

Numerical Study of Vortex Nucleation in Two-Band Superconductors

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Abstract— In this study, numerical aspects of the two-dimensional, isothermal, isotropic two-band time-dependent Ginzburg-Landau (TB TDGL) equations in the presence of an external magnetic field are presented. The stability of finite element approximations of the solutions are discussed. Numerical experiments are presented for real two-band superconductor such as MgB₂.

Keywords— Ginzburg-Landau theory; multi-band superconductivity; vortex lattice

I. INTRODUCTION

The conventional time-dependent Ginzburg-Landau (TDGL) model for single band superconductors was suggested many years ago [1]. This theory has been widely accepted as a successfully phenomenological model for a single-band superconductor. Last year many classes of multiband superconductors such as MgB₂, borocarbides and FeAs based superconductors were discovered. Therefore, the TDGL model presented in [1] is not a correct model for multiband superconductivity. In paper [2], the breakdown of the anisotropic GL model for study of MgB₂ is investigated. The TB-TDGL model generalizes the TDGL model by adding coupling terms of the two distinct order parameters to the free energy functional.

Up to now Ginzburg-Landau theory remains a powerful method in study of some physical properties of superconductors. The vortices nucleation in the single-band isotropic superconductors was originally studied by using Ginzburg-Landau equations for single-band isotropic superconductors [3-5]. It is important to note that, the GL theory was generalized for the case superconductors with unconventional order parameter symmetry - d-wave symmetry [6]. GL equations also are useful in study of fluctuational effects on physical properties near T_c [7] in single band isotropic superconductors. TDGL theory was used for calculations of fluctuation conductivity near T_c by Aslamazov-Larkin [8].

Previously, time independent two-band GL equations were successfully used for study the physical properties of recently discovered superconductors such as magnesium diboride (MgB₂) [9, 10] and nonmagnetic $Y(Lu)Ni_2B_2C$ borocarbide compounds [11,12]. In this study, we present the vortex nucleation of the external magnetic field in the framework of a TB TDGL equations. Firstly, we drive time-dependent GL

equations for two-band superconductors. Secondly, we apply these equations for numerical modeling of vortex nucleation in thin superconducting film of two-band superconductor MgB₂ with perpendicular external magnetic field. We use the modified forward Euler method for numerical experiments.

II. TIME DEPENDENT GL EQUATIONS FOR TWO-BAND SUPERCONDUCTORS

The GL free energy functional for an isotropic two-band superconductor can be written as follows [9-12]:

$$F_{SC} = \int d^3r (F_1 + F_{12} + F_2 + H^2 / 8\pi) \quad (1)$$

where

$$F_i = \frac{\hbar^2}{4m_i} \left| \left(\nabla - \frac{2\pi i \vec{A}}{\Phi_0} \right) \Psi_i \right|^2 + \alpha_i(T) \Psi_i^2 + \beta_i \Psi_i^2 / 2 \quad (2)$$

$$F_{12} = \varepsilon (\Psi_1^* \Psi_2 + c.c.) + \varepsilon_1 \left\{ \left(\nabla + \frac{2\pi i \vec{A}}{\Phi_0} \right) \Psi_1^* \left(\nabla - \frac{2\pi i \vec{A}}{\Phi_0} \right) \Psi_2 + c.c. \right\} \quad (3)$$

In these equations m_i denotes the masses of electrons belonging to different bands ($i = 1, 2$); $\alpha_i = \gamma_i(T - T_{ci})$ represents the quantities linearly dependent on the temperature; β and γ_i are constant coefficients; ε and ε_1 describe the interaction between the band order parameters and their gradients, respectively; H is the external magnetic field; and Φ_0 is the magnetic flux quantum. Notation *c.c.* in Eq. (3) means complex conjugate term. In Eqs. (1) and (2), the order parameters are assumed to be slowly varying in space. Minimization procedure of the free-energy functional yields the time-independent GL equations describing the two-band superconductors in equilibrium state [9-12].

Time-dependent equations in two-band Ginzburg-Landau theory can be obtained from Eqs. (1-3) using minimization procedure in analogical way to [13]:

$$\Gamma_1 \left(\frac{\partial}{\partial t} + i \frac{2e}{\hbar} \phi \right) \Psi_1 = - \frac{\delta F}{\delta \Psi_1^*}, \quad (4a)$$

$$\Gamma_2 \left(\frac{\partial}{\partial t} + i \frac{2e}{\hbar} \phi \right) \Psi_2 = - \frac{\delta F}{\delta \Psi_2^*}, \quad (4b)$$

$$\sigma_n \left(\frac{\partial \bar{A}}{\partial t} + \nabla \phi \right) = - \frac{1}{2} \frac{\delta F}{\delta \bar{A}} \quad (4c)$$

Here we use notations similar to [13]. In Eqs. (4) ϕ means electrical scalar potential, $\Gamma_{1,2}$ is relaxation time of order parameters, σ_n is conductivity of sample in two-band case. Choosing corresponding gauge invariance we can eliminate scalar potential from system of Equations (4) [13]. Under such calibration and magnetic field in form, $\vec{H} = (0, 0, H)$ without any restriction of generality, time-dependent equations in two-band Ginzburg-Landau theory can be written as

$$\Gamma_1 \frac{\partial \Psi_1}{\partial t} = - \frac{\hbar^2}{4m_1} \left(\frac{d^2}{dx^2} - \frac{x^2}{l_s^2} \right) \Psi_1 + \alpha_1(T) \Psi_1 + \varepsilon \Psi_2 + \varepsilon_1 \left(\frac{d^2}{dx^2} - \frac{x^2}{l_s^2} \right) \Psi_2 + \beta \Psi_1^3 = 0 \quad (5a)$$

$$\Gamma_2 \frac{\partial \Psi_2}{\partial t} = - \frac{\hbar^2}{4m_2} \left(\frac{d^2}{dx^2} - \frac{x^2}{l_s^2} \right) \Psi_2 + \alpha_2(T) \Psi_2 + \varepsilon \Psi_1 + \varepsilon_1 \left(\frac{d^2}{dx^2} - \frac{x^2}{l_s^2} \right) \Psi_1 + \beta \Psi_2^3 = 0 \quad (5b)$$

$$\sigma_n \left(\frac{\partial \bar{A}}{\partial t} - \nabla \phi \right) = - \text{rot} \bar{A} + \frac{2\pi}{\Phi_0} \left\{ \frac{\hbar^2}{4m_1} n_1(T) \left(\frac{d\phi_1}{dr} - \frac{2\pi A}{\Phi_0} \right) + \right. \quad (5c)$$

$$\left. \varepsilon_1 (n_1(T) n_2(T))^{0.5} \cos(\phi_1 - \phi_2) + \frac{\hbar^2}{4m_2} n_2(T) \left(\frac{d\phi_2}{dr} - \frac{2\pi A}{\Phi_0} \right) \right\}$$

where $l_s^{-2} = \frac{\hbar c}{2eH}$ is the so-called magnetic length. In the general case, the signs of the parameters of interband interaction in Eq. (3) can be arbitrary. These signs of coefficients ε and ε_1 are determined by the microscopic nature of the interaction of electrons belonging to different bands. If ε and ε_1 are both zero, the inter-band interaction vanishes, Eqs. (5a) and (5b) convert into the usual GL equations with the critical temperatures T_{c1} and T_{c2} . In Eqs. (5) $\phi_{1,2}(\vec{r})$ phase of

order parameters $\Psi_{1,2}(\vec{r}) = |\Psi_{1,2}| \exp(i\phi_{1,2})$, $n_{1,2}(T) = 2|\Psi_{1,2}|^2$ - density of superconducting electrons in different bands, expressions for which are presented in [9–12]. Natural boundary conditions to Eqs. (5) has a form:

$$\left\{ \frac{1}{4m_1} \left(\nabla - \frac{2\pi i \bar{A}}{\Phi_0} \right) \Psi_1 + \varepsilon_1 \left(\nabla - \frac{2\pi i \bar{A}}{\Phi_0} \right) \Psi_2 \right\} \bar{n} = 0 \quad (6a)$$

$$\left\{ \frac{1}{4m_2} \left(\nabla - \frac{2\pi i \bar{A}}{\Phi_0} \right) \Psi_2 + \varepsilon_1 \left(\nabla - \frac{2\pi i \bar{A}}{\Phi_0} \right) \Psi_1 \right\} \bar{n} = 0, \quad (6b)$$

$$(\bar{n} \times \bar{A}) \times \bar{n} = \vec{H}_0 \times \bar{n} \quad (6c)$$

First two conditions correspond to absence of supercurrent through boundary of two-band superconductor, third condition corresponds to the continuity of normal component of

magnetic field to the boundary superconductor-vacuum.

As shown in [9–12], temperature dependence of some physical quantities become nonlinear, in contrast to single-band G-L theory. It means that dynamics of order parameters in two-band superconductors differ from those in single-band superconductors. In this study we introduce unconventional scales to non-dimensionalize the TB TDGL system of equations. Mostly, we are focusing on experiments performed with TB TDGL system, and claiming that our model yields realistic results for recently discovered compound MgB_2 .

III. APPLICATION TO THIN SUPERCONDUCTING FILM: RESULT AND DISCUSSION

In this part, we will focus our study on the following two-dimensional simulation topics: steady-state vortex lattices under the effect of a steady applied magnetic field. This includes the cases involving samples consisting of Type-I/Type-II and Type-II/Type-II condensates, with two distinct critical temperatures. We will present the results of many simulations and show that the composite and noncomposite lattice phenomena mentioned above appear only with special combinations of values of the coupling parameters ε , ε_1 and the applied field He , different phenomena appear in other combinations of the values of ε , ε_1 and He . We consider a finite homogeneous superconducting film of uniform thickness, subject to a constant magnetic field. We also consider that the superconductor is in rectangular shape. In this case our two-band GL model becomes two-dimensional [14]. The order parameters Ψ_1 and Ψ_2 vary in the plane of the film, and vector potential \mathbf{A} has only two nonzero components, which lie in the plane of the film. Therefore, we identify the computational domain of the superconductor with a rectangular region $\Omega \in R^2$, denoting the Cartesian coordinates by x and y , and the x - and y - components of the vector potential by $A(x, y)$ and $B(x, y)$, respectively. Before modeling we use so-called bond variables [14] in order to provide the discretization of time-dependent two-band G-L equations

$$W(x, y) = \exp(i\kappa \int^x A(\zeta, y) d\zeta), \quad (7a)$$

$$V(x, y) = \exp(i\kappa \int^y B(x, \eta) d\eta) \quad (7b)$$

Such variables make obtained discretized equations gauge-invariant. In order to get spatially discretization we use forward Euler method [15]. In this method we begin with partitioning the computational domain $\Omega = [0, N_{xp}] \times [0, N_{yp}]$ into two subdomains, denoted by Ω_{2n} and Ω_{2n+1} such that

$$\Omega_{2n} = \Omega \Big|_{i+j=2n} \text{ and } \Omega_{2n+1} = \Omega \Big|_{i+j=2n+1} \quad (8)$$

for

$$i = 0, \dots, N_{xp}, j = 0, \dots, N_{yp},$$

where

$$N_{xp} = N_x + 1, N_{yp} = N_y + 1.$$

For numerical calculations in two-band GL theory, we assume that the size of superconducting film is $40\lambda \times 40\lambda$, where λ denotes London penetration depth of external magnetic field on superconductor [9–12]. Under modeling we also introduce another dimensionless parameters

$$\begin{aligned} \vec{r}' &= \frac{\vec{r}}{\lambda}; \Psi'_{1,2} = \frac{\Psi_{1,2}}{\Psi_{(1,2)0}}; \vec{A} = \frac{\vec{A}}{\lambda H_c \sqrt{2}}; \\ F'(\Psi'_{1,2}, A') &= \frac{F(\Psi_{1,2}, A)}{\alpha_0^2 |\Psi_{1,0}|^2 + \alpha_1^2 |\Psi_{2,0}|^2} \end{aligned} \quad (9)$$

Expressions for $\Psi_{(1,2)0}$, and for thermodynamic magnetic field H_c are presented in [9–12]. The calculations were performed by using the following values of parameters: $T_c = 40$ K; $T_{c1} = 20.0$ K; $T_{c2} = 10$ K

$$\frac{\varepsilon^2}{\gamma_1 \gamma_2 T_c^2} = 3/8$$

$$\eta = \frac{T_c m_2 \varepsilon_1 \gamma_2}{\hbar^2 \varepsilon} = -0.016.$$

These parameters were used for the calculation of another physical properties of two-band superconductor MgB_2 [9–12]. External magnetic field was measured in units of thermodynamic magnetic field H_c .

To solve of corresponding discretized GL equations we will use method of adaptive grid [15]. Results of numerical modelling in different cases are presented in Fig. 1-3. In figures 1-2 we present profile of the order parameters Ψ_1 and Ψ_2 in the absence of interaction between order parameters.

Fig.1 corresponds to the nucleation of magnetic field in superconductor. In Fig. 2 we plot order parameter profile in more high magnetic field, in which vortex numbers arise to four. The case of inter order parameter interaction and drag effects (intergradient interaction) are presented in Fig. 3. As followed from this calculations, due to interband interaction, order parameters in different bands become stronger and as a result distance between vortexes increased. Also, it is clear that at initial stage of penetration of magnetic field into two-band superconductor, the symmetry of Abrikosov vortex lattices has a square character. Similar square lattice was observed experimentally in $LuNi_2B_2C$ compound (see [12]). Also it is clear that, magnetic field penetrate into two-band

superconductor by lateral way. It is necessary to note that, external magnetic field penetration to two-band superconductor is different from those in single-band superconductor. At high magnetic field, when distance between vortexes is small, we must take into account nonuniform distribution of magnetic field in cross-section of single vortex [16]. Detailed analysis of vortex lattices at high magnetic field is the subject of our future investigations.

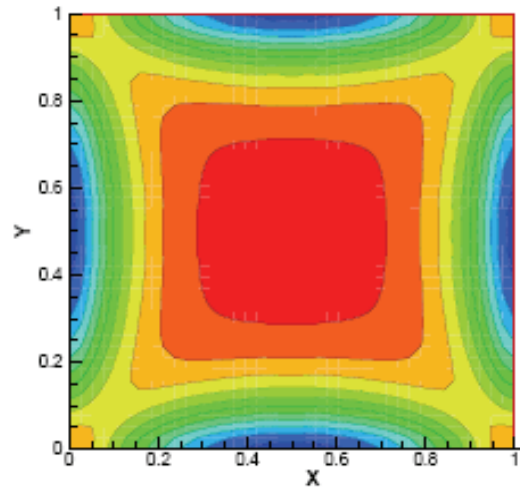


Figure.1a) $\Psi_1; \varepsilon = \varepsilon_1 = 0, H_e = 1$

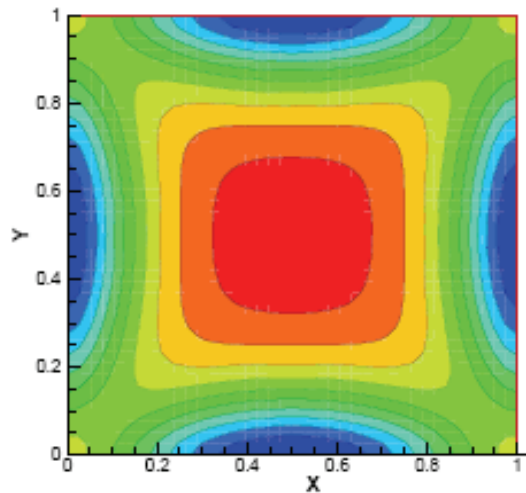


Figure.1b) $\Psi_2; \varepsilon = \varepsilon_1 = 0, H_e = 1$

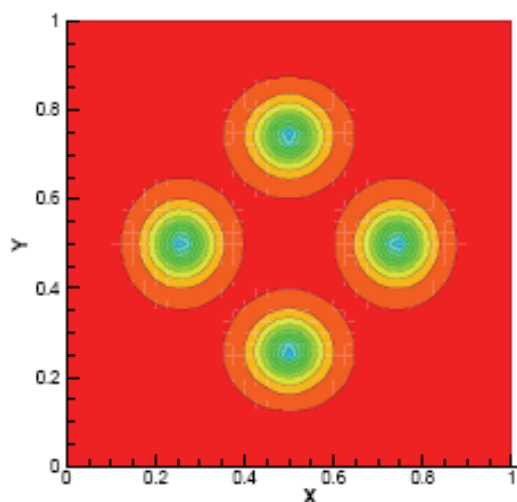


Figure. 2a) Ψ_1 ; $\varepsilon = \varepsilon_1 = 0, H_e = 1.8$

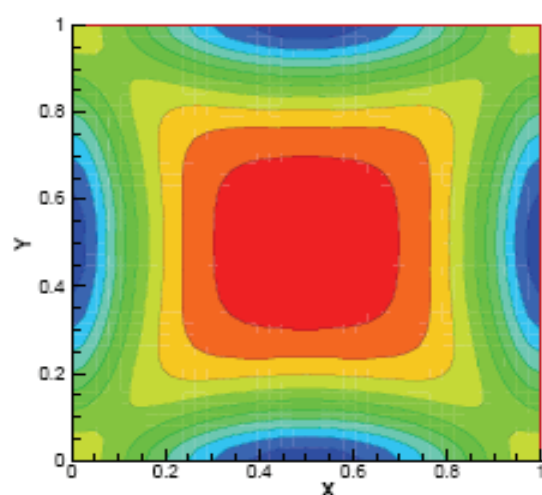


Figure. 3b) Ψ_2 ; $\varepsilon^2 = 3/8; \eta = -0.016, H_e = 1$

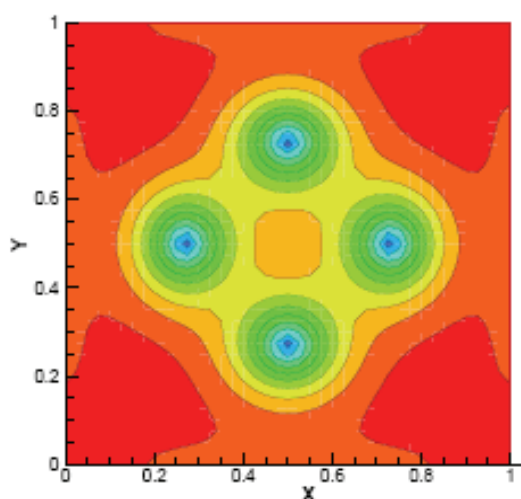


Figure. 2b) Ψ_2 ; $\varepsilon = \varepsilon_1 = 0, H_e = 1.8$

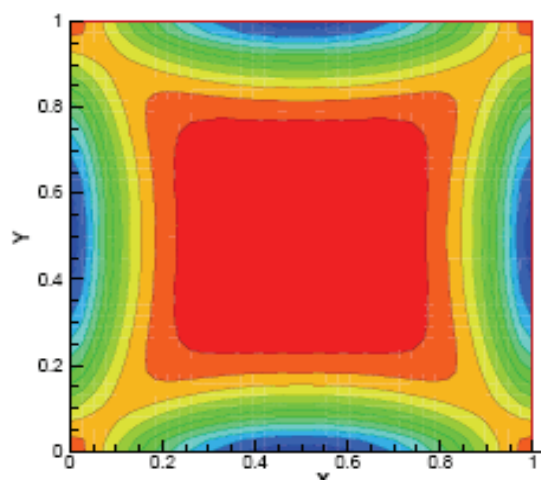


Figure.3a) Ψ_1 ; $\varepsilon^2 = 3/8; \eta = -0.016, H_e = 1$

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