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Pressure induced FFLO instability in multi-band superconductors

I T Padilha and M A Continentino

Instituto de Física, Universidade Federal Fluminense, Campus da Praia Vermelha, 24210-340, Niterói, JR, Brazil

E-mail: mucio@if.uff.br

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Abstract
Multi-band systems such as inter-metallic and heavy fermion compounds have quasi-particles arising from different orbitals at their Fermi surface. Since these quasi-particles have different masses or densities, there is a natural mismatch of the Fermi wavevectors associated with different orbitals. This makes these materials potential candidates to observe exotic superconducting phases as Sarma or FFLO phases, even in the absence of an external magnetic field. The distinct orbitals coexisting at the Fermi surface are generally hybridized and their degree of mixing can be controlled by external pressure. In this work we investigate the existence of an FFLO type of phase in a two-band BCS superconductor controlled by hybridization. At zero temperature, as hybridization (pressure) increases we find that the BCS state becomes unstable with respect to an inhomogeneous superconducting state characterized by a single wavevector q.

1. Introduction

Asymmetric superfluidity refers to Cooper pairing in systems with mismatched Fermi surfaces. This phenomenon includes the FFLO state [1, 2] where an external magnetic field produces a mismatch between bands with different spin orientations. It also occurs in cold atom systems where the mismatch is due to different numbers of interacting fermions [3, 4]. Also it may appear in the interior of neutron stars where the pairing of up and down quarks in different numbers can give rise to color superconductivity (see for example, [5, 6]).

In multi-band metallic systems such as inter-metallic compounds and heavy fermions, electrons arising from distinct atomic orbitals coexist at a common Fermi surface [7, 8]. Since these electrons have different effective masses or occur in different numbers per atom, there is a natural mismatch of the Fermi wavevectors of these quasi-particles. As a consequence, we may expect to find the physics associated with asymmetric superconductivity in these systems, even in the absence of an external magnetic field. In general, the wave functions of electrons in different orbitals hybridize and it turns out that the mismatch of the Fermi wavevectors is affected by hybridization. Since pressure controls hybridization [9], we show that in multi-band superconductors it plays a role similar to that of an external magnetic field in the study of FFLO phases. The pressure induced FFLO phase does not compete with the orbital effects which arise when applying an external magnetic field to a superconductor.

The problem of superconductivity in systems with overlapping bands was treated originally by Suhl *et al* [10]. These authors did not consider inter-band pairing as this is negligible in the case where the critical temperature is much smaller than the effective inter-band splitting.

Recently, we have investigated asymmetric superconductivity in multi-band metallic systems in the presence of intra- and inter-band interactions [11]. We have studied the different types of homogeneous ground states which appear as hybridization is changed. In the inter-band case, as hybridization increases there is a first order transition from the BCS state [12] to the normal state. Between these states there is a gapless metastable phase with similarities to the Sarma phase [13] which has had renewed interest in recent years [14, 6]. The instability of the BCS state is related to the appearance of a soft mode at a characteristic wavevector [11, 14]. This suggests that an alternative ground state as hybridization increases is an inhomogeneous superconductor of the FFLO type. In this paper we investigate the existence of such a state. Differently from [10], we consider the situation where the dispersion relations of the bands overlap at the Fermi surface such that their Fermi wavevectors are equal. In this case inter-band interactions must be taken into account. Also we neglect intra-band pairing, assuming that these are suppressed by a strong on-site repulsion. In this case we expect inter-orbital repulsion to be relatively weaker such that the net attractive interaction between different orbitals turns out to be larger than that for intra-band channels.

2. Model and formalism

The effective Hamiltonian describing the two-band metallic system, hybridization and pairing of quasi-particles with a net momentum q is given by

$$\begin{aligned}\mathcal{H}_{\text{eff}} &= \sum_k \left(\epsilon_k^a a_k^+ a_k + \epsilon_k^b b_k^+ b_k\right) \\ &+ \sum_k \left(\Delta_q a_{k+\frac{q}{2}}^+ b_{-k+\frac{q}{2}}^+ + \Delta_q^* b_{-k+\frac{q}{2}} a_{k+\frac{q}{2}}\right) \\ &+ \sum_k V_k \left(a_{k+\frac{q}{2}}^+ b_{k+\frac{q}{2}} + b_{k+\frac{q}{2}}^+ a_{k+\frac{q}{2}}\right),\end{aligned} \tag{1}$$

where the inhomogeneous superconducting order parameter is

$$\Delta_q = -g \sum \left\langle b_{-k+\frac{q}{2}} a_{k+\frac{q}{2}} \right\rangle, \tag{2}$$

where g is the strength of the attractive interaction and the symbol $\langle \cdots \rangle$ stands for the thermodynamic average at $T \neq 0$ or to the expectation value of the product operators in the superconducting ground state at zero temperature. The dispersion of the quasi-particles is given by

$$\epsilon_k^i = \xi_i(k) - \mu_i, \qquad i = a, b \tag{3}$$

where

$$\xi_i(k) = \alpha_i k^2, \begin{cases} \alpha_a = 1 \\ \alpha_b = \alpha = \frac{m_a}{m_b} \end{cases} \tag{4}$$

and $\alpha < 1$ is the ratio of the effective masses.

The Green's function method is used to obtain the BCS-like order parameter

$$\left\langle b_{-k+\frac{q}{2}} a_{k+\frac{q}{2}} \right\rangle = \int \mathrm{d}\omega\, f(\omega) \left[\mathrm{Im} \left\langle\left\langle a_{k+\frac{q}{2}}; b_{-k+\frac{q}{2}} \right\rangle\right\rangle_\omega\right], \tag{5}$$

where $f(\omega)$ is the Fermi function and $\langle\langle a; b\rangle\rangle_\omega$ is the frequency dependent anomalous Green's function in the notation of Tyablikov [15] and Zubarev [16].

In order to calculate the relevant Green's functions we obtain their equations of motion. In particular for the anomalous Green's function $\langle\langle a_{k+\frac{q}{2}}; b_{-k+\frac{q}{2}}\rangle\rangle_\omega$ this is given by

$$\begin{aligned}\omega \left\langle\left\langle a_{k+\frac{q}{2}}; b_{-k+\frac{q}{2}} \right\rangle\right\rangle_\omega &= \left\langle\left\langle \left[a_{k+\frac{q}{2}}, \mathcal{H}_{\text{eff}}\right]; b_{-k+\frac{q}{2}} \right\rangle\right\rangle_\omega \\ &+ \frac{1}{2\pi} \left\langle \left\{a_{k+\frac{q}{2}}, b_{-k+\frac{q}{2}}\right\} \right\rangle.\end{aligned} \tag{6}$$

After some long calculations we obtain for the anomalous Green's function,

$$\left\langle\left\langle a_{k+\frac{q}{2}}; b_{-k+\frac{q}{2}} \right\rangle\right\rangle_\omega = \frac{D_x(\omega)}{D(\omega)} \tag{7}$$

with

$$D_x(\omega) = \Delta_q \left[\left(\omega - \epsilon_{k-\frac{q}{2}}^b\right)\left(\omega + \epsilon_{-k+\frac{q}{2}}^a\right) - \left(\left|\Delta_q\right|^2 - V_k^2\right)\right] \tag{8}$$

and

$$\begin{aligned}D(\omega) &= \left(\omega + \epsilon_{-k+\frac{q}{2}}^b\right)\left(\omega - \epsilon_{k-\frac{q}{2}}^a\right)\left(\omega - \epsilon_{k+\frac{q}{2}}^b\right)\left(\omega + \epsilon_{-k+\frac{q}{2}}^a\right) \\ &- V_k^2\left[\left(\omega + \epsilon_{-k+\frac{q}{2}}^b\right)\left(\omega + \epsilon_{-k+\frac{q}{2}}^a\right) + \left(\omega - \epsilon_{k-\frac{q}{2}}^a\right)\left(\omega - \epsilon_{k+\frac{q}{2}}^b\right)\right] \\ &- \left|\Delta_q\right|^2\left[\left(\omega - \epsilon_{k+\frac{q}{2}}^b\right)\left(\omega + \epsilon_{-k+\frac{q}{2}}^a\right) + \left(\omega + \epsilon_{-k+\frac{q}{2}}^b\right)\left(\omega - \epsilon_{k+\frac{q}{2}}^a\right)\right] \\ &+ \left(V_k^2 - \left|\Delta_q\right|^2\right)^2.\end{aligned} \tag{9}$$

The poles of the Green's function, $D(\omega) = 0$, in equation (9) yield the excitations of the system. Substituting the dispersion relation of the bands,

$$\begin{aligned}\epsilon_{\pm k+\frac{q}{2}}^a &= k^2 + \frac{q^2}{4} \pm \vec{k}.\vec{q} - \mu_a \\ \epsilon_{\pm k+\frac{q}{2}}^b &= \alpha k^2 + \alpha\frac{q^2}{4} \pm \alpha\, \vec{k}.\vec{q} - \mu_b\end{aligned}$$

in equation (9), we obtain a complete fourth degree equation for the energy ω of the excitations,

$$D = \omega^4 + b\omega^3 + c\omega^2 + \mathrm{d}\omega + e = 0, \tag{10}$$

where

$$\begin{aligned}b &= -2v_{\mathrm{F}} q X (1+\alpha) \\ c &= -\left[\epsilon_k^{a2} + \epsilon_k^{b2} + 2\left(V_k^2 + \left|\Delta_q\right|^2\right)\right] \\ d &= 2v_{\mathrm{F}} q X \left[\epsilon_k^{b2} + \alpha\epsilon_k^{a2} + (1+\alpha)\left(V_k^2 + \left|\Delta_q\right|^2\right)\right] \\ e &= \left[\epsilon_k^a \epsilon_k^b - \left(V_k^2 - \left|\Delta_q\right|^2\right)\right]^2 \\ X &= \frac{\vec{k}.\vec{q}}{kq} = \cos\theta\end{aligned} \tag{11}$$

where v_{F} is the Fermi velocity and we have neglected terms of $\mathrm{O}(q^2)$ as usual.

In order to solve this equation we introduce the change of variable

$$\omega \to u - \frac{b}{4} = u + v_{\mathrm{F}} q \frac{(1+\alpha)}{2} \cos\theta, \tag{12}$$

which yields a *depressed* equation of the fourth degree

$$u^4 + \beta u^2 + \gamma u + \lambda = 0, \tag{13}$$

where

$$\begin{aligned}\beta &= \frac{-3b^2}{8} + c = -2(V^2 + \Delta_q^2) - \epsilon_k^{a2} - \epsilon_k^{b2} \\ \gamma &= \frac{b^3}{8} - \frac{bc}{2} + d = -q v_{\mathrm{F}} X (1-\alpha)(\epsilon_k^{a2} - \epsilon_k^{b2}) \\ \lambda &= \frac{-3b^4}{256} + \frac{cb^2}{16} - \frac{bd}{4} + f = (\epsilon_k^a \epsilon_k^b - V^2 + \Delta_q^2)^2\end{aligned}$$

up to linear terms in q. In the case $V = 0$, $\alpha = 1$, $\epsilon_k^a = \epsilon_k^b$, the fourth order equation reduces to a product of two identical second order equations. The roots of this second order equation yield the excitations found in the usual FFLO problem.

3. The FFLO state induced by mixing

The problem above is still quite intractable. This is due to the different masses ($\alpha \neq 1$) of the quasi-particles, that in combination with mixing, has a very strong destabilizing effect on the FFLO state. The effects of hybridization are stronger at the points in k-space where the bands cross, i.e., for $\epsilon^a_{k_c} = \epsilon^b_{k_c}$. Analytical progress can be made if we assume the case of homotectic bands, i.e., we take $\epsilon^b_k = \alpha\epsilon^a_k$ and $\epsilon^a_k = \epsilon_k$. The crossing of the bands takes place exactly at the Fermi surface, at $\epsilon^i_k = 0$, which is just the situation where inter-band interactions are most relevant [10]. Furthermore, to make analytical progress we consider that the ratio between the masses of the quasi-particles α is very close to unity, i.e., we write $\alpha = 1 - \varepsilon$, and neglect terms of order ϵ^2. In this case we can find a solution for the depressed fourth order equation given by equation (13).

The energies of the excitations in this case are given by $\omega = \omega^{\pm}_{12}(k)$, where

$$\omega^{\pm}_{12}(k) = \pm\omega_{12} + \delta\mu \tag{14}$$

with

$$\omega_{12}(k) = \sqrt{A_k \pm \sqrt{B_k}}. \tag{15}$$

The quantity $\delta\mu = -b/4 = v_F q[(1+\alpha)/2]\cos\theta$. Also,

$$A_k = (1-\varepsilon)\epsilon_k^2 + V^2 + \Delta_q^2 + \mathrm{O}[\epsilon]^2 \tag{16}$$

and

$$B_k = 4V^2[(1-\varepsilon)\epsilon_k^2 + \Delta_q^2] + \mathrm{O}[\epsilon]^2. \tag{17}$$

These equations yield

$$\omega_{12}(k) = \xi_k \pm V, \tag{18}$$

where

$$\xi_k = \sqrt{(1-\varepsilon)\epsilon_k^2 + \Delta_q^2}.$$

When calculating the gap function, Δ_q, we find, after a change of variables, the following integral,

$$G_k(\delta\mu) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} \mathrm{d}\omega D_x(\omega+\delta\mu)\,\mathrm{Im}\left[\frac{1}{D(\omega)}\right] f(\omega+\delta\mu),$$

where $f(\omega)$ is the Fermi function, $D_x(\omega)$ is given by equation (8) above and the denominator of the anomalous Greens function is given by

$$D = (\omega^2 - \omega_1^2)(\omega^2 - \omega_2^2).$$

Using that,

$$\frac{1}{(\omega^2-\omega_1^2)(\omega^2-\omega_2^2)} = \frac{1}{8V\xi_k}\left\{\frac{1}{\omega_1}\left[\frac{1}{\omega-\omega_1} - \frac{1}{\omega+\omega_1}\right] - \frac{1}{\omega_2}\left[\frac{1}{\omega-\omega_2} - \frac{1}{\omega+\omega_2}\right]\right\}.$$

Recalling that in the equation above, $\omega \to \omega + \mathrm{i}\epsilon$, and taking the imaginary part, we obtain that $G_k(\delta\mu)$ is a sum of three terms, $G_k(\delta\mu) = G^1_k(\delta\mu) + G^2_k(\delta\mu) + G^3_k(\delta\mu)$ with

$$G^1_k(\delta\mu) = \frac{\Delta_q}{4\xi_k}\left\{2 - \sum_\sigma [f(E^1_{k\sigma}) + f(E^2_{k\sigma})]\right\},$$

$$G^2_k(\delta\mu) = \frac{-\Delta_q[(1-\alpha)\epsilon_k + 2\alpha\vec{k}.\vec{q}]}{8V\xi_k} \times \left\{\sum_{j=1,2}(-1)^{j-1}[f(E^j_{k+}) + f(E^j_{k-})]\right\}$$

and

$$G^3_k(\delta\mu) = \frac{\Delta_q(1+\alpha)\epsilon_k}{8\xi_k(\xi_k^2 - V^2)}\vec{k}.\vec{q} \times \left\{2 + \sum_{j=1,2}(-1)^{j-1}[f(E^j_{k+}) - f(E^j_{k-})]\right\},$$

where $E^1_{k\sigma} = \xi_k + \sigma(V + \delta\mu)$ and $E^2_{k\sigma} = \xi_k + \sigma(V - \delta\mu)$ with $\sigma = \pm$. We have omitted terms of $\mathrm{O}(q)^2$ and $\mathrm{O}(\varepsilon)^2$. When calculating the gap equation $\Delta_q = \sum_{\vec{k}} G_k(\delta\mu)$ at zero temperature, the Fermi functions are expressed in terms of θ functions and this imposes severe restrictions on the sums over $\vec{k}$. When these sums are performed and angular integrations are carried out, the only contribution which remains is that arising from $G^1_k(\delta\mu)$. The gap equation can finally be written as

$$-1 + \frac{g}{2}\int\frac{\mathrm{d}^3k}{(2\pi)^3}\frac{1}{\xi_k} = \frac{g}{4}\int\frac{\mathrm{d}^3k}{(2\pi)^3}\frac{1}{\xi_k}\sum_\sigma[\theta(-E^1_{k\sigma}) + \theta(-E^2_{k\sigma})]. \tag{19}$$

Subtracting the $T = 0$ gap equation for a BCS superconductor,

$$-1 + \frac{g}{2}\int\frac{\mathrm{d}^3k}{(2\pi)^3}\frac{1}{\sqrt{\alpha\epsilon_k^2 + \Delta_0^2}} = 0, \tag{20}$$

with $\alpha \approx 1$, from the left-hand side of equation (19), we obtain in the weak coupling approximation,

$$\frac{g\rho}{2\sqrt{\alpha}}\ln\frac{\Delta_0}{\Delta_q} = \frac{g}{4}\int\frac{\mathrm{d}^3k}{(2\pi)^3}\frac{1}{\xi_k}\sum_\sigma[\theta(-E^1_{k\sigma}) + \theta(-E^2_{k\sigma})],$$

where ρ is the density of states at the Fermi level. The integrals over k ($\int \mathrm{d}k$) on the right-hand side are performed taking into account the constraints imposed by the θ functions. They yield

$$\frac{g\rho}{4\sqrt{\alpha}}\sum_\sigma\int\frac{\mathrm{d}\Omega}{4\pi}\sinh^{-1}\left[\frac{\sqrt{(V+\sigma\delta\mu)^2 - \Delta_q^2}}{\Delta_q}\right].$$

This equation has real solutions only if $V + v^*_F q > \Delta_q$, where $v^*_F = v_F(1+\alpha)/2$. Let us consider the case $\sigma = -1$, Recalling that $\delta\mu = v^*_F q\cos\theta$, the integral above can be rewritten as

$$\frac{g\rho}{4\sqrt{\alpha}}\frac{1}{2v^*_F q}\int_{-v^*_F q}^{v^*_F q}\mathrm{d}x\,\sinh^{-1}\left[\frac{\sqrt{(V+x)^2 - \Delta_q^2}}{\Delta_q}\right],$$

where we used the change of variables, $x = -v^*_F q\cos\theta$. In fact the integrals are independent of σ and the result is simply twice that for a given sign. Respecting the limits of integration in different cases to obtain a real result, the final gap equation is given by

$$\frac{g\rho}{2\sqrt{\alpha}}\ln\frac{\Delta_0}{\Delta_q}=\frac{g\rho}{4\sqrt{\alpha}}\frac{\Delta_q}{v_F^*q}\left[G\left(\frac{v_F^*q+V}{\Delta_q}\right)+G\left(\frac{v_F^*q-V}{\Delta_q}\right)\right], \tag{21}$$

where $G(x)$ is the function [17]

$$\begin{aligned} G(x) &= x\cosh^{-1}x-\sqrt{x^2-1}, \qquad |x|>1\\ &= 0, \qquad |x|\leqslant 1\\ &= -G(-x), \qquad x<0. \end{aligned}$$

Notice that the mass ratio α cancels out explicitly in the gap equation, equation (21). Its role at least for $\alpha\approx 1$ is just to renormalize the Fermi velocity. From this equation we find that for the FFLO state to be a solution it is necessary that $\overline{q}=q/(V/v_F^*)>1$. Also, since $G(|x|\leqslant 1)=0$, the solution for $V<V_1^c(\overline{q})=\Delta_0/(1+\overline{q})$ is always $\Delta_q=\Delta_0$, i.e., the BCS state. Thus a necessary condition for the FFLO state is $V>V_1^c(\overline{q})$. The upper critical value of the hybridization $V_2^c(\overline{q})$ below which the FFLO state can be a solution of the gap equation is obtained taking the limit of equation (21) for $\Delta_q\to 0$. The results can be expressed as [5, 17]

$$V_2^c(\overline{q})=\frac{\Delta_0 e}{2(\overline{q}+1)}\left|\frac{\overline{q}+1}{\overline{q}-1}\right|^{\frac{\overline{q}-1}{2\overline{q}}}.$$

In figure 1 we plot $V_1^c(\overline{q})$ and $V_2^c(\overline{q})$ as a function of the reduced wavevector, and it is clear that there is a range of values for the hybridization $V_c^1<V<V_c^2$ for which a FFLO phase may exist. The maximum value of V_2^c occurs for $\overline{q}=\overline{q}_c\approx 1.2$, which when substituted in the equation above yields $V_c=V_2^c(\overline{q}_c)\approx 0.75\Delta_0$. This value of $\overline{q}$ is that which minimizes the free energy in the range of stability of the FFLO phase [5, 17]. The value $V_1^c(\overline{q})$ above marks the limit of stability of the FFLO phase. The actual value of the hybridization for which the first order phase transition occurs is obtained considering the energies of these states. The argument is similar to that of Chandrasekhar and Clogston [18] to obtain the critical field in BCS superconductors. Here we have to consider the hybrid bands. In the limit of very small mass differences their dispersion relations can be easily obtained and are given by $\omega_{1,2}=[(1+\alpha)/2]\epsilon_k\pm V$. On the other hand the condensation energy for a system of unequal masses was obtained in [19]. This is similar to that of a system of identical particles with the mass m replaced by $2m_r$, where the reduced mass $m_r=m_am_b/(m_a+m_b)=m_a/(1+\alpha)$ in our notation. The chemical potential is also modified and given by $\mu^*=(\mu_a+\mu_b)/2=[(1+\alpha)/2]\mu_a$. Then the effective particles have dispersion $\epsilon_k^*=[(1+\alpha)/2]\epsilon_k$. Comparing the condensation energy of these quasi-particles, $E_c=(1/2)\rho^*\Delta_0^2$, with the energy associated with hybridization, $E_V=\rho^*V^2$, one obtains a critical hybridization, $V_c=\Delta_0/\sqrt{2}\approx 0.71\Delta_0$, above which BCS superconductivity becomes unstable. In these expressions, ρ^* is the density of states at the Fermi level of particles with dispersion relation $\epsilon_k^*=[(1+\alpha)/2]\epsilon_k$. Consequently, there is a window of values for the hybridization $(0.71\Delta_0<V<0.75\Delta_0)$ where we can expect an FFLO phase to occur. The transition at V_2^c is a continuous second order transition from the FFLO to the normal state.

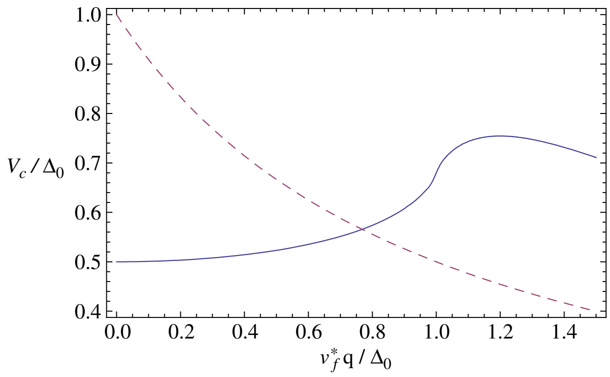

Figure 1. V_1^c (dashed) and V_2^c as a function of the reduced wavevector.

(This figure is in colour only in the electronic version)

Notice that in multi-band systems, even at zero pressure, hybridization is always present, such that the bands in equation (1) already contain some degree of mixing. Then the critical values of the hybridization obtained above refer to changes in this parameter introduced by applying pressure in the system.

4. Conclusions

Our results have a close similarity to the usual FFLO approach for a superconductor in an external magnetic field. This was anticipated from the form of the dispersion relations, equation (18), where V enters formally as an external magnetic field[1]. However, the analogy with the usual FFLO stops there. The Green's functions in the present case have four poles, instead of two, and the numerator of the anomalous Green's function (equation (8)) is much more complex and includes an angular dependence. At the level of the Hamiltonian, equation (1), V mixes different states and from this point of view it acts like a *transverse field* and not as a polarizing longitudinal field. The latter only repopulates the states while the former changes the nature of the quantum states.

The FFLO phase in condensed matter systems has long been sought and now there is much evidence that it has been found in organic superconductors [20]. Here we point out the possibility of attaining an inhomogeneous superconducting state by applying pressure in a multi-band superconductor. The existence of quasi-particles belonging to different orbitals in a common Fermi surface provides a natural mismatch. It can be controlled by pressure and this, as we have shown, offers the possibility of finding new inhomogeneous superconducting states by tuning this external parameter. This zero field type of FFLO phase is distinct from the field induced FFLO state in that superconducting regions alternate with normal regions and not with spin-polarized ones as in the original proposal. Another mechanism for a zero field FFLO state has also been proposed [21]. In our case it is very useful that we can use pressure as a control parameter.

[1] See, for example, equation 2.13 of [17].

We have considered the simplest situation of an FF state with the modulation of the order parameter described by a single wavevector [1], although we referred to it generically as an FFLO state. In the original FF state a magnetic field raises the degeneracy of the spin up and down bands, introducing a mismatch between them. In our case, hybridization creates a repulsion between the bands, varying the mismatch of their Fermi wavevectors. In both cases the wavevector controlling the modulation of the order parameter is related to this mismatch and can be tuned by an external parameter, the magnetic field or pressure, respectively.

The study of heavy fermion superconductors probes the phase diagram of these systems in a large region of applied pressures and magnetic fields [22]. Many of these systems can be doped allowing one to tune the Fermi level and hybridization [23]. This type of study can be also carried out in inter-metallic systems, which are best candidates to observe the phase proposed here.

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