Analytic proposal for $p + ip$ coupling in three-band Ginzburg-Landau model

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Abstract. In this contribution, we propose a theoretical Josephson coupling for a superconducting system in the three-component time-dependent Ginzburg-Landau model. We study a system with three superconducting bands $\psi_1$, $\psi_2$, and $\psi_3$ in the superconducting condensate. The coupling between bands is of the form $\gamma_{12}$, $\gamma_{13}$ and $\gamma_{23}$, taking into account couplings of each of the bands with the other two. We show the mathematical development of the final form of the complete set of acopled non-linear time-dependent Ginzburg-Landau differential equations, considering the coupling between the three bands, also we show that this coupling imposes a phase difference between the different components of the superconducting order parameter.

1. Introduction

The discovery of superconductors based in iron ($F_e$) [1–3], has increased the interest of theoretical and experimental researchers in multiband superconducting systems. As is know, these materials have two or more coupled superconducting bands [4, 5]. This coupling allows new physics not present in single-band or two-band superconducting materials, leading to non-conventional vortex states with broken time-reversal symmetry due to the pairing interaction among Fermi surfaces.

Yanagisawa T, et al. found a solution with time-reversal symmetry breaking, that is, a chiral solution when there is such a frustration, resulting in the existence of fractional vortices on the domain wall of $Fe$-pnictides [6]. Nunes T, et al., analyzed the influence of the deGennes extrapolation length $b$ on the vortex configuration in a two-band superconducting square with a central defect. They found a non-conventional vortex state due to the repulsive-short range (or attractive-long) potential between the vortices and show that at the limit of the thin film, a two-band system behaves like a three-band system [7]. Also, the effect of the Josephson and bi-quadratic coupling types on the vortex state, the magnetization in a two-band superconducting disk was studied by Aguirre C, et al., using the two bands Ginzburg-Landau time-dependent theory. They found that there is a predominant band in this type of material for weak coupling, this is also supported by the ab-initio study in magnesium diboride ($MgB_2$) samples [8].

Gilles S, et al., using three-component Ginzburg-Landau simulations, show novel vortex states in mesoscopic three-band superconductors. They found chiral states, with non-trivial phase differences between the bands, and they report the broken-symmetry vortex states, the chiral...
states where vortex cores in different band condensates do not coincide (split-core vortices), as well as fractional vortex states with broken time-reversal symmetry [9]. Orlova N, et al., analyzed the influence of the mesoscopic confinement on the broken time-reversal symmetry states. They studied a system with one strong superconducting band, which couples to two other bands which are only superconducting due to the interaction with the first band. They found non-trivial phase differences between the bands [10].

Takabatake Y, et al., investigated theoretically the tunneling conductance of the \((d+ip)\)-wave superconductor utilizing the quasi-classical Eilenberger theory, they obtain the pair potentials and the differential conductance of the normal-metal-\((d+ip)\)-wave superconductor junction and conclude that spin-triplet p-wave surface subdominant order is feasible [11]. Hayes M, et al., observed the non-zero polar Kerr effect in uranium telluride \((UTe_2)\), indicating that this material is characterized by a two-component spin-triplet superconductivity order parameter that breaks time reversal symmetry [12].

The study of superconducting systems at low critical temperatures has regained the interest of the scientific community, discoveries, such as topology, multi-components [10, 13–16]. So, the time dependence Ginzburg-Landau (TDGL) theory is a very strong tool to study the vortex dynamics and thermo-magnetic properties in superconducting systems [17–21]. With this, in the present work, we show the analytical implementation for a three-band superconducting system, taking into account a Josephson coupling between the three bands. The importance of phase dynamics has been studied previously in the references [22–27]. We think that magnetic and thermodynamics properties of three-orbital superconducting systems such as oxido(oxo)cobalt \((CoO_2)\), iron dioxide \((FeO_2)\) and nickel dioxide \((NiO_2)\) can be analyzed by three-band Ginzburg-Landau model.

2. Physical model

In the three band Ginzburg-Landau model, the superconducting order parameter is a complex pseudo-function defined as \(\psi_i = |\psi_i|e^{i\theta_i}\), and their conjugate complex \(\psi_i^* = |\psi_i|e^{-i\theta_i}\), being \(\theta_i\) its phase. So, the Ginzburg-Landau functional considering a Josephson coupling \(\gamma_{i,j}\), between the bands \(i\) and \(j\) is Equation (1).

\[
\mathcal{G} = \int dV \left[ \sum_i^3 (\alpha_i|\psi_i|^2 + \frac{\beta_i}{2} |\psi_i|^4 + \frac{v_i}{2m_i} (i\hbar \nabla + 2eA)|\psi_i|^2 + \frac{1}{2\mu_0} |\nabla \times A|^2 + \mathcal{H}(\psi_i) \right],
\]

where \(\mathcal{H}(\psi_i)\) is defined by Equation (2).

\[
\mathcal{H}(\psi_i) = \gamma (\psi_1^* \psi_2 \psi_3 + \psi_1 \psi_2^* \psi_3^*) + \gamma (\psi_1^* \psi_2^* \psi_3^* + \psi_1 \psi_2 \psi_3^*) + \gamma (\psi_1^* \psi_2 \psi_3^* + \psi_1 \psi_2^* \psi_3). \tag{2}
\]

Here, the applied magnetic field \(B\) is implemented by giving \(A\) a boundary condition such that \(\nabla \times A = B\) on the boundary. \(\alpha_i, \beta_i\) are phenomenological parameters, \(\alpha_i = \alpha_0 (1 - T/T_c)\) in the Equation (1) and Equation (2). The parameter \(v_i\) in the Equation (1) indicates the height of the kinetic energy or velocity of the superconducting Cooper pairs (also related to the super-current) in the \(i\)-band. Therefore for the conisered dominant band \(\nu_{dominant-band} >> \nu_{non-dominand-band}\), in equilibrium, the free energy has a minimum with respect to \(\psi_i^*\) and \(A\), which in London gauge \(\nabla \cdot A = 0\), after the dimensionless form, gives the Equation (3) to Equation (5).

\[
\frac{\partial \psi_1}{\partial t} = (1 - T - |\psi_1|^2) \psi_1 - (-i\nabla - A)^2 \psi_1 + \gamma_{23}, \tag{3}
\]

\[
\frac{\partial \psi_2}{\partial t} = (1 - \frac{T}{T_{r_2}} - |\psi_2|^2) \psi_2 - m_{r_2} \alpha_{r_3}^{-1} (-i\nabla - A)^2 \psi_2 + \sqrt{\frac{\alpha_2}{\beta_2}} \frac{\alpha_2}{\beta_2} \gamma_{13}, \tag{4}
\]

\[
\frac{\partial \psi_3}{\partial t} = (1 - \frac{T}{T_{r_3}} - |\psi_3|^2) \psi_3 - m_{r_3} \alpha_{r_2}^{-1} (-i\nabla - A)^2 \psi_3 + \sqrt{\frac{\alpha_2}{\beta_3}} \frac{\alpha_2}{\beta_3} \gamma_{12}, \tag{5}
\]
where $\gamma_{23}$, $\gamma_{13}$, and $\gamma_{12}$ are defined by Equation (6) to Equation (8).

\begin{align*}
\dot{\gamma}_{23} &= \gamma|\psi_2||\psi_3|e^{i\theta_1}\left[\cos(\theta_3 + \theta_2 - \theta_1) + 3i\sin(\theta_3 + \theta_2 - \theta_1)\right], \\
\dot{\gamma}_{13} &= \gamma|\psi_1||\psi_3|e^{i\theta_2}\left[\cos(\theta_3 - \theta_2 + \theta_1) + 3i\sin(\theta_3 - \theta_2 + \theta_1)\right], \\
\dot{\gamma}_{12} &= \gamma|\psi_1||\psi_2|e^{i\theta_3}\left[\cos(-\theta_3 + \theta_2 + \theta_1) + 3i\sin(-\theta_3 + \theta_2 + \theta_1)\right],
\end{align*}

and $\frac{\partial A}{\partial t}$ by Equation (9).

\[
\frac{\partial A}{\partial t} = v_1\Re[\psi_1(i\nabla - A)\psi_1^*] + v_2\Re\left[\frac{\beta_{23}}{\alpha_{23}}\psi_2(i\nabla - A)\psi_2^*\right] + v_3\Re\left[\frac{\beta_{13}}{\alpha_{13}}\psi_3(i\nabla - A)\psi_3^*\right] + \kappa^2 \Delta A. \tag{9}
\]

In the Ginzburg-Landau Equations (Equation (3) to Equation (9)), we defined: $T_{r2} = T_2/T_1$, $T_{r3} = T_3/T_3$; $\alpha_{r2} = \alpha_{30}/\alpha_{20}$, $\alpha_{r3} = \alpha_{03}/\alpha_{30}$, $m_{r2} = m_2/m_3$, $m_{r3} = m_3/m_2$, $\beta_{r2} = \beta_3/\beta_2$, $\beta_{r3} = \beta_2/\beta_3$. We express the temperature $T$ in units of the critical temperature $T_c$, length in units of the coherence length $\xi_{10} = h/\sqrt{-2\alpha_{30}}$, the order parameters in units of $\psi_{10} = \sqrt{-\alpha_{20}/\beta_1}$. We choose the zero-scalar potential gauge, $\phi = 0$ at all times. $\kappa$ is the Ginzburg-Landau parameter. The TDGL equations are solved using the method of the link variables or $\Psi - U$ method [28–32]. Now, the parameter $v_i$ in the equation 9 is related to the height of the super-current in the $i$-band. The convergence relationship is $\Delta t \leq 0.25\min(\delta, \Delta \kappa^{-2})$ with $\delta = \delta_x^2 + \delta_y^2 + \delta_z^2$. where $\delta_x$, $\delta_y$, and $\delta_z$ are the grid space used of the computationally mesh.

3. Josephson coupling for a 3-band system

From Gibbs energy density, (Equation (1)), we considered the Josephson coupling for three order parameters $\psi_1$, $\psi_2$, and $\psi_3$, thought the isotropic inter-band coupling $\gamma$ as Equation (10).

\[
\mathcal{H}(\psi_1, \psi_2, \psi_3) = \gamma(\psi_1^*\psi_2\psi_3 + \psi_1\psi_2^*\psi_3^*) + \gamma(\psi_1\psi_2^*\psi_3 + \psi_1^*\psi_2\psi_3^*) + \gamma(\psi_1\psi_2\psi_3^* + \psi_1^*\psi_2^*\psi_3). \tag{10}
\]

Then, replacing $\psi_i = |\psi_i|e^{i\theta_i}$, $i = 1, 2, 3$, in the first part of the Equation (10) we have the Equation (11).

\[
\gamma(\psi_1^*\psi_2\psi_3 + \psi_1\psi_2^*\psi_3^*) = \gamma(|\psi_1||\psi_2||\psi_3|e^{i(\theta_3+\theta_2-\theta_1)}) = 2\gamma|\psi_1||\psi_2||\psi_3|\cos(\theta_3 + \theta_2 - \theta_1). \tag{11}
\]

Now, in a similar way, we can write the second part of Equation (10) as Equation (12).

\[
\gamma(\psi_1\psi_2^*\psi_3 + \psi_1^*\psi_2\psi_3^*) = \gamma(|\psi_1||\psi_2||\psi_3|e^{i(\theta_3-\theta_2+\theta_1)}) = 2\gamma|\psi_1||\psi_2||\psi_3|\cos(\theta_3 - \theta_2 + \theta_1), \tag{12}
\]

and the third part of Equation (10) we can write as Equation (13).

\[
\gamma(\psi_1\psi_2\psi_3^* + \psi_1^*\psi_2^*\psi_3) = \gamma(|\psi_1||\psi_2||\psi_3|e^{i(-\theta_3+\theta_2+\theta_1)}) = 2\gamma|\psi_1||\psi_2||\psi_3|\cos(-\theta_3 + \theta_2 + \theta_1). \tag{13}
\]

Now, making the functional derivative of the Equation (11) to Equation (13) respect to $\psi_i^*$. We show the analysis for $\theta_3 + \theta_2 - \theta_1$ phase, obtaining Equation (14).

\[
\partial \psi_i^*[2\gamma|\psi_1||\psi_2||\psi_3|\cos(\theta_3 + \theta_2 - \theta_1)] = 2\gamma|\psi_2||\psi_3|\partial \psi_i^*\left[|\psi_1|\cos(\theta_3 + \theta_2 - \theta_1)\right]. \tag{14}
\]
Then, making the derivate of the last term in the Equation (14), obtain the Equation (15).
\[
\partial \psi_1^* \left( |\psi_1| \cos(\theta_3 + \theta_2 - \theta_1) \right) = \left[ \partial \psi_1^* |\psi_1| \right] \cos(\theta_3 + \theta_2 - \theta_1) + |\psi_1| \partial \psi_1^* (\cos(\theta_3 + \theta_2 - \theta_1)),
\]
(15)
derivating the first term of the Equation (15), obtain the Equation (16).
\[
\partial \psi_1^* \left[ \cos(\theta_3 + \theta_2 - \theta_1) \right] = \partial \psi_1^* \sqrt{\psi_1 \psi_1^*} \cos(\theta_3 + \theta_2 - \theta_1) = \frac{\psi_1}{2|\psi_1|} \cos(\theta_3 + \theta_2 - \theta_1)
\]
(16)
derivating the first term of the Equation (15), obtain the Equation (17).
\[
|\psi_1| \partial \psi_1^* (\cos(\theta_3 + \theta_2 - \theta_1)) = |\psi_1| \sin(\theta_3 + \theta_2 - \theta_1) \left[ - \frac{\partial \theta_1}{\partial \psi_1^*} \right]
\]
(17)
and for the phase: \( \psi_1^* = |\psi_1|e^{-i\theta_1} \), then, \( \theta_1 = -i \ln |\psi_1| + i \ln \psi_1^* \). Applying the functional discrete (Equation (18)).
\[
\frac{\partial \theta_1}{\partial \psi_1^*} = -i \partial \psi_1^* [\ln |\psi_1|] + i \partial \psi_1^* \ln \psi_1^* = -i \left[ \frac{\psi_1}{2|\psi_1|} \right] + i \psi_1^*
\]
(18)

Finally taking from the Equation (14) to Equation (18) for \( \dot{\gamma}_{23} \), we define new phase variable \( \rho = \theta_3 + \theta_2 - \theta_1 \) as example (Equation (19) to Equation (23)).
\[
\dot{\gamma}_{23} = 2 \gamma |\psi_2| |\psi_3| \left[ \frac{\psi_1}{2|\psi_1|} \right] \cos(\rho) + \left[ i \frac{\psi_1}{2|\psi_1|^2} + i \psi_1^* \right] |\psi_1| \sin(\rho)
\]
(19)
\[
= \gamma |\psi_2| |\psi_3| \frac{\psi_1}{|\psi_1|} \cos(\rho) + i \gamma |\psi_2| |\psi_3| |\psi_1|^2 \sin(\rho) + \frac{2i \gamma |\psi_1| |\psi_2| |\psi_3|}{\psi_1^*} \sin(\rho)
\]
(20)
\[
= \gamma |\psi_2| |\psi_3| |\psi_1| \cos(\rho) + \gamma |\psi_2| |\psi_3| \frac{\psi_1}{|\psi_1|} \sin(\rho) + \frac{2i \gamma |\psi_1| |\psi_2| |\psi_3|}{\psi_1^*} \sin(\rho)
\]
(21)
Then:
\[
\dot{\gamma}_{23} = \gamma |\psi_2| |\psi_3| e^{i\theta_1} \left[ \cos(\rho) + i \sin(\rho) \right] + 2i \gamma |\psi_2| |\psi_3| e^{i\theta_1} \sin(\rho)
\]
(22)
\[
= \gamma |\psi_2| |\psi_3| e^{i\theta_1} \left[ \cos(\rho) + 3i \sin(\rho) \right]
\]
(23)

Thus, we show that from the Equation (19) to the Equation (23) lead to the Equation (6). In an analogous way we can find the coupling \( \dot{\gamma}_{13} \) and \( \dot{\gamma}_{12} \).

\( \gamma_{ij} \) simulates the probability of superconducting electrons tunneling between the \( j \) and \( j \) band, with just two possible values \( \dot{\gamma}_{ij} > 0 \) and \( \dot{\gamma}_{ij} < 0 \). Also the parameter \( u_i > 0 \) and \( v_i < 0 \) represent the high of the super-current in the \( i \) band in the case in which is considered \( |\gamma_{ij}| = |u_i| \) equals in all bands. So, there are several different possibilities of combination of these two parameters, we show only some of these possible combinations in the Table 1. It is very important to note that the chosen value of \( \gamma \) is decisive for there to be a numerical convergence in the solution of the three-band Ginzburg-Landau equations (Equation (3) to Equation (9)). Our simulations show that one possible optimal value for these parameters are \( |\gamma| \sim 10^{-3} \), and for the dominant band \( v_{dominant} = 1.0 \) and \( v_{non-dominant} \sim 10^{-3} \).
Table 1. Some possibilities combinations of $\hat{\gamma}_{ij}$ and $\nu_i$ values, considering only the sign of the parameters, and $|\gamma_{12}| = |\gamma_{23}| = |\gamma_{13}| = |\zeta_i|$, equals in all bands. (+(-) means values positives (negatives) for $\hat{\gamma}$ and $\nu$).

| Combination | 1  | 2  | 3  | 4  | 5  | 6  | 7  | 8  | 9  | 10 | 11 | 12 | 13 | 14 |
|-------------|----|----|----|----|----|----|----|----|----|----|----|----|----|----|
| $\hat{\gamma}_{23}$ | + | − | + | + | + | + | − | + | − | − | − | − | + |
| $\hat{\gamma}_{13}$ | + | + | − | + | + | + | − | + | − | − | − | − | + |
| $\hat{\gamma}_{12}$ | + | + | + | − | + | + | − | − | − | + | − | − | + |
| $\nu_1$ | + | + | + | + | − | + | − | − | − | − | − | − | − |
| $\nu_2$ | + | + | + | + | − | − | − | − | − | − | − | + | + |
| $\nu_3$ | + | + | + | + | + | − | − | − | − | − | − | − | − |

| Combination | 15 | 16 | 17 | 18 | 19 | 20 | 21 | 22 | 23 | 24 | 25 | 26 | 27 | 28 |
|-------------|----|----|----|----|----|----|----|----|----|----|----|----|----|----|
| $\hat{\gamma}_{23}$ | + | − | − | − | − | − | + | − | + | − | − | − | + | + |
| $\hat{\gamma}_{13}$ | + | + | − | − | − | − | + | + | − | + | − | − | + | + |
| $\hat{\gamma}_{12}$ | − | + | + | + | − | − | + | + | − | − | + | + | − | − |
| $\nu_1$ | − | − | + | + | − | + | + | + | + | + | − | − | − | − |
| $\nu_2$ | − | − | − | + | − | + | + | + | + | + | − | − | − | − |
| $\nu_3$ | − | − | − | − | + | − | − | − | − | − | − | + | + | + |

4. Conclusions

In this contribution, we show the analytic form of the time-dependent Ginzburg-Landau equations applied to a three-band superconducting system. The coefficient of each term of the Gibbs free energy is expressed in terms Josephson coupling factor. We show that the possibilities difference of phases between the order parameters of each band are $\rho = \theta_3 + \theta_2 - \theta_1$, $\varrho = \theta_3 - \theta_2 + \theta_1$ and $\varsigma = -\theta_3 + \theta_2 + \theta_1$. In addition, the choice of the values of the parameter $\gamma$ and $\nu$ is a very important point to study the chirality of this type of superconductors. We believe that this analytical guide will help researchers interested in to solve problems at a theoretical level considering chiral superconducting state with broken time-reversal symmetry, as is well know, a bi- and three-dimensional multi-band superconductor exhibit an interesting variety of different vortex structures that are not possible in uni-dimensional samples.

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