Frustrated multiband superconductivity

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Abstract

We show that a clean multiband superconductor may display one or several phase transitions with increasing temperature from or to chiral superconducting states with broken time-reversal symmetry with continuous evolution of the relative phases of the superconducting order parameters. These transitions may occur when more than two bands are involved in the formation of the superconducting phase and when the number of repulsive interband interactions is odd. These transitions are signalled by slope changes in the temperature dependence of the superconducting gaps. In the case of quasi-2D superconductors, such transitions also occur with increasing in-plane magnetic field.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

The possibility of multiple bands contributing to the formation of a superconducting phase has been considered in the case of transition metals [1–3], superconducting copper oxides [4] and magnesium diboride [5–7]. More recently, sign-reversed two-band superconductivity has been proposed for the iron-based layered pnictides [8, 9]. In the two-band case, the relative phase of the superconducting gap function associated to each band is determined by the sign of the interband interaction, being zero (\(\pi\)) for attractive (repulsive) interband coupling. However, if more than two electronic bands have to be considered in the study of the superconducting phase, the relative phases are not uniquely defined by the signs of the interband interactions and, in particular, frustration may occur if the number of repulsive interband interactions is odd [10–13].

There is a close analogy between such frustrated multiband superconductors and the well studied problem of frustrated Josephson junction arrays since the interband pairing may be regarded as an interband Josephson coupling [14]. For example, a squared Josephson junction array with a \(\pi\) magnetic flux per plaquette is frustrated with a degenerate ground state since the effect of the \(\pi\) magnetic flux is the change of the sign of the Josephson coupling from positive to negative, i.e., a \(\pi\)-junction [15]. Such \(\pi\)-junctions are also present without magnetic flux as a consequence of d-wave pairing symmetry. In the case of a frustrated (odd number) loop of \(\pi\)-junctions, a spontaneous current will be present. A repulsive interband interaction in a multiband superconductor plays a similar role to that of a \(\pi\)-junction in a Josephson junction array.

Studies of frustrated Josephson junction arrays usually assume symmetric junctions. The case of multiband superconductivity is more closely analogous to the case of an array of asymmetric Josephson junctions [16]. A three-band superconductor can also be pictured as a Josephson junction between a two-gap superconductor and a single-band s-wave superconductor. Recently, the possibility of chiral states with broken time-reversal symmetry in such systems has been discussed [10, 11]. Due to a repulsive interband pairing in the two-band superconductor (which may be interpreted as an internal Josephson junction), a sign-reversed two-band pairing state would occur, but the introduction of Josephson tunnellings from the two-band superconductor to the s-wave superconductor draws a frustrated triangular array of Josephson tunnellings. There is a close analogy between these chiral states and the chiral spin states which were proposed long ago [17]. In very recent works, the possibility of chiral states in a simplified three-band superconductor with repulsive interband interactions but zero interband interactions has been discussed using the BCS approach [11, 13] or a phenomenological Ginzburg–Landau description [12]. A particularly symmetric situation was considered in [11] with two identical interband pairings.

In this paper, we address a feature which is specific to a superconducting system and that has no parallel in magnetically frustrated systems, namely the influence of the temperature dependence of the superconducting gap functions.
on the chiral properties of the multiband superconductor. When temperature is increased, strong modifications of the ratios of the interband Josephson tunnelling rates may occur due to the relative changes of the superconducting gaps which are known to happen in multiband superconductors [3]. These relative changes are larger when the repulsive or attractive interband couplings are weaker than the intraband attractive interactions. We show in this paper that this may lead to one or several phase transitions with increasing temperature from or to frustrated configurations of the relative phases of the superconducting order parameters (which correspond to the double degenerate chiral ground states of a classical XY model). The effects reported in this paper are not expected either in the temperature range where the Ginzburg–Landau approach is valid [12] (since the gap functions have constant ratios in this temperature range) or when all intraband interactions are zero [11, 13]. Furthermore, these transitions may occur induced by variation of other parameters that affect the gap function value. We discuss the case of quasi-2D multiband superconductors in a parallel magnetic field and show that Zeeman splitting may play a similar role to that of temperature. In this paper, we concentrate on the case of a three-band superconductor with one or more repulsive interband couplings. This study can easily be generalized to any number of superconducting bands.

The remaining part of this paper is organized in the following way. In section 2, the model is defined. In section 3, the zero temperature phase diagram for the three-band superconductor is presented. The influence of temperature is discussed in section 4. In section 5, we discuss Zeeman splitting effects in the case of a quasi-2D three-band superconductor. In section 6, we conclude.

2. Hamiltonian

We adopt the Hamiltonian introduced by Suhl et al [3] to describe two-band superconductors, generalized for n bands,

\[
H = \sum_{i, k \sigma} \varepsilon_k c_{i k \sigma}^\dagger c_{i k \sigma} - \sum_{i, j, k, l} V_{ij} c_{i k \uparrow}^\dagger c_{i k \downarrow} c_{j l \uparrow}^\dagger c_{j l \downarrow},
\]

with \(\varepsilon_k = \varepsilon_k - \mu\) and where \(i, V_{ij}\) and \(\mu\) are respectively the band index \((i = 1, \ldots, n)\), the interaction constant and the chemical potential. The \(k\) sums in the interaction term follow the usual BCS restrictions. S-wave symmetry is assumed throughout the paper for simplicity. The interaction constants are assumed to be positive (attractive interactions) for electrons in the same band \((i = j)\), and one has \(V_{ij} = V_{ji}\). The interband interactions may be attractive or repulsive. It is reasonable to expect that the interband interactions are weaker than the intraband interactions, if the Fermi surfaces of the bands participating the superconducting state are distant from each other. We will nevertheless discuss the effects of both large and small interband pairings.

3. Zero temperature phase diagram

In this section, we follow the seminal discussion of [14]. We start by restricting the \(n\)-band superconducting system to the subspace constructed from the set of BCS states,

\[
|F(\Delta, \Phi)\rangle = \prod_{j \neq k} \left(\prod_{\sigma} (u_{jk} e^{\pm i\phi_{jk}}) |\Phi_0\rangle\right),
\]

where \(\Delta = (\Delta_1, \ldots, \Delta_n)\) and \(\Phi = (\phi_1, \ldots, \phi_n)\) are the absolute values of the superconducting gaps and the respective phases, and with the usual BCS definition of superconducting order parameters

\[
u_{jk} \equiv \frac{\Delta_j}{\sqrt{\Delta_j^2 + |\Delta_k|^2}}.
\]

and \(u_{jk}^2 + \nu_{jk}^2 = 1\). Such states with different values of \(\Delta_j\) are orthogonal in the thermodynamic limit since their inner product gives a Dirac \(\delta\)-function [14]. Defining the operators \(\Psi_i = \sum_k c_{i k \uparrow} c_{i k \downarrow}\), which are diagonal in the previous basis in the thermodynamic limit,

\[
\Psi_j |F(\Delta, \Phi)\rangle = \Psi_j |F(\Delta, \Phi)\rangle = \sum_{k} u_{jk} \nu_{jk} e^{-i\phi_{jk}} |F(\Delta, \Phi)\rangle
\]

one may write a simple expression for the eigenvalues of the Hamiltonian which is also diagonal in this basis,

\[
E = \sum_j f_j (|\Psi_j|^2) - \sum_j V_{ij} |\Psi_j|^2 - \sum_{i \neq j} V_{ij} |\Psi_j| |\Psi_j| \cos(\phi_j - \phi_i),
\]

where \(f_j (|\Psi_j|^2)\) is the kinetic energy contribution of the respective band term in the Hamiltonian and has an elaborate dependence on the superconducting parameters \(\Delta_j\). The other terms result from the intraband and interband pairing terms in the Hamiltonian.

The phases associated with the superconducting parameters, \(\Psi_i = |\Psi_i| e^{i\phi_i}\), only affect the interband contributions for the ground state energy. The minimization of this energy with respect to the phases \(\phi_i\) gives

\[
\frac{\partial E}{\partial \phi_i} = 0, \forall i \Rightarrow \sum_j V_{ij} |\Psi_j| \sin(\phi_j - \phi_i) = 0, \forall i.
\]

These equations motivate a simple analogy with a system of \(n\) two-component classical spins governed by the Heisenberg Hamiltonian \(H = \sum_{i \neq j} J_{ij} \vec{S}_i \cdot \vec{S}_j\). The two-component classical spin is written as \(\vec{S}_i = S_i (\cos \phi_i, \sin \phi_i)\). The energy of this system for a given set of magnitudes \(\{S_i\}\) and angles \(\{\phi_i\}\) is \(E(\{\phi_i\}) = \sum_{i < j} J_{ij} S_i S_j \cos(\phi_i - \phi_j) = \sum_{i < j} \vec{J}_{ij} \cdot (\vec{S}_i \times \vec{S}_j)\), where \(\vec{J}_{ij} = J_{ij} S_i S_j\). The last form of this energy can also be interpreted as the energy of a circuit of Josephson junctions with couplings \(J_{ij}\). The classical ground state configuration is obtained from the minimization of this energy with respect to the angles \(\phi_i\) which leads to the condition \(\sum_j \vec{J}_{ij} \cdot (\vec{S}_j - \vec{S}_i) = 0\) for each \(i\), analogous to (6) with the correspondence \(\vec{J}_{ij} \rightarrow -2V_{ij} |\Psi_i| |\Psi_j|\). Note that if a set of angles \(\{\phi_i\}\) is a solution of the previous set of equations, then the set \([-\phi_i]\) also is. This implies that non-degenerate solutions must have \(\phi_i - \phi_i = 0, \pm \pi\). Other values correspond
to frustrated configurations (degenerate ground states which are chirally different and break the time-reversal symmetry).

We will now restrict our study to three bands \((n = 3)\) but the arguments are easily generalized to arbitrary \(n\). We impose for a matter of convenience that \(\phi_1 = 0\) (with no loss of generality). Solving \((6)\) we get several solutions corresponding to extreme or saddle points of the interband energy contribution, the non-frustrated solutions being \(\phi_1, \phi_2, \phi_3\) \(= (0, 0, 0), (0, \pi, 0), (0, 0, \pi), (0, \pi, \pi), (0, \pi, 0)\) and the chiral solutions being

\[
\phi_1, \phi_2, \phi_3 = \pm \left[ 0, \cos^{-1}(a^-), -\text{sgn} \left( \frac{a}{b} \right) \cos^{-1}(a^+) \right],
\]

where

\[
\alpha^\pm = \frac{\pm a^2 \mp b^2 - a^2 b^2}{2 a b y^\pm},
\]

\(\gamma = b, \gamma^- = a, a = \tilde{J}_{12}/\tilde{J}_{23}\) and \(b = \tilde{J}_{31}/\tilde{J}_{23}\). These chiral solutions exist only if \(|\alpha^\pm| \leq 1\).

In figures 1(a) and (b) we show a frustrated array of three classical spins and a non-frustrated array, respectively. In figures 1(c) and (d), the respective plots of \(E_j\) as function of the phases \(\phi_2\) and \(\phi_3\) as well as the respective contour plots are displayed. The locations of the solutions of the minimization equations are indicated by the red spheres in the contour plots. As \(\tilde{J}_{31}\) is varied from 1 to 0.2, the chiral solutions in figure 1(c) continuously converge to the saddle point \((\phi_2, \phi_3) = (0, \pi)\) and to the equivalent location \((0, -\pi)\) and disappear when reaching this point (with \((0, \pi)\) becoming a local minimum). This is a typical second-order phase transition.

In figure 2, the \(\tilde{J}_{31}/\tilde{J}_{23}\) versus \(\tilde{J}_{12}/\tilde{J}_{23}\) phase diagram of the three classical spin system is displayed in the case when one of the interband \(\tilde{J}_{ij}\) is negative. Note that in this case, the ratios of the couplings determine the signs of the couplings fully. The phase diagram of the three classical spin system when one of the interband \(\tilde{J}_{ij}\) is positive can be easily obtained from the former using, for example, the transformation \(\phi_3 \to \phi_3 + \pi\), which leads to \(J_{23} \to -J_{23}\) and \(J_{31} \to -J_{31}\). For example, the symmetrically frustrated case \(\tilde{J}_{12} = \tilde{J}_{23} = \tilde{J}_{31} = 1\) has the frustrated solutions \((\phi_1, \phi_2, \phi_3) = \pm(0, 2\pi/3, -2\pi/3)\). These solutions using

Figure 2. The \(\tilde{J}_{31}/\tilde{J}_{23}\) versus \(\tilde{J}_{12}/\tilde{J}_{23}\) phase diagram of three classical spins when one of the interactions \(\tilde{J}_{ij}\) is negative. The non-frustrated regions have \((\phi_1, \phi_2, \phi_3) = (0, 0, 0), (0, \pi, 0), (0, 0, \pi), (0, \pi, \pi)\). The boundaries of the regions of frustration correspond to second-order phase transitions.
the previous transformation correspond to the frustrated case \( J_{12} = 1 \) and \( J_{23} = J_{13} = -1 \) and \((\phi_1, \phi_2, \phi_3) = (0, \pi/3, 2\pi/3)\). Recalling the relation with the multiband superconductor, one has \( J_{13}/J_{23} \rightarrow (V_{13}/V_{23}) \cdot (|\Psi_1|/|\Psi_2|) \) and \( J_{12}/J_{23} \rightarrow (V_{12}/V_{23}) \cdot (|\Psi_1|/|\Psi_2|) \), so that the location of the multiband superconducting system in this phase diagram is determined not only by the interband pairings but also by the superconducting parameters \(|\Psi_i|\).

We have discussed in this section the minimization with respect to the superconducting phases. Given a certain phase configuration, the remaining minimization of (5) with respect to the absolute values of the superconducting order parameters gives the following result for \( n \) bands:

\[
\Delta_{ik} = \sum_{j,k'} V_{jk}^{i/} \cos(\phi_j - \phi_i) u_{j,k'} v_{k'}(1 - 2 f_{i,k}), \quad (9)
\]

so that the effect of the superconducting phase differences is the renormalization of the interband coupling.

### 4. Finite temperature

The same reasoning can be followed at finite temperature. One must consider the free fermion entropy contribution for the free energy as well as the non-zero occupation of quasiparticle states. One has

\[
\Psi_i = \sum_k u_{i,k} v_{i,k} e^{-\beta \phi_i} (1 - 2 f_{i,k}), \quad (10)
\]

and the interband pairing term has the same expression as that of (5). Since the other terms in the free energy do not depend on the superconducting phases, the minimization with respect to the superconducting phases generates the same set of equations as for zero temperature. Minimizing the free energy with respect to the absolute values of the superconducting parameters [18, 14, 19], one obtains a system of coupled gap equations

\[
\Delta_{ik} = \sum_{j,k'} V_{jk}^{i/} \cos(\phi_j - \phi_i) u_{j,k'} v_{k'}(1 - 2 f_{i,k}), \quad (11)
\]

with \( j = 1, \ldots, n \), which, following the usual steps [18, 19], can be written as

\[
\Delta_i = \sum_j V^{i/} \cos(\phi_j - \phi_i) \int_0^{\omega_D} d\xi_j K_j(\xi_j, \Delta_i, T) \Delta_j, \quad (12)
\]

with

\[
K_j(\xi, \Delta, T) = \frac{N_j(\xi)}{E} \tanh \frac{E}{2T}, \quad (13)
\]

where \( E = \sqrt{\xi^2 + \Delta^2} \), \( \omega_D \) is the usual frequency cutoff, \( N_j(\xi) \) is the density of states of the \( j \)-band and \( t = k_b T \). We assume equal constant density of states for all bands, \( N_i(\xi) = N_i(0) = N \), as a simplification. The differences in the density of states could also be absorbed in the definition of the couplings.

The finite temperature minimization process with respect to the superconducting phases is the same as that described for zero temperature (with the same analogy to the classical spin system), but now the couplings \( \tilde{J}_i \) are temperature dependent. Let us consider the case where the interband couplings, \( V_i \), are finite, but much smaller (in absolute value) than the attractive intraband pairings, \( \tilde{V}_i \). The bands are indexed according to their uncoupled critical temperatures (critical temperatures associated with each band when all interband couplings are zero), starting at the highest \( T_c \) and ending at the lowest.

In the uncoupled situation, the superconducting gaps display steep decreases at the respective critical temperatures with temperature regions where only \( \Delta_3 \) is zero (from \( T_{c3} \) to \( T_{c2} \)) and both \( \Delta_3 \) and \( \Delta_2 \) are zero (from \( T_{c2} \) to \( T_{c1} \)). The modifications relative to the uncoupled case, when the interband couplings \( V_i \) are small, are larger in these temperature ranges.

Note that the coupling of the gap equations implies that if \( \Delta_1 \) is non-zero at a local minimum, then \( \Delta_2 \) and \( \Delta_3 \) are also non-zero. In the non-frustrated situation one expects for the three-band superconducting gaps an analogous temperature dependence to that of a two-band superconductor (with an extra gap function) [3].

However, the coupling \( \tilde{J}_1 \) depends strongly on the values of the superconducting parameters \(|\Psi_1|\) and \(|\Psi_2|\), which, for weak interband interactions, follow approximately the behaviour of the uncoupled gap functions, i.e., undergo sharp decreases around the respective uncoupled critical temperatures. Therefore one should expect a fast increase in the absolute value of \( J_{13}/J_{23} \rightarrow (V_{13}/V_{23}) \cdot (|\Psi_1|/|\Psi_2|) \) around the uncoupled critical temperature \( T_{c2} \) and a similar increase of \( J_{12}/J_{23} \rightarrow (V_{12}/V_{23}) \cdot (|\Psi_1|/|\Psi_2|) \) around the uncoupled critical temperature \( T_{c3} \). Such variations may lead to crossings from a frustrated region of the phase diagram to a non-frustrated region or vice versa. This is shown in figure 3(c) for a three-band superconductor which is initially non-frustrated and completely crosses the frustration region with increasing temperature. This system has weak (one repulsive and two attractive) interband couplings: \( V_{12} = -0.0045 \), \( V_{22} = 0.95 \), \( V_{23} = 0.016 \), \( V_{31} = 0.016 \) and \( V_{33} = 0.85 \), in units of \( V_{11} \). A plot of the superconducting gap functions as function of the normalized temperature for this system is shown in figure 3(b). The associated superconducting phases are displayed in figure 3(a) (only one of the frustrated solutions is shown, the other being symmetric). These graphs were obtained by solving numerically the minimization conditions, (6) and (11). In figure 3(b), slope changes are observed in the lower superconducting gap which reflect a second-order phase transition from or to a chiral phase configuration as shown in figure 3(a). The vertical dotted lines indicate these transitions. Tiny slope changes also occur in the other superconducting gap curves. These changes are very small because the interband contribution to the respective gap function values is much smaller than the intraband contribution. In figure 3(a), the superconducting phases do not reach the point \((\phi_1, \phi_2, \phi_3) = (0, \pi/3, 2\pi/3)\) corresponding to maximum frustration. This is because the \([J_{ij}]\) are never simultaneously equal to one as one increases temperature.

It is more difficult for the transitions to or from chiral configurations to occur if the interband pair tunnelling is of the order of or stronger than the intraband pairing, since the ratios of the superconducting gaps in this case have little
The transitions described in section 4 occur due to the relative change of the superconducting gap functions with increasing temperature. They may also occur induced by variation of other parameters that modify the ratios of the gaps. In this section, we address the case of quasi-2D multiband superconductors in a parallel magnetic field and show that the Zeeman splitting may play a similar role to that of temperature. In the case of a quasi-two-dimensional superconductor under in-plane magnetic fields, orbital frustration can be neglected and the suppression of spin-singlet superconductivity is dominated by Zeeman pair breaking. With increasing magnetic field at zero temperature, a first-order transition from the homogeneous superconducting phase to the normal phase will occur. The paramagnetic limit $H_p$, also designated as the Pauli limit or Chandrasekhar–Clogston limit [20, 21], is the zero temperature critical field associated with this first-order transition. The low temperature first-order transition line ends at a tricritical point around $T \approx 0.56T_c$ where a high temperature second-order phase transition line begins [22, 18].

Quasi-2D two-band superconductors with weak interband interactions display besides this first-order transition curve an additional low temperature first-order transition curve within the superconducting region of the phase diagram, characterized by a large reduction of the superconducting gap in one of the bands [19]. This is shown in figure 5(b), while in figure 5(a) the behaviour of the superconducting gaps above the tricritical temperature is presented. These curves were obtained from (11), (12) and (13) with the substitution $\tanh \tilde{\gamma} \rightarrow \frac{1}{2}(\tanh \frac{\Delta_1}{2T_c} + \tanh \frac{\Delta_2}{2T_c})$ in (13), reflecting the replacement of the energy dispersion $\xi_k$ in the Hamiltonian given by (1) by $\xi_{k\sigma} = \xi_k - \sigma h$ with $h = \mu_B H$, and where
and $\mu_B$ are respectively the magnetic field and the Bohr magneton. As the interband coupling grows, the transition within the superconducting region of the phase diagram approaches the first-order transition to the normal phase and disappears after a certain interband coupling value [19].

For weak interband couplings, a cascade of low temperature first-order transitions occurs in the multiband case within the superconducting region of the phase diagram. In the case of a three-band superconductor, one has two such transitions. Note in figure 5(b) that up to first discontinuity, the zero temperature gap functions remain constant, and after the transition, the gap functions remain almost constant. Consequently, at zero temperature, the path followed by the three-band superconductor in the phase diagram of figure 2, when the magnetic field is increased, can be described in the following way: a single point up to the first transition point; an almost horizontal jump due to the transition and to the respective discontinuities of the gap functions, followed by a very short path; and a second jump, almost vertical at the second transition point, again followed by a very short path. Depending on the initial point in the phase diagram of figure 2, the system may have a first-order transition between chiral states (phase discontinuities) or even jump over the chiral phase region.

Above the tricritical temperature, the dependence of the superconducting phases and gap functions on magnetic field becomes similar to the dependence on temperature, as one can observe in figures 6(a) and (b). There is, however, a steeper magnetic field dependence of $\Delta_1$ near $H_c$ in (a), which reflects the fact that the system is close to the tricritical point where the second-order transition curve becomes of first-order leading to a reentrant behaviour of $\Delta_1(H)$ [19]. Again, slope changes are clearly observed in the lowest gap function at the transition points and a continuous path describes the evolution of the system in the $J_{12}/J_{23}$ phase diagram as shown in figure 6(c).

6. Discussion

We have shown that transitions from or to chiral phase configurations with broken time-reversal symmetry may occur in a three-band superconductor induced by temperature or Zeeman splitting, if one or more of the interband interactions are repulsive. The critical temperatures associated with these transitions can be estimated in the limit of very weak interband couplings. These transitions can be expected to occur in the close vicinity of the uncoupled superconducting critical temperatures associated with bands 2 and 3 (critical temperatures in the absence of interband couplings). For zero interband coupling, the temperature dependence of the gap function $\Delta_3$ follows the BCS mean-field curve, and near $T_{c3}$, is approximately given by $\Delta_3(T) \approx 1.74\Delta_3(0)(1 - T/T_{c3})^{1/2}$. Assuming $\Delta_2 \approx \Delta_2(0)$ and $\Delta_1 \approx \Delta_1(0)$ in this temperature range, one has

$$
\left(1 - \frac{T}{T_{c3}}\right)^{\frac{1}{2}} \approx \frac{1}{1.74} \frac{|V_{12}|\Delta_2(0)}{V_{31}\Delta_3(0)} \left[\frac{V_{31}\Delta_1(0)}{V_{23}\Delta_2(0)} + 1\right],
$$

Figure 5. Superconducting gap functions versus normalized magnetic field for a two-band superconductor for (a) $T = 0.6T_c$ and (b) $T = 0$. The steep behaviour of $\Delta_1$ near $H_c$ in (a) reflects the fact that the system is close to the tricritical point where the second-order transition curve becomes of first-order leading to a reentrant behaviour of $\Delta_i(H)$ [19]. In (b), two discontinuities are present reflecting the existence of two first-order phase transitions in the temperature versus magnetic field phase diagram of a two-band superconductor [19]. Parameters: $V_{12} = \pm 0.045$ and $V_{22} = 0.9$, in units of $V_{11}$.

Figure 6. Same as figure 3, but as a function of the normalized magnetic field at $T = 0.6T_c$. Two phase transitions to and from chiral states are clearly observed as slope changes in the lowest gap function. Parameters: $V_{12} = -0.004$, $V_{22} = 0.95$, $V_{23} = 0.016$, $V_{31} = 0.016$ and $V_{33} = 0.88$, in units of $V_{11}$.
assuming a situation similar to that of figure 3, and where \( T^+ \) and \( T^- \) are respectively the critical temperatures associated to the transitions to and from a chiral state. A similar reasoning can be followed for the transition temperatures of figures 4 and 6.

For an \( n \)-band superconductor in the neighbourhood of the critical temperature \( T_c \) of the transition from the superconducting state to the normal state, the superconducting gap parameters are very small and we can write the system of gap equations in this limit as an eigenvalue equation, \( \Delta \cdot A = \frac{1}{2}\Delta \), where \( A_{ij} = \cos(\phi_j - \phi_i)N^\dagger_i(0) \) and with

\[
S = \int \frac{\omega_0}{\xi} \frac{\tanh(\beta_\omega \xi)}{\xi} \, d\xi \approx \ln \left( \frac{1.36\hbar\omega_0}{T_c} \right),
\]  

where \( \omega_0 \) is the Debye frequency and \( \hbar \) is the Planck constant divided by \( 2\pi \). The minimization of the free energy with respect to the phases \( \phi_i \) gives the stable phase configuration, as previously. The maximum positive eigenvalue of the \( A \) matrix will generate the higher critical temperature. The other solutions will be associated with maxima or saddle points of the free energy (or unphysical solutions). Since all gap functions will be proportional in this limit, no phase transition will occur from or to chiral states near \( T_c \). Note that if, as considered in [11], one assumes a symmetric case where two interband couplings are equal and interband pairings are absent, the possibility of having only two finite gaps and one zero gap must be considered. This result is understood by noting that if \( \Delta_1 = -\Delta_2 \), the Josephson currents from these bands to the third band are symmetric and therefore the third band effectively decouples from the others. The introduction of intraband pairings as well as differences in the Fermi level densities of states of the third band and more obviously different interband couplings forces the existence of three finite gaps.

One should emphasize that there is an important difference between the two-band case and the frustrated three-band case, which is the fact that for the two-band case, the transition between sign-reversed order parameters (the so-called \( s_{\pm} \) scenario, proposed by Mazin et al [9] for the iron-based superconductors) and equal sign order parameters involves always a discontinuity in the relative superconducting phase, while in a frustrated three-band superconductor, one has a continuous evolution of the superconducting phases between a state with equal sign order parameters (\( s \)-wave like state) and a state where one of the order parameters has opposite sign to that of the other two order parameters, as shown in figure 3(c). This also reflects the basic fact that the interband Josephson current must be zero in the two-band case, but a persistent interband Josephson current is possible in a ‘circuit’ of three bands. This difference should be perceptible in properties which are directly or indirectly functions of the relative superconducting phases.

One example is the sensitivity to nonmagnetic and magnetic scattering in a multiband superconductor. It is well known that an isotropic one-band superconductor with \( s \)-wave symmetry is insensitive to nonmagnetic impurities (as stated by Anderson’s theorem). If some anisotropy is present, it will be reduced by the introduction of such impurities. However, superconducting states with a sign change in the gap function such as a \( d \)-wave symmetry state suffer from pair breaking due to the presence of nonmagnetic impurities and this leads to a reduction of the critical temperature as well as to a finite density of states at the Fermi level. In contrast, magnetic impurities have a pair breaking effect for both \( s \)-wave and \( d \)-wave symmetries. Similar behaviour has been found for the sign-reversed two-band superconductor [23]. Strong suppression of the critical temperature due to nonmagnetic interband scattering is expected in the \( s_{\pm} \) scenario if the two gap functions are similar in magnitude. In contrast, only magnetic interband scattering is pair breaking if the two gaps have equal magnitudes and signs. Also, as the impurity concentration is increased, in-gap states appear and with increasing concentration of impurities a gapless superconducting state is reached [23].

We expect the three-band case with gaps of equal signs to behave similarly to the conventional \( s \)-wave superconductor so that a ‘discrete’ Anderson’s theorem is followed. That is, the effect of nonmagnetic impurities should be the averaging of the three gap values, reducing the differences in the values of the order parameters. The case where one of the three gaps has opposite sign to the other two can be viewed as a two-band \( s_{\pm} \) state with one anisotropic gap. In this case, we expect the nonmagnetic interband scattering between the two bands with equal sign gaps to reduce such anisotropy, but the other interband scattering processes (between bands with opposite sign gaps) to be pair breaking just like in the usual \( d \)-wave case. In this paper, we have described a continuous evolution between the former and the latter with increasing temperature. Therefore, along the ‘frustrated’ path of figure 3(c), the behaviour described for equal sign gaps will be continuously modified into that of the latter (where one of the three gaps has opposite sign). The presence of a maximum in one of the gap phases (see figure 3(a)) may induce some peculiar behaviour in this transformation.

Finite in-gap density of states is known to occur in the \( s_{\pm} \) case with nonmagnetic impurities [24–26], reflecting the existence of bound states which appear easily in the case of sign-reversed two-band superconductivity, but not when the order parameters of the two-band superconductor have equal signs. The condition for the appearance of these bound states depends on the relative phase of the gap functions and on the ratio of the superconducting gaps [24]. We argue that for the frustrated three-band superconductor a similar condition should exist and this would imply that the bound states first appear when the three-band superconducting system is in a chiral configuration. That is, when following a temperature-induced path such as that of figure 3(c), no finite in-gap density of states would be present up to a certain point (and respective temperature) within the region of chirality. Beyond this point (or equivalently above the respective temperature), the in-gap density of states should grow until the transition temperature to the \((0, 0, \pi)\) region of figure 3(c) is reached.

Note also that the phase diagram of figure 2 should be modified by the presence of impurities. It has been suggested by several authors that nonmagnetic impurities in
a two-band superconductor induce a local ferromagnetic Josephson between the two bands, therefore reducing effectively the antiferromagnetic (repulsive) interband pairing [24, 27, 28]. Extrapolating this for the three-band case, this would imply that the introduction of nonmagnetic impurities would displace the regions of chirality away from the origin in figure 2. This is in agreement with [23] where it is claimed that with increasing nonmagnetic scattering a crossover from a state with opposite signs to an equal sign isotropic state occurs in a two-band superconductor.

As far as we know, there are at the present no experimental reports of the temperature-induced phase transitions reported in this paper. One should recall that the necessary conditions for the existence of such effects are: (i) more than two bands participating in the superconducting state; (ii) attractive intraband interactions; (iii) weak interband pair tunnellings; (iv) odd number of repulsive interband interactions. Furthermore, the slope changes due to the second-order phase transitions to or from frustrated configurations are only clearly observed in temperature ranges where the interband contribution is dominant at least for one of the gap functions. Among the several examples of superconductors where the possibility of multiple bands contributing to the formation of a superconducting phase has been considered, the iron-based layered pnictides seem to be the more suitable candidates for the observation of these effects due to the complex band structure with more than two Fermi surfaces (hole and electron like). The possibility of a frustrated multiband scenario in the iron-based superconductors has indeed been mentioned recently [11, 29, 30]. Another possibility for the observation of temperature-induced transitions is a Josephson junction between a sign-reversed two-band superconductor and a single band superconductor [10, 11]. In our opinion, the fact that the interband pairing is in principle considerably larger than the Josephson tunnelling between the superconductors may make the observation of these effects difficult (note that the chiral phase is ‘centred’ at $J_{31}/J_{23} = J_{12}/J_{23} \approx 1$). Three species of cold bosonic atomic gases in a triangular lattice may also provide a testing ground for the observation of the effects described here. In fact, it has been shown in [31] that phase factors for atom hopping between optical potential minima equivalent to the Peierls phase due to an effective magnetic field can be introduced in optical lattices, and the possibility of frustration and chiral states in optical lattices has been considered, for example, in [32].

To summarize, we have studied a three-band superconductor considering frustration effects due to the existence of repulsive interband interactions. With increasing temperature and in the case of small interband couplings one may have second-order phase transitions to or from chiral configurations of the superconducting phases which lead to slope changes in the temperature dependence of the superconducting gaps. These effects may also occur induced by Zeeman splitting if parallel magnetic fields are applied to a quasi-2D multiband superconductor.

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