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# Ginzburg–Landau theory of multi-band superconductivity and applications to Fe pnictides

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ABSTRACT

We investigate multi-component superconductors, in relation to iron pnictides, by using the Ginzburg–Landau theory. We show that a three-band superconductor exhibits several significant properties that are not found in single-band or two-band superconductors. The frustrating pairing interaction among Fermi surfaces may lead to a time-reversal symmetry broken pairing state. In fact, we have a solution with time-reversal symmetry breaking, that is, a chiral solution when there is such a frustration. The Ginzburg–Landau equation for three-component superconductors leads to a double sine-Gordon equation. A kink solution exists to this equation that results in the existence of fractional-quantum flux vortices on the domain wall.



## 1. Introduction

Since the discovery of oxypnictides $LaFeAsO_{1-x}F_x$ [1], $BaFe_2As_2$ [2], LiFeAs [3,4] and $Fe_{1+x}Se$ [5,6], the Fe pnictides high-temperature superconductors have attracted extensive attention. There are numerous experimental studies regarding the electronic states of the new family of iron-based superconductor [7–12]. The undoped samples exhibit the antiferromagnetic transition [9,10], and show the superconducting transition with electron doping [1]. The band structure calculations indicate that the Fermi surfaces are composed of two hole-like cylinders around $\Gamma$, a three-dimensional Fermi surface, and two electron-like cylinders around $M$ for LaFeAsO [13]. This family of iron pnictides is characterized by multi Fermi surfaces.

The objective of this paper is to show novel properties of multi-component superconductors on the basis of Ginzburg–Landau theory. An importance of multi-band structure is obviously exhibited in recent measurements of the Fe isotope effect [14,15]. The inverse isotope effect in $(Ba,K)Fe_2As_2$ can be understood by the multi-band model with competing inter-band interactions [16]. The two-gap theory of superconductivity has a long history, which is the generalization of the BCS theory to the case with two conduction bands [17,18]. We show that an extension to a three-band model provides us remarkable new properties.

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## 2. Hamiltonian and Ginzburg–Landau functional

Let us consider the multi-band BCS model

$$H = \sum_{i\sigma} \int dr \psi^+_{i\sigma} K_i(r) \psi_{i\sigma}(r) - \sum_{ij} g_{ij} \int dr \psi^+_{i\uparrow}(r)\psi^+_{i\downarrow}(r)\psi_{j\downarrow}(r)\psi_{j\uparrow}(r) \tag{1}$$

where $i$ and $j$ (=1, 2, ...) are band indices. $K_i(r)$ stands for the kinetic operator and we assume that $g_{ij} = g^*_{ji}$. The second term is the pairing interaction and $g_{ij}$ are coupling constants. The mean-field Hamiltonian is

$$H = \sum_i \int dr \left[ \sum_\sigma \psi^+_{i\sigma} K_i(r) \psi_{i\sigma}(r) + \Delta_i(r)\psi^+_{i\uparrow}(r)\psi^+_{i\downarrow}(r) + \Delta^*_i(r)\psi_{i\downarrow}(r)\psi_{i\uparrow}(r) \right] \tag{2}$$

where the gap function is

$$\Delta_i(r) = -\sum_j g_{ij} \langle \psi_{j\downarrow}(r)\psi_{j\uparrow}(r) \rangle \tag{3}$$

We define the Green's function,

$$F^+_{j\sigma\sigma}(x - x') = \langle T_\tau \psi^+_{j\sigma}(x)\psi^+_{j\sigma'}(x') \rangle \tag{4}$$

$T_\tau$ is the time ordering operator and we use the notation $x = (t, r)$. The gap functions satisfy

$$\Delta^*_i(r) = \sum_j g^*_{ij} F^+_{j\downarrow\uparrow}(\tau' = \tau + 0; r, r) = \sum_j g^*_{ij} \frac{1}{\beta} \sum_n F^+_{j\downarrow\uparrow}(i\omega_n; r, r) \tag{5}$$

This yields the gap equation,

$$\Delta_i = \sum_j g_{ij} N_j \Delta_j \int d\xi_j \frac{1}{E_j} \tanh\left(\frac{E_j}{2T}\right) \tag{6}$$

where $E_j = (\xi_j^2 + |\Delta_j|^2)^{1/2}$ and $T$ is the temperature. We set the Boltzmann constant $k_B$ to unity and $N_j$ is the density of states at the Fermi surface. At the critical temperature $T = T_c$ this equation reads

$$\Delta_i = \ln\left(\frac{2e^{\gamma_E}\omega_c}{\pi T_c}\right) \sum_j g_{ij} N_j \Delta_j \tag{7}$$

Here $\omega_c$ is the cutoff energy and $\gamma_E$ is the Euler constant. We assume the same cutoff energy $\omega_c$ in all channels of attractive interactions. Following the method by Gor'kov [19], we obtain a set of differential equations

$$\Delta_j^*(r) = \ln\left(\frac{2e^{\gamma_E}\omega_c}{\pi T_c}\right) \sum_\ell g_{j\ell}^* N_\ell \Delta_\ell^*(r) + \frac{7\zeta(3)}{48(\pi T_c)^2} \times \sum_\ell g_{j\ell}^* N_\ell v_\ell^2 \left(\nabla - i\frac{2e}{\hbar c}A\right)^2 \Delta_\ell^*(r) - \frac{7\zeta(3)}{8(\pi T_c)^2} \times \sum_\ell g_{j\ell}^* N_\ell \Delta_\ell^*(r) |\Delta_\ell(r)|^2 \tag{8}$$

Here, $e$ is the charge of the electron and $v_l$ is the electron velocity at the Fermi surface in the $l$th band. From this set of equations, the Ginzburg–Landau free energy for three-gap superconductors is written as

$$F = \int dr \left[\sum_{j=1}^3 \alpha_j |\psi_j|^2 + \frac{1}{2}\sum_{j=1}^3 \beta_j |\psi_j|^4 + \sum_{j=1}^3 K_j \left|\left(\nabla + i\frac{2\pi}{\phi_0}\right)\psi_j\right|^2 + \frac{1}{8\pi}H^2 - (\gamma_{12}\psi_1^*\psi_2 + \gamma_{21}\psi_2^*\psi_1) - (\gamma_{23}\psi_2^*\psi_3 + \gamma_{32}\psi_3^*\psi_2) - (\gamma_{31}\psi_3^*\psi_1 + \gamma_{13}\psi_1^*\psi_3)\right] \tag{9}$$

$\beta_j$ are constants and $\varphi_0$ is the flux quantum,

$$\phi_0 = \frac{hc}{|e^*|} = \frac{hc}{2|e|} \tag{10}$$

The coefficients of bilinear terms are expressed in terms of the matrix $G = (g_{ij})$ as

$$\alpha_j = -\left[N_j \ln\left(\frac{2e^\gamma \omega_c}{\pi T}\right) - (G^{-1})_{jj}\right] \tag{11}$$

$$\gamma_{ij} = -(G^{-1})_{ij} \tag{12}$$

where $G^{-1}$ is the inverse of the matrix $G$.

## 3. Chiral ground states

The order parameter is written as

$$\psi_j = \rho_j e^{i\theta_j} \tag{13}$$

where $\rho_j = |\psi_j|$. The importance of phase dynamics has been pointed out previously [20–26]. We assume that the coefficients of the Josephson terms are real: $\gamma_{ij} = \gamma_{ji}^* = \gamma_{ji}$. Then the free energy density is

$$f = \sum_j \alpha_j \rho_j^2 + \frac{1}{2}\sum_j \beta_j \rho_j^4 - \sum_j K_j \rho_j e^{-i\theta_j}\left(\nabla + i\frac{2\pi}{\phi_0}A\right)^2 (\rho_j e^{i\theta_j}) + \frac{1}{8\pi}H^2 - 2\gamma_{12}\rho_1\rho_2\cos(\theta_1 - \theta_2) - 2\gamma_{23}\rho_2\rho_3\cos(\theta_2 - \theta_3) - 2\gamma_{31}\rho_3\rho_1\cos(\theta_3 - \theta_1) \tag{14}$$

We focus on the role of phases of the order parameters and define new phase variables

$$\varphi_1 = \theta_1 - \theta_2, \quad \varphi_2 = \theta_2 - \theta_3, \quad \varphi_3 = \theta_3 - \theta_1 \tag{15}$$

We examine the ground state of the system with the potential

$$V = -2\gamma_{12}\rho_1\rho_2\cos(\theta_1 - \theta_2) - 2\gamma_{23}\rho_2\rho_3\cos(\theta_2 - \theta_3) - 2\gamma_{31}\rho_3\rho_1\cos(\theta_3 - \theta_1) = \Gamma_1\cos\varphi_1 + \Gamma_2\cos\varphi_2 + \Gamma_3\cos\varphi_3 \tag{16}$$

We assume that the absolute values $|\Gamma_i|$ are equal in magnitude. When all the $\Gamma_i$ are negative, we have the minimum at $\varphi_1 = \varphi_2 = \varphi_3 = 0$. If we change the sign of $\Gamma_3$, this produces a frustration effect and the ground state is at $(\pi/3, \pi/3, 2\pi/3)$. $\varphi_i$ ($i = 1, 2, 3$) take fractional values. When all the $\Gamma_i$ are positive, we have a minimum at $(\varphi_1, \varphi_2, \varphi_3) = (2\pi/3, 2\pi/3, 2\pi/3)$, as shown in Fig. 1. In these two cases, the order parameters are complex and thus the time-reversal symmetry is broken [25,26]. In this time-reversal symmetry broken state, the two eigenvalues of the gap equation in Eq. (7) are degenerate so that we have complex eigenvectors with SU(2) symmetry [27]. We can generalize the condition, that $|\Gamma_i|$ are equal, to obtain general time-reversal symmetry broken states [28].

## 4. Double since-Gordon equation and kinks

Here we consider the case $\gamma_{12} = \gamma_{23}$ and find a solution satisfying $\varphi_1 = \varphi_2 \equiv \varphi$. In this case we obtain the double sine-Gordon equation,

$$K\nabla^2\varphi - \gamma_{12}\sin\varphi - \gamma_{31}\sin(2\varphi) = 0 \tag{17}$$

We investigate the energy functional

$$E = \int \left[\frac{1}{2}K_0\left(\frac{d\varphi}{dx}\right)^2 + V(\varphi)\right]dx \tag{18}$$

where $K_0 = 2K\rho^2$ and the potential $V$ is

$$V(\varphi) = V_0\left(\cos\varphi + \frac{u}{2}\cos(2\varphi)\right) \tag{19}$$

We defined $V_0 = -\gamma_{12}\rho^2$ and $u = \gamma_{31}/\gamma_{12}$.

First consider the case $V_0 > 0$. In the case $u > 1/2$, we have a chiral state at $\varphi = \varphi_0 = \arccos(-1/(2u))$ and a kink solution that travels from one minimum to the other minimum. The stationary condition with respect to $\varphi$ leads to the double sine-Gordon equation,

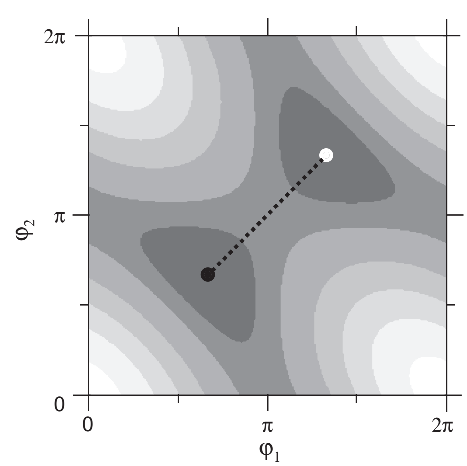


**Fig. 1.** Contour map of V for $\Gamma_1 = \Gamma_2 = \Gamma_3 > 0$. Black and white dots indicate minima of the potential V. Dotted line is the path in the valley connecting two minima.