Model of collective modes in three-band superconductors with repulsive interband interactions

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Model of collective modes in three-band superconductors with repulsive interband interactions

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I consider a simple model of a three-band superconductor with repulsive interband interactions. The frustration, associated with the odd number of bands, leads to the possible existence of intrinsically complex time-reversal symmetry breaking (TRSB) order parameter. In such state the fluctuations of the *different* gaps are strongly coupled, and this leads to the development of novel collective modes, which mix phase and amplitude oscillations. I study these fluctuations using a simple microscopic model and derive the dispersion for two physically distinct modes, which are gapped by energy less than 2Δ, and apparently present for all values of interband couplings.

I. INTRODUCTION

Study of the collective modes in superfluids and superconductors has a long history. In the case of single-band systems there are two well-known modes – Bogoliubov-Anderson[1,2] and Schmid[3], representing oscillations of the phase or the amplitude of the order parameter, respectively. In superfluids Bogoliubov-Anderson is a gapless Goldstone mode, but in superconductors it couples to the electromagnetic field and is gapped by energy of the order of the plasma frequency. Schmid mode is always gapped by at least 2Δ (and thus is always damped by interaction with quasiparticles). In superconductors yet another mode, which couples phase oscillations with charge currents, appears close to T_c[4] (it is known as Carlson-Goldman).

In multiband and multicomponent superconductors the situation is even richer. This was first realized by Leggett[5], who considered a two-band superconductor, in which the bands are coupled via Josephson-like term. In such system, apart from the Bogoliubov-Anderson and Schmid modes, another collective mode, representing oscillations of the relative phase of the two gaps, is possible (observation of this mode in MgB_2 has been reported[6]). The Leggett mode is gapped in both superconductors and superfluids (for discussion of Leggett and Carson-Goldman modes in dirty two-band superconductor see Ref. 7). There are analogs of this mode in systems with two-component order parameters (see, for example, Refs. 8 and 9), and it has been argued that there is a related mode in strongly correlated superconductors[10]. This mode exists if the different bands are weakly coupled *and* superconducting even in the case the interband coupling vanishes. In such case there are two non-trivial mean-field (MF) superconducting states (with phase difference between the two gaps equal to 0 or π). One of these states is metastable (which one depends on the sign of the interband coupling). When the interband interactions become dominant the metastable state and the Leggett mode disappear[5].

Recently, multiband superconductivity has attracted a lot of attention in connection with the iron-based high-temperature superconductors, since these materials may have up to four or five superconducting gaps on disconnected pieces of the Fermi surface[11]. One interesting feature of these compounds is the likely existence of a strong *repulsive* interband interactions. In the case of two-band superconductors such interactions lead to an unconventional state with a relative minus sign between the gaps (the so-called $s_\pm$ state)[12]. The three-band case is even more interesting, since in such system there is an intrinsic frustration, and several possible superconducting states compete[13–21] (schematically shown on Fig.1). First, the system can effectively behave as a two-gap $s_\pm$ superconductor, with one of the bands remaining normal. There is also a three-gap $s_\pm$ state, with a π phase difference between two of the gaps and the third one. The most interesting possibility appears if the three interband interactions are roughly comparable in strength (and thus the two- and three-gap $s_\pm$ states are close in energy) – then the system can develop an intrinsically complex order parameter, with non-trivial relative phases between the different gaps. Such complex superconducting state breaks the time-reversal symmetry. Even if such

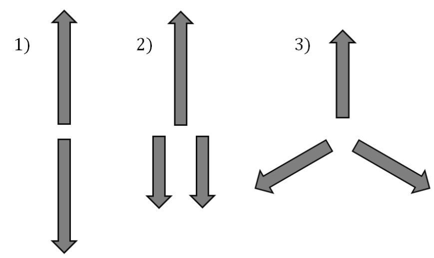

FIG. 1. The possible superconducting states in a three-band system. The angles between the arrows represent the relative phase between the different gaps. On the left is the effective two-gap $s_\pm$ state, in the middle the three-gap $s_\pm$ state, and on the right the TRSB three-gap state (see Ref. 14 for details). The complex state is possible if one or three of the interband pairing terms are repulsive.

order parameter is absent in bulk iron-based superconductors (which are more likely in some variation of the $s_\pm$ state[22]), a related order parameter can be induced by bringing in contact a iron-based and conventional $s-$wave superconductors[13,14]. Frustration between the s-wave and the $s_\pm$ state at the interface can induce on the pnictide side a relative phase, different from the bulk π value. Thus the TRSB state can be stabilized close to the boundary, at least under some circumstances (see also Ref. 23).

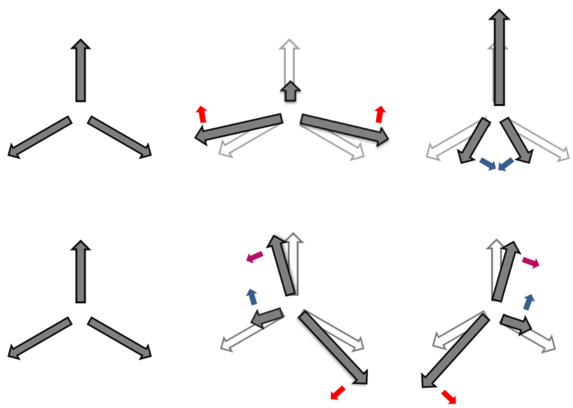

FIG. 2. The two possible phase-amplitude modes around the TRSB state. The red/blue/purple arrows represent phase oscillations coupled with increase/decrease/no change of the amplitude of a given gap.

In such intrinsically complex TRSB states there is a new phenomena – mixed phase-amplitude collective modes. They replace the more conventional Leggett modes and appear because phase and amplitude fluctuations of the gaps on the *different* bands are coupled (unlike the case of multiband s or $s_\pm$ states), due to the non-trivial relative phase angle. Recently these modes have been discussed in Refs. 18 and 20 using phenomenological Ginsburg-Landau (GL) theory[24]. Within this approach it was shown that such modes can have arbitrary low mass. In this paper I study the intergap coupling using alternative – microscopic – description. This approach is very similar in spirit to the one used in Refs. 15 and 19. There, however, the coupling between the phase and amplitude modes have been mostly neglected. In this work I show that such coupling is unavoidable and it creates true collective modes, which are gapped by energy less than 2Δ, and seem to exist for all interband interactions.

Note that coupling between amplitude and phase fluctuations is mandated by the Galilean invariance even in the single-gap case. However, these mixing terms can be neglected in the long-wavelength limit[25]. In contrast, the coupling between phase and amplitude fluctuations of the *different* gaps in the TRSB state has a different physical origin and survives even in the long-wavelength limit.

II. PAIR SUSCEPTIBILITY AND LINEAR RESPONSE

To study the problem I start from a simple generalization of the Bardeen-Cooper-Schrieffer (BCS) model for a three-band case:

$$\mathcal{H} = \sum_{\mathbf{p}} \xi_{\mathbf{p},\alpha} c^\dagger_{\mathbf{p}\alpha} c_{\mathbf{p}\alpha} + \sum_{\mathbf{p}\mathbf{p}'\mathbf{q},\alpha\beta} V^{\alpha\beta}_{\mathbf{p}\mathbf{q}} c^\dagger_{\mathbf{p}\alpha} c^\dagger_{\mathbf{p}'\alpha} c_{\mathbf{q}\beta} c_{\mathbf{q}'\beta}, \quad (1)$$

where α is a band index, the spin indexes are suppressed for the moment, and $V^{\alpha\beta}_{\mathbf{p}\mathbf{q}}$ is the pairing interaction matrix, which has both intraband ($\alpha = \beta$) and interband ($\alpha \neq \beta$) components. The TRSB state exists when one or three of the interband interactions are repulsive, and for concreteness I concentrate on the latter case. The intraband interactions can be both negative (attractive) or positive (repulsive), but even then the system can become superconducting, if the interband interactions are sufficiently strong.

I decouple the interaction terms in a standard BCS fashion. This leads to multiband weak-coupling Hamiltonian

$$\mathcal{H} = \sum_{\mathbf{p}} \xi_{\mathbf{p}\alpha} c^\dagger_{\mathbf{p}\alpha} c_{\mathbf{p}\alpha} + \sum_{\mathbf{p}\mathbf{p}',\alpha} \Delta_{\mathbf{p},\alpha} c^\dagger_{\mathbf{p}+\mathbf{p}'\alpha} c^\dagger_{-\mathbf{p}'\alpha} + \text{h.c.}, \quad (2)$$

where from the self-consistency condition

$$\Delta_{\mathbf{p},\alpha} = V^{\alpha\beta} \sum_{\mathbf{q}\beta} \langle c_{\mathbf{p}+\mathbf{q},\beta,\uparrow} c_{-\mathbf{q},\beta,\downarrow} \rangle$$

(restoring the spin indexes). I will assume that the bands are identical – a rather artificial case, but it simplifies the calculations considerably (for several examples of non-iron based compounds for which this model may apply see Ref. 26). Thus $\xi_{p,1} = \xi_{p,2} = \xi_{p,3} \equiv \xi$, $V^{12} = V^{13} = V^{23} \equiv J$, $V^{11} = V^{22} = V^{33} \equiv V$. It is useful to expressed Δ's through the auxiliary variables d:

$$d_{\mathbf{p},\alpha} = \sum_{\mathbf{q}} \langle c_{\mathbf{p}+\mathbf{q},\alpha,\uparrow} c_{-\mathbf{q},\alpha,\downarrow} \rangle,$$

for which it is straightforward to get:

$$d_1 = \frac{J(\Delta_2 + \Delta_3) - (J+V)\Delta_1}{(J-V)(2J+V)} \quad (3)$$

and analogous expressions for d_2 and d_3.

To study the fluctuations around the TRSB state I use standard linear response theory[27]. In the case of identical bands the free energy below T_c is minimized by the (uniform) state $\Delta_{1,MF} = \Delta_0$, $\Delta_{2,MF} = \Delta_0 e^{2\pi i/3}$, $\Delta_{3,MF} = \Delta_0 e^{4\pi i/3}$ (up to an arbitrary overall phase)[14]. The other mean field solutions – the two and three gap $s_\pm$ states – are degenerate and separated from the TRSB state by finite energy. I introduce small fluctuations around the TRSB state, and get

$$\Delta_1 = \Delta_0 + \rho_1 + i\theta_1,$$
$$\Delta_2 = \Delta_0 e^{2\pi i/3} - \frac{1-i\sqrt{3}}{2}\rho_2 - \frac{\sqrt{3}+i}{2}\theta_2,$$
$$\Delta_3 = \Delta_0 e^{4\pi i/3} - \frac{1+i\sqrt{3}}{2}\rho_3 + \frac{\sqrt{3}-i}{2}\theta_3,$$

Here $\rho(\mathbf{r},t)$ and $\theta(\mathbf{r},t)$ represent the amplitude and phase fluctuations, respectively (note that both have dimension of energy). With this the Hamiltonian can be split into two parts – $\mathcal{H} = \mathcal{H}_0 + \mathcal{H}'$, where $\mathcal{H}_0$ contains all the one-particle and mean-field terms, and $\mathcal{H}'$ can be regarded as a (time-dependent) perturbation:

$$\mathcal{H}' = \sum_{\mathbf{pq}} \Big[\Psi^\dagger_{\mathbf{p+q},1}(\rho_1\sigma_1 + \theta_1\sigma_2 + e\phi\sigma_3)\Psi_{\mathbf{p},1} + \Psi^\dagger_{\mathbf{p+q},2}\left(\frac{-\sigma_1+\sqrt{3}\sigma_2}{2}\rho_2 - \frac{\sqrt{3}\sigma_1+\sigma_2}{2}\theta_2 + e\phi\sigma_3\right)\Psi_{\mathbf{p},2} + \Psi^\dagger_{\mathbf{p+q},3}\left(\frac{\sigma_1+\sqrt{3}\sigma_2}{2}\rho_3 + \frac{\sqrt{3}\sigma_1-\sigma_2}{2}\theta_3 + e\phi\sigma_3\right)\Psi_{\mathbf{p},3}\Big] e^{-i\omega t}, \quad (4)$$

where I used Nambu 2-spinors $\Psi^\dagger_{\mathbf{p},\alpha} = [c^\dagger_{\mathbf{p},\alpha,\uparrow}, c_{\mathbf{p},\alpha,\downarrow}]$, the Pauli matrices σ_i, momentum-frequency representation of θ and ρ, and added scalar potential ϕ.

The response of the superconducting state to a perturbation $\mathbf{h}_\alpha = [\rho_\alpha, \theta_\alpha, e\phi]$ around its mean field value can be written as:

$$g^i_\alpha(\mathbf{p},\omega) = \sum_j \Pi^{ij}_{\alpha\alpha}(\mathbf{p},\omega) h^j_\alpha(\mathbf{p},\omega), \quad (5)$$

where $g^i_\alpha = \mathrm{Tr}\sum\langle\Psi^\dagger_{\mathbf{p},\alpha}\sigma_i\Psi_{\mathbf{p+q},\alpha}\rangle e^{-i\omega t}$. Using Matsubara frequencies formalism the polarization tensor is:

$$\Pi^{ij}_{\alpha\alpha}(\mathbf{p},\omega) = \mathrm{Tr}\; T\sum_{\mathbf{q},\mathbf{q}',\nu}\sigma_i\hat{\mathcal{G}}^{\alpha\alpha}_{\mathbf{q},\mathbf{q}'}(\nu)\sigma_j\hat{\mathcal{G}}^{\alpha\alpha}_{\mathbf{q-p},\mathbf{q}'-\mathbf{p}}(\omega-\nu)$$

where $\hat{\mathcal{G}}$ is the electronic Green's functions in a superconductor:

$$\hat{\mathcal{G}}^{\alpha\alpha}_{\mathbf{p},\mathbf{p}'}(\omega) = -\langle\Psi^\dagger_{\mathbf{p},\alpha}\Psi_{\mathbf{p}',\alpha}\rangle = -\frac{\xi_{p,\alpha}\sigma_3 + i\omega\sigma_0 - \Delta_\alpha\sigma_1}{\omega^2 + |\Delta_\alpha|^2 + \xi^2_{p,\alpha}}\delta_{\mathbf{p},\mathbf{p}'}$$

In writing the linear response in Eqs.(5) I have used the fact that $\hat{\mathcal{G}}$ is *diagonal* in band indexes and there are no $\Pi^{ij}_{\alpha\beta}$ terms with $\alpha \neq \beta$. This means that the coupling between fluctuations in different bands enters only through the self-consistency equations. Furthermore, in absence of supercurrents, the matrix elements coupling amplitude to phase fluctuations of the same gap, and to the scalar potential field vanish in the long-wavelength limit ($\Pi^{12}_{\alpha\alpha} = \Pi^{21}_{\alpha\alpha} = \Pi^{13}_{\alpha\alpha} = \Pi^{31}_{\alpha\alpha} = 0$ for each band). Finally, in the model with identical bands $\Pi^{ij}_{11} = \Pi^{ij}_{22} = \Pi^{ij}_{33} \equiv \Pi^{ij}$.

With this Eqs.(5) can be written in a relatively simple form. Using the d variables (note that Eq. (3) holds for each $(\mathbf{p},\omega)$ component) the equation for the purely real amplitude fluctuations of the first gap can be written as

$$2\mathrm{Re}(d_1(\mathbf{p},\omega)) - \Pi^{11}\rho_1(\mathbf{p},\omega) = 0.$$

It is convenient to define

$$A = \frac{J}{\nu_0(J-V)(2J+V)}, \quad B = \frac{V}{\nu_0(J-V)(2J+V)},$$

and write the expression for d_1:

$$\mathrm{Re}(d_1) = -\nu_0(A+B)\mathrm{Re}(\Delta_1) + \nu_0 A(\mathrm{Re}(\Delta_2) + \mathrm{Re}(\Delta_3))$$
$$= -\nu_0(A+B)\rho_1 - \frac{\nu_0 A}{2}[(\rho_2+\rho_3) + \sqrt{3}(\theta_2-\theta_3)],$$

where ν_0 denotes the density of states.

The equation for the phase fluctuations of Δ_1 is

$$2\mathrm{Im}(d_1(\mathbf{p},\omega)) - \Pi^{22}(\mathbf{p},\omega)\theta_1(\mathbf{p},\omega) - \Pi^{23}(\mathbf{p},\omega)e\phi(\mathbf{p},\omega) = 0,$$

with:

$$\mathrm{Im}(d_1) = -\nu_0(A+B)\theta_1 + \frac{\nu_0 A}{2}[\sqrt{3}(\rho_2-\rho_3) - (\theta_2+\theta_3)].$$

I also define $Q^{23} \equiv \Pi^{23}/\nu_0$, $\Pi^{ii}/\nu_0 + 2\int d\xi \tan(\sqrt{\xi^2+\Delta_0^2}/2T)/\sqrt{\xi^2+\Delta_0^2} \equiv Q^{ii}$, and express the integral through A and B using the gap equations (for details see Ref. 27 and 28). Utilizing these definitions and the equivalence of the bands Eqs.(5) can be written in compact matrix form:

$$\begin{bmatrix} Q^{11}-2A & A & A & 0 & \sqrt{3}A & -\sqrt{3}A & 0 \\ A & Q^{11}-2A & A & -\sqrt{3}A & 0 & \sqrt{3}A & 0 \\ A & A & Q^{11}-2A & \sqrt{3}A & -\sqrt{3}A & 0 & 0 \\ 0 & -\sqrt{3}A & \sqrt{3}A & Q^{22}-2A & A & A & Q^{23} \\ \sqrt{3}A & 0 & -\sqrt{3}A & A & Q^{22}-2A & A & Q^{23} \\ -\sqrt{3}A & \sqrt{3}A & 0 & A & A & Q^{22}-2A & Q^{23} \\ 0 & 0 & 0 & Q^{32} & Q^{32} & Q^{32} & Q^{33}-p^2/(4\pi e^2) \end{bmatrix} \begin{bmatrix} \rho_1 \\ \rho_2 \\ \rho_3 \\ \theta_1 \\ \theta_2 \\ \theta_3 \\ e\phi \end{bmatrix} = 0 \quad (6)$$

The Poisson equation has been used in the last element of the lowest matrix row. Note that the coupling constants J and V appear in the matrix only as a combination in A, which controls all intergap fluctuation couplings. This is due to the high symmetries of the model with identical bands we are considering. In the case of non-identical bands the couplings between the phase-phase and phase-amplitude fluctuations are generally different and the matrix becomes 19×19.

III. COLLECTIVE MODES

The collective modes of the system can be obtained after analytically continuing to real frequencies. They are given by the eigenvectors of the matrix with eigenvalues equal to zero. The explicit expressions are quite unwieldy, but analysing them reveals a relatively simple picture. There are six eigenvectors, and two of them represent locked-in oscillations of the phase or amplitude of the three gaps, which are trivial generalization of the single-gap Bogoliubov-Anderson and Schmid modes. As in the single-gap case, the Bogoliubov-Anderson mode couples to the electromagnetic field (which gives it a mass), while the Schmid mode does not (but is nonetheless gapped by $2\Delta_0$). The remaining eigenvectors represent the new coupled amplitude and phase fluctuations modes (see Fig. 2). There are four eigenvectors and two eigenvalues, so each eigenvalue is two-fold degenerate. The energy spectrum of the modes can be obtained by solving the equation

$$-6A + Q^{11} + Q^{22} \pm \sqrt{36A^2 + (Q^{11} - Q^{22})^2} = 0. \quad (7)$$

For simplicity I consider only the case $T = 0$ (no thermally excited quasiparticles). If Q^{ii} are small they can be expanded to the lowest order in p and ω[27,28]:

$$Q^{11} \approx -\frac{\omega^2 - c^2p^2 - 4\Delta_0^2}{4\Delta_0^2}, \quad Q^{22} \approx -\frac{\omega^2 - c^2p^2}{4\Delta_0^2}, \quad Q^{23} \approx \omega,$$

where $c = v_F/\sqrt{3}$ gives the mode velocity. Using these results Eq.(7) simplifies to

$$\omega^2 = 2\Delta_0^2 \left(-6A + 1 \pm \sqrt{36A^2 + 1}\right) + c^2p^2 \quad (8)$$

Obviously, the first term on the right side gives the energy gap ω_0 of the mixed modes.

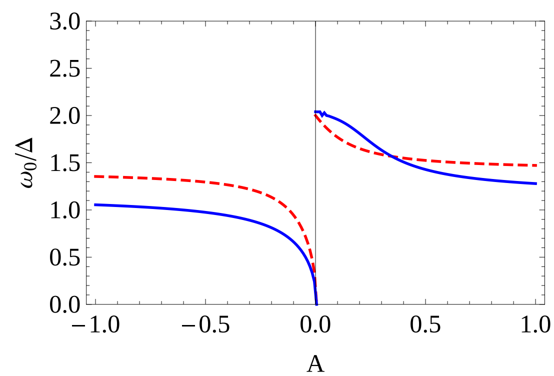

FIG. 3. The energy gap of the mixed modes as function of A, as derived from Eqs.(7) (blue curve) and Eqs.(8) (red dashed curve). Apparently the modes can exist both for small and large J (negative and positive A).

Before considering the eigenmodes let's look at the possible values of A. As seen from its definition, it can be positive or negative. When V is finite and attractive (i.e. negative) A has infinite discontinuity at $J = |V|/2$ and is negative/positive for smaller/larger values of J. In the case both interactions are repulsive (positive) superconductivity can exist only for $J > V$, and A is always positive and decreasing function of J.

To obtain ω_0 these equations have to be solved. Eq.(7) can only be solved numerically, while Eq.(8) allows analytic treatment. In both cases it is easy to see that the mixed modes are well defined (ω_0 is real and below $2\Delta_0$) for positive (negative) A for the plus (minus) sign in the equation. Thus for each A there are two distinct collective modes (schematically shown on Fig. 2) with identical dispersion. The exact and the approximate solutions for ω_0 are plotted on Fig. 3 and from it we see that these modes appear to exist for any given A in the interval $(-\infty, \infty)$. As the coupling between the different gaps decreases ($J \to 0$, small negative A) ω_0 also becomes smaller.

Now let me compare these modes with the well-known collective modes in one- and two-band superconductors. Note that despite the fact that the mixed modes involve amplitude oscillations, they are gapped by less than $2\Delta_0$. This is quite surprising and is entirely due to the phase-amplitude coupling. In contrast, purely amplitude modes cannot have energy less then twice the gap. The dispersion of the mixed modes is similar to that of the Leggett mode, but again there are important differences. As the results above indicate, the mixed modes are present for all values of J, in sharp contrast to the Leggett mode, which only exists for weak interband interactions. There is one crucial difference between the two- and the three-band superconductors, which may explain this – in the former the number of the mean-field solutions reduces from two to one when the interband interaction starts to dominate. In the three-band case such reduction does not occur, and there can be three mean-field order parameters, even if the intraband interactions are set to zero. However, the reader should be warned that using the above results in the region of small and positive A may be problematic, for at least two reasons. First, this region is formally outside of the regime of validity of the weak-coupling calculation (since in this region J is large). Second, and more physical reason, is that when interband interactions dominate it is unclear if well defined relative phase even exist.

Several features of the above results are due to the peculiarity of the particular case with identical bands. First, the electromagnetic potential does not couple to the mixed modes. In the general case such coupling should be expected, since phase fluctuations are conjugate to density fluctuations, and changes in the relative density produce charge imbalance, which couples to the field. Second, there are two degenerate in energy, but physically different modes (shown on Fig. 2). The degeneracy is due to the fact the two metastable $s_\pm$ states (states 1 and 2 on Fig. 1) have the same energy. In the case of non-identical bands these states split, and there are two different modes with distinct dispersions.

More detailed and sophisticated calculations are necessary to study the possible existence of such modes in real superconductors, such as iron pnictides. These modes can be observed experimentally, for example by Raman scattering[6,19], and their presence can be used as a probe of the TRSB state.

IV. CONCLUSIONS

In conclusion, I have considered a simple microscopic model of a three-band superconductor with repulsive interband interactions. In such a system the frustration associated with the odd number of bands can lead to intrinsically complex TRSB state. In this state two distinct collective modes develop, which necessarily mix the phase and amplitude oscillations of the *different* gaps. These modes appear to be gapped by energy less than 2Δ both in the cases of weak and strong interband couplings.

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