulated the system with the external field $\mathbf{H} = \mathbf{0}$ starting from the arbitrary chosen state $[\psi_{\boldsymbol{k}}]_v^0 = 0.25$, $[\boldsymbol{a_k}]_v^0 = \mathbf{0}$. The exact solution of GL equations in this case is $\Psi_{\text{exact}}(x,y,z) = 1$, $\mathbf{A}_{\text{exact}}(x,y,z) = \mathbf{0}$. Other parameters of the problem are: $\varkappa = 0.2$ (type-I superconductor), $L_x = L_y = L_z = 1.6$.

The convergence to the exact solution is demonstrated in figure 2: during the simulation, the free energy approaches the exact value $F_{\text{exact}} = -L_xL_yL_z/2$.

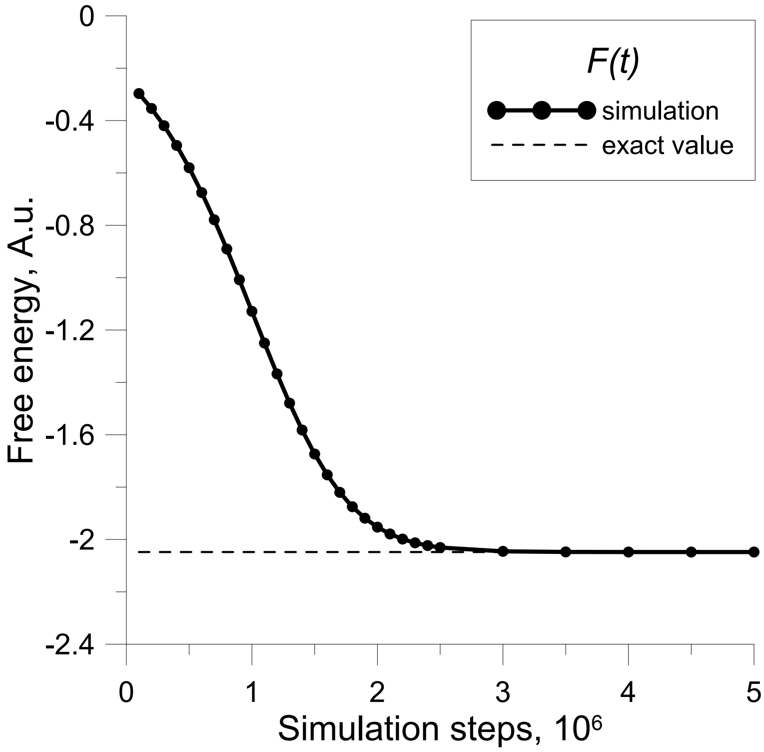

Figure 2. Test of stability and convergence of the suggested approach using the pseudoviscosity method. Parameters of the calculation are $\Delta t = 10^{-6}$, $\Delta z = 0.1$, $l_{\min} = 0$, $l_{\max} = 1$. It can be seen that the free energy of the film approaches exact value $F_{\text{exact}} = -2.048$ during the calculation.

4. Conclusion

In this article, we presented the approach for numerical determination of quantum state of superconductor using the pseudospectral method to solve the Ginzburg-Landau equations. Due to reduction of the problem dimensionality and application of efficient numerical algorithms, this method can sufficiently reduce the amount of calculations needed, and can speed-up the process of solution. All the relations needed for realization are shown. The suggested approach was applied to the problem with known exact solution, to demonstrate the stability and convergence of the algorithm.

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