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NUMERICAL STUDY OF VORTEX PATTERN IN FRAMEWORK OF TWO-BAND GINZBURG-LANDAU THEORY

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Abstract. Numerical modeling of vortex nucleation in external magnetic field in two-band superconductor using modified Ginzburg-Landau theory is conducted. Results of simulation experiments for a two-band superconducting films MgB_2 near the critical temperature in perpendicular magnetic field is presented. Obtained results seems interesting from the point of investigation of pecularities of vortex dynamics in systems with complex order parameter and another possible applications.

1. Introduction

Despite a large period of time that passed since the discovery of the high-temperature superconductivity in cuprate compounds in 1987, the question concerning the nature of this phenomenon is still open. It is clear that, many properties of superconductors can be analyzed in framework of Ginzburg-Landau (GL) theory [1]. The GL theory which was proposed in 1950 years on phenomenological ground as a generalization of phase transition theory to the quantum state [1]. In 1957, Abrikosov predicted the existence of type-II superconductors based on GL theory [2]. According to Abrikosov classification, there are type-I and type-II superconductors. The value of Ginzburg-Landau parameter $\kappa = \frac{\lambda}{\xi} = \frac{1}{\sqrt{2}}$ separate type-II superconductors ($\kappa > \frac{1}{\sqrt{2}}$) from those of type-I ($\kappa < \frac{1}{\sqrt{2}}$). It means that a type-II superconductor at magnetic fields higher than the lower critical field H_{c1}, an applied magnetic field starts to penetrate a superconductor in the form of quantum flux Φ_0 (mixed state). In homogeneous uniform superconductors vortex pattern reveal hexagonal symmetry [2]. This leads to global minimum for energy functional. Furthermore, the vortex pattern in mixed state is often affected by the locations at which the initial seed (or seeds) are placed. A vortex consists of a normal-like region called the core with a radius equal to the coherence length ξ , and a region of circulating current with a radius equal to London penetration depth λ [2]. High

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temperature superconductors are type-II superconductors with a large value of the Ginzburg-Landau parameter $\kappa >> 1$. The GL theory has been modified to account high-Tc superconductivity (see below).

The energy band structure in many superconductors exhibits a complicated character; in particular, there are several overlapping energy bands near the Fermi level. An two-band Bardeen–Cooper–Schriffer (BCS) model was used [3,4] to calculate the dependence of the critical temperature T_c on the carrier concentration n. It should be noted that the two-band BCS model was originally proposed long years ago [6, 7]. In recent years, a generalized electron–phonon Eliashberg theory for two-band superconductors was used to study the properties of magnesium diboride [8] and nonmagnetic $Y(Lu)Ni_2B_2C$ borocarbides [9]. As shown by experimental investigations, this compound seems to be first real objects of two-band superconductors [8-9]. Many new models has been suggested last years for describing physical properties of many band superconductors. Up to now GL remains powerful method in study of some physical properties. The vortices nucleation in the single-band isotropic superconductors was originally studied by using Ginzburg–Landau equations for single-band isotropic superconductors [10-12]. It is important to note that, the GL theory was generalized for the case superconductors with non-conventional order parameter symmetry- d-wave symmetry [13]. GL equations also are useful in study of fluctuational effects on physical properties near T_c [14] in single band isotropic superconductors. Time-dependent single-band GL theory was used for calculations of fluctuation conductivity neat T_c by Aslamazov-Larkin [15].

Previously, time independent two-band GL equations were successfully used to study the physical properties of recently discovered superconductors such as magnesium diboride (MgB_2) [16, 17] and nonmagnetic $Y(Lu)Ni_2B_2C$ borocarbide compounds [18,19]. In the present study, the vortices nucleation of vortex in external magnetic field in the framework of a two-band model two-band GL equations. Firstly we will drive time-dependent GL equations for two-band superconductors. Secondly we apply this equations for numerical modeling for vortex nucleation in the case thin superconducting film of two-band superconductor MgB_2 with perpendicular external magnetic field. We could use the modified forward Euler method for numerical experiments. Finally, a conclusion remarks will be made.

2. Time-dependent GL equations for two-band superconductors

The GL free energy functional for an isotropic two-band superconductor can be written as follows /16-19/:

$$F_{SC} = \int d^3r(F_1 + F_2 + F_{12} + \frac{H^2}{8\pi} \tag{2.1}$$

where

$$F_i = \frac{\hbar^2}{4m_i}\left|\left(\nabla - \frac{2\pi i\overrightarrow{A}}{\Phi_0}\right)\Psi_i\right|^2 + \alpha_i(T)\Psi_i^2 + \beta_i\Psi_i^2/2 \tag{2.2}$$

$$F_{12} = \varepsilon(\Psi_1^*\Psi_2 + c.c.) + \varepsilon_1\left\{\left(\nabla + \frac{2\pi i\vec{A}}{\Phi_0}\right)\Psi_1^*\left(\nabla - \frac{2\pi i\vec{A}}{\Phi_0}\right)\Psi_2 + c.c.\right\} \tag{2.3}$$

m_i are the masses of electrons belonging to different bands ($i = 1,\ 2$); $\alpha_i = \gamma_i(T - T_{ci})$ are 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. In Eqs. (2.1) and (2.2), the order parameters are assumed to be slowly varying in space. Minimization procedure of the free-energy functional yields the GL equations describing the two-band superconductors. For an isotropic superconductor in the case (not limiting the generality) of $A = (0, Hx, 0)$, the time-independent GL equations take the following form:

$$-\frac{\hbar^2}{4m_1}(\frac{d^2}{dx^2} - \frac{x^2}{l_s^4})\Psi_1 + \alpha_1(T)\Psi_1 + \varepsilon\Psi_2 + \varepsilon_1(\frac{d^2}{dx^2} - \frac{x^2}{l_s^4})\Psi_2 + \beta_1\Psi_1^3 = 0, \tag{2.4}$$

$$-\frac{\hbar^2}{4m_2}(\frac{d^2}{dx^2} - \frac{x^2}{l_s^4})\Psi_2 + \alpha_2(T)\Psi_2 + \varepsilon\Psi_1 + \varepsilon_1(\frac{d^2}{dx^2} - \frac{x^2}{l_s^4})\Psi_1 + \beta_2\Psi_2^3 = 0 \tag{2.5}$$

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 Eqs. (2.4) and (2.5) can be arbitrary. These signs are determined by the microscopic nature of the interaction of electrons belonging to different bands. If the inter-band interaction vanishes, Eqs. (2.4) and (2.5) convert into the usual GL equations with the critical temperatures T_{c1} and T_{c2}. In the general case (irrespective of the sign of ε), the superconducting transition takes place at a temperature T_c, which is higher than both T_{c1} and T_{c2} and is determined by the following equation [16–19]:

$$(T_c - T_{c1})(T_c - T_{c2}) = \frac{\varepsilon^2}{\gamma_1\gamma_2}, \tag{2.6}$$

Time-dependent equations in two-band Ginzburg-Landau theory can be obtained from Eqs. (1-3) in analogical way to [20]:

$$\begin{aligned} \Gamma_1(\frac{\partial}{\partial t} + i\frac{2e}{\hbar}\phi)\Psi_1 &= -\frac{\delta F}{\delta\Psi_1^*}, \\ \Gamma_2(\frac{\partial}{\partial t} + i\frac{2e}{\hbar}\phi)\Psi_2 &= -\frac{\delta F}{\delta\Psi_2^*}, \\ \sigma_n(\frac{\partial\vec{A}}{\partial t} + \nabla\phi)\Psi_1 &= -\frac{1}{2}\frac{\delta F}{\delta\vec{A}} \end{aligned} \tag{2.7}$$

Here we use notations similar to [20]. In Eqs. (2.7) ϕ means electrical scalar potential, $\Gamma_{1,2}$ -relaxation time of order parameters, σ_n-conductivity of sample in two-band case. Choosing corresponding gauge invariance we can eliminate scalar potential from system of equations (2.7) [20]. 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

$$\Gamma_1 \frac{\partial \Psi_1}{\partial t} = -\frac{\hbar^2}{4m_1}(\frac{d^2}{dx^2} - \frac{x^2}{l_s^4})\Psi_1 + \alpha_1(T)\Psi_1 + \varepsilon\Psi_2 + \varepsilon_1(\frac{d^2}{dx^2} - \frac{x^2}{l_s^4})\Psi_2 + \beta_1\Psi_1^3 = 0, \quad (2.8)$$

$$\Gamma_2 \frac{\partial \Psi_2}{\partial t} = -\frac{\hbar^2}{4m_2}(\frac{d^2}{dx^2} - \frac{x^2}{l_s^4})\Psi_2 + \alpha_2(T)\Psi_2 + \varepsilon\Psi_1 + \varepsilon_1(\frac{d^2}{dx^2} - \frac{x^2}{l_s^4})\Psi_1 + \beta_2\Psi_2^3 = 0, \quad (2.9)$$

$$\begin{array}{l} \sigma_n(\frac{\partial \vec{A}}{\partial t} - \nabla\phi) = -rot\vec{A} + \frac{2\pi}{\Phi_0}\{ \frac{\hbar^2}{4m_1}n_1(T)(\frac{d\varphi_1}{dr} - \frac{2\pi A}{\Phi_0}) \\ +\varepsilon_1(n_1(T)n_2(T))^{0.5}\cos(\varphi_1 - \varphi_2) + \frac{\hbar^2}{4m_2}n_2(T)(\frac{d\varphi_2}{dr} - \frac{2\pi A}{\Phi_0}) \} \end{array} \quad (2.10)$$

where $\varphi_{1,2}(\vec{r})$ phase of order parameters $\Psi_{1,2}(\vec{r}) = |\Psi_{1,2}|\exp(i\varphi_{1,2})$, $n_{1,2}(T) = 2|\Psi_{1,2}|^2$-density of superconducting electrons in different bands, expressions for whichs are presented in [16–19] with so-called natural boundary conditions

$$\left\{ \frac{1}{4m_1}(\nabla - \frac{2\pi i\vec{A}}{\Phi_0})\Psi_1 + \varepsilon_1(\nabla - \frac{2\pi i\vec{A}}{\Phi_0})\Psi_2 \right\}\vec{n} = 0 \quad , \quad (2.11)$$

$$\left\{ \frac{1}{4m_2}(\nabla - \frac{2\pi i\vec{A}}{\Phi_0})\Psi_2 + \varepsilon_1(\nabla - \frac{2\pi i\vec{A}}{\Phi_0})\Psi_1 \right\}\vec{n} = 0, \quad (2.12)$$

$$(\vec{n} \times \vec{A}) \times \vec{n} = \vec{H}_0 \times \vec{n} \quad (2.13)$$

First two conditions correspond to absence of supercurrent through boundary of two-band superconductor, third conditions correspond to the contiunity of normal component of magnetic field to the boundary superconductor-vacuum.

In this study we introduce unconventional scales to non-dimensionalize the time-dependent two-band G-L system of equations. As shown in [16–19], temperature dependence of some physical quantities becomes nonlinear in contrast to single-band G-L theory. It is well known that, G-L parameter κ for single-band superconductors is temperature independent, while in two-band G-L theory κ grows with decreasing of temperature [18–19]. This implies about possibility changing of type of superconductivity with lowering of temperature. It means that dynamics of order parameters in two-band superconductors differs from those of in single-band superconductors. In this study, we focus mostly on experiments performed with two-band time-dependent GL system, and claim that our model yields realistic results.

3. **Application of TD TB GL equations to thin superconducting film**

We consider a finite homogeneous superconducting film of uniform thickness, subject to a constant magnetic field. We also consider that the superconductor is rectangular in shape. In this case our two-band GL model becomes two-dimensional [16–19]. The order parameters Ψ_1 and Ψ_2 varies in the plane of the film, and vector potential **A** has only two nonzero components, which lie in the plane of the film. Therefore, we identify the compuational domain of the superconductor with a rectangular region $\Omega \in \mathrm{R}^2$, denoting the Cartesian coordinates by x and y, and the $x-$ and $y-$ components of the vector potential by $A(x, y)$ and $B(x, y)$, recpectively. Before modeling we use so-called bond variables [20,21] for the discretization of time-dependent two-band G-L equations

$$W(x, y) = \exp(i\kappa \int^{x} A(\zeta, y) d\zeta),$$

$$V(x, y) = \exp(i\kappa \int^{y} B(x, \eta) d\eta) \tag{3.1}$$

Such variables make obtained discretized equations gauge-invariant. For spatially discetization we use forward Euler method [22]. 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

$$\Omega_{2n} = \Omega_{i+j=2n}; \Omega_{2n+1} = \Omega_{i+j=2n+1} \tag{3.2}$$

for $i = 0, ...; N_{xp}, j = 0, ...; N_{yp}$, where $N_{xp} = N_x + 1$, $N_{yp} = N_y + 1$. Schematical presentation of such partition are shown in Fig. 1, in which Ω_{2n} denoted by normal cycles and Ω_{2n+1} denoted by full cycles. In calculations we could use two different approach. The first approach (zero-field –cooled) is assume that sample that has is initially in a perfect superconducting state is cooled to a temperature below the critical Tc in the absence of applied magnetic field, and then a magnetic field of an appropriate strength is suddenly turned out. The second approach (field-cooled) is to assume that a sample that is cooled to a temperature at or above the critical temperature is in a normal state under magnetic field of appropriate strength, and then the temperature is suddenly decreased below the critical temperature.

For numerical calculations in two-band GL theory we assume that the size of superconducting film is $40\lambda \times 40\lambda$, where λ London penetration depth of external magnetic field on superconductor [16–19]:

$$\lambda^{-2}(T) = \frac{4\pi e^2}{c^2}\left(\frac{n_1(T)}{m_1} + 2\varepsilon_1 (n_1(T) n_2(T))^{0.5} + \frac{n_2(T)}{m_2}\right) \tag{3.3}$$

Under modeling we also introduce another dimensionless parameters

$$\vec{r'} = \frac{\vec{r}}{\lambda}; \Psi_{1,2}^{'} = \frac{\Psi_{1,2}}{\Psi_{(1,2)0}}; \vec{A} = \frac{\vec{A}}{\lambda H_c \sqrt{2}}; F'(\Psi'_{1,2}, A') = \frac{F(\Psi_{1,2}, A)}{\alpha_0^2 \left|\Psi_{1,0}\right|^2 + \alpha_1^2 \left|\Psi_{2,0}\right|^2} \tag{3.4}$$

Expressions for $\Psi_{(1,2)0}$, and for thermodynamic magnetic field H_c are presented in [16–19]. The calculations were performed for the following values of parameters: $T_c = 40$ K; T_{c1} =20.0 K; $T_{c2} = 10$ K, $\frac{\varepsilon^2}{\gamma_1 \gamma_2 T_c^2} = 3/8$; $\eta = \frac{T_c m_2 \varepsilon_1 \gamma_2}{\hbar^2 \varepsilon} = -0.016$. This parameters was used for the calculation another physical properties of two-band superconductor MgB_2 [16–19].

For solving of corresponding discretized GL equations we will use method of adaptive grid [22]. Results of numerical modelling in the case of zero-field-cooled process presented in Fig. 2. We assume that the sample, which is initially in a perfect superconducting state, is cooled through T_c in the absence of applied magnetic field, and then a magnetic field of an appropriate strenght is suddenly turned out. Mathematically it means that, the initial state is achieved by letting$|\Psi'_{1,2}(\vec{x})\ | = 1, \quad A_0(\vec{x}) = 0$ for all $\vec{x} \in \Omega$.

In figure 2, we present a a contour plot of superconducting electrons. GL parameter for sample is the $\kappa = 5$. We can observe a partial hexagonal pattern , yet we do not observe the physically exact hexagonal pattern, as expected of homogeneous samples with uniform thickness.

Secondly we simulate the field cooled case. In (x_0, y_0)a temperature at or above the critical temperature, is in a normal state under a magnetic field of appropriate strenght, and then the temperature is suddenly reduced to below T_c. In matematical denotes, the initial states is achieved by letting

$$A_0(x, y) = (0, xH, 0), \quad |\ \Psi'_{1,2}\ (x, y)| = \begin{cases} 0, if(x, y) \neq (x_0, y_0) \\ c_{1,2}, f(x, y) = (x_0, y_0) \end{cases},$$

where $c_{1,2}$ is a small constant representing the magnitude of the seed, and (x_0, y_0) is the location of a seed in the sample. We can conclude that (Fig. 3) the result vortex pattern depends upon where and how many seeds are placed into the sample. Existence of Meissner state is shown by numerical calcutions using both (zero-field-cooled and field cooled) approachs. It means that at fixed Ginzburg-Landau parameter κ and external magnetic field $H < H_{c1}$ no nucleation of vortexes of external magnetic field.

As shown in [23] structure of magnetic field in section of vortex in two-band superconductor differs from single-band superconductor. Nonsymmetric angular magnetic field distriburion in vortex change their interaction force between them and total energy of superconductor with such vortexes differs from single band one. In high density vortex pattern effects of influence of nonsymmetric angular dependence becomes crusial. Detail analysis of influence of asymmetric character of sectional magnetic field distribution on the parameters of hexagonal vortex pattern is the object of future investigations.

4. **Conclusions**

In this study we obtain time-dependent GL equations taking into account two-band character of the superconducting state, which was originally developed by Schmid for single band superconductors. Furthermore, we perform numerical modeling of vortex nucleation in external magnetic field in two-band superconducting films $MgB2$ using two-band Ginzburg-Landau theory. It was shown that the vortex configuration in the mixed state depends upon initial state of the sample and that the system does not seem to yield hexagonal pattern for finite size homogeneous samples of uniform thickness with the natural boundary conditions. On the other hand, the time-dependent two-band GL equations leads to the expected hexagonal pattern, i.e. global minimizer of the energy functional.

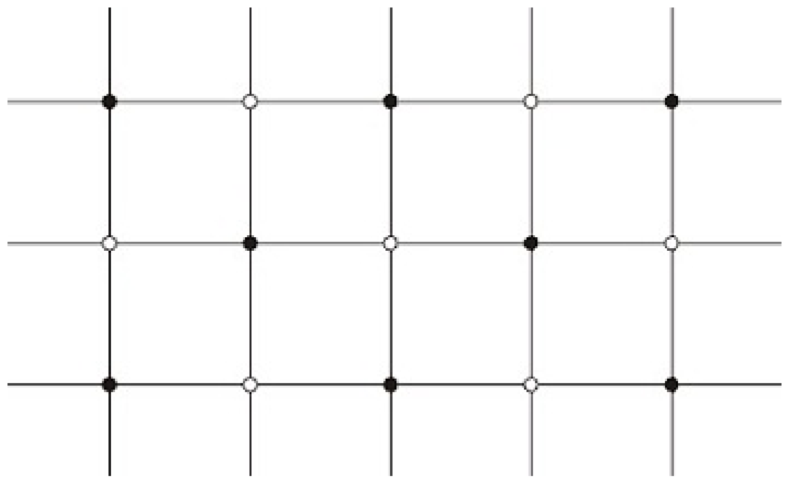

Fig. 1: A partition of Ω into two subdomains; Ω_{2n}(normal cicles), and Ω_{2n+1} (full cicles)

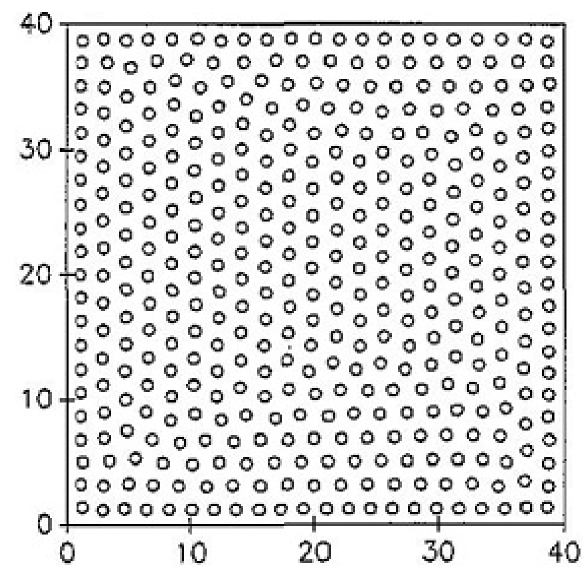

Fig. 2: A hexagonal vortex pattern in the case of zero-field-cooled process

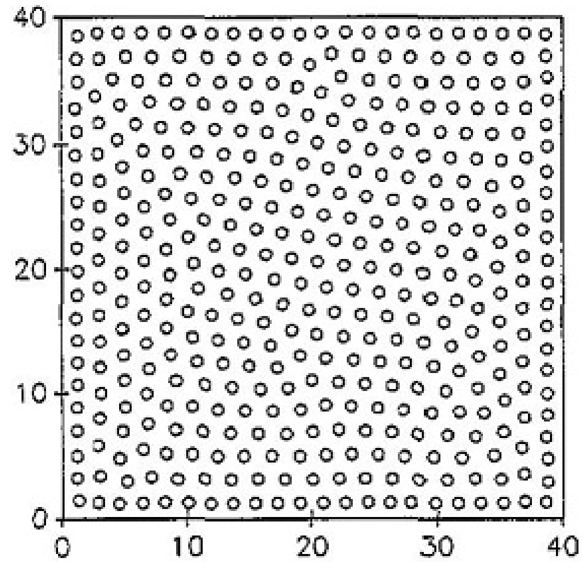

Fig. 3: A hexagonal vortex pattern in the field cooled case

ÖZET: Modife olunmuş Ginzburg-Landau teorisi kapsamında dış manyetik alana yerleştirilmiş süper iletkenlerde girdap örgüsünün oluşması sayısal olarak modellenmiştir. Kritik sıcaklık civarında manyetik alana dik yönde yerleştitrilmiş MgB_2 ince filmi için sayısal deneylerin sonuçu verilmektedir. Elde edilen sonuçlar basit olmayan düzlenme parametreli sistemlerde girdap dinamiğinin özelliklerinin araştırılması ve diğer mümkün uygulamalar için önemlidir.

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