Coexistence of spin density wave, d-wave singlet and staggered $\pi$-triplet superconductivity

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Abstract
We have studied the competition and coexistence of staggered triplet superconductivity (SC) with d-wave singlet SC and spin density waves (SDWs) in the mean-field approximation. Detailed numerical studies demonstrate that particle–hole asymmetry mixes these states and therefore they are simultaneously present. Even more interesting were the results of our study of the influence of a uniform magnetic field. We observe novel transitions that show the characteristics of Fulde–Ferrel phases, yet they concern transitions to different combinations of the above orders. For example, above a given field, in a particle–hole symmetric system we observe a transition from d-wave singlet SC to a state in which d-wave singlet SC coexists with staggered triplet SC and SDWs. We believe our results may provide, among others, a direct explanation of recent puzzles about the Fulde–Ferrel like states that are apparently observed in CeCoIn$_5$.

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

1. Introduction

Some of the most intriguing research problems in the field of strongly correlated electrons concern the coexistence of superconductivity (SC) with itinerant antiferromagnetism, namely the spin density wave (SDW) state [1–3]. Most of the electronic systems that have been proposed to exhibit such a coexisting phase, are thought to be unconventional superconductors [4]. The quasi-one-dimensional organic salts based on TMTSF were the first to exhibit clearly the proximity of the SDW state with SC [5]. More recent experiments on the same salts have established that there is a region of macroscopic coexistence of these two phases [6]. Similar phenomena have also been observed in organic quasi-two-dimensional (quasi-2D) superconductors like $\kappa$–$(ET)_2$Cu(NCS)$_2$, high-$T_c$ oxides in the underdoped regime and heavy-fermion compounds such as uranium based UBe$_{13}$, UPt$_3$ or cerium based CeRhIn$_5$ just to name a few [7]. Many controversies still remain about the type of SC involved, and in particular whether SC is singlet or triplet.

In the present paper we study the coexistence of singlet d-wave SC with SDWs and in particular we focus on the induced staggered triplet SC component and new behavior that may result because of the presence of these three order parameters. Several studies of the competition of unconventional SC with SDWs and the possibility of an emergent staggered $\pi$-triplet pairing are available [8–13]. For example, in [10, 12] scattering by non-magnetic impurities is shown to stabilize a phase with all three order parameters (OPs) whereas in [11, 13] the induced $\pi$-pairing is studied in the context of deviations from half-filling.

We associate here for the first time the coexistence and competition of the above triplet of phases with the recent experimental evidence of a Fulde–Ferrel–Larkin–Ovchinnikov (FFLO) [14, 15] state in the high field–low temperature phase diagram regime of CeCoIn$_5$ [16, 17]. This quasi-2D compound has remarkable features separating it from other HF superconductors, such as the highest SC $T_c$ among all Ce and U compounds. Its gap symmetry is considered to be d-wave and its Fermi surface consists of quasi-cylindrical sheets (for a recent review, see [18]). There is no clear evidence so far for AFM ordering in CeCoIn$_5$. Nevertheless, its proximity to CeRhIn$_5$, which is an AFM unconventional
superconductor [7], and recent nuclear magnetic resonance (NMR) experiments suggest that CeCoIn$_5$ is close to a magnetic quantum critical point situated at a slightly negative pressure [19].

Using an eight component spinor formalism and a mean-field approach we study the influence of varying temperature, doping and external magnetic field on the competition of d-wave singlet SC with SDWs and staggered $\pi$-triplet SC. We have considered only the Zeeman splitting of an in-plane magnetic field which is the relevant term in the context of a FFLO formulation in a thin film superconductor whose thickness is smaller than its coherence length. In such a case, orbital effects can safely be neglected. The layered CeCoIn$_5$ meets well these requirements. Bearing in mind the above, we show how particle–hole asymmetry mixes the above states as proposed before in slightly different contexts. Most importantly, we produce novel field-induced transitions that bear remarkable similarities to the experimentally observed FFLO phases.

2. Model—formalism

Our starting point is the generalized mean-field Hamiltonian which corresponds to the coexistence of d-wave singlet SC, $\pi$-triplet (or $Q$-triplet) SC and SDW order parameters under the influence of an external magnetic field:

$$\mathcal{H} = \sum_{k,\alpha} \xi_{k\alpha} c_{k\alpha}^\dagger c_{k\alpha} - \sum_{k,\alpha,\beta} (\sigma \cdot n)_{\alpha\beta} M_k c_{k\alpha}^\dagger c_{k\beta} + \text{h.c.}$$

$$\mathcal{H} = \sum_{k,\alpha} \xi_{k\alpha} c_{k\alpha}^\dagger c_{k\alpha} - \sum_{k,\alpha,\beta} (\sigma \cdot n)_{\alpha\beta} M_k c_{k\alpha}^\dagger c_{k\beta} + \text{h.c.}$$

$$= \sum_{k,\alpha,\beta} \sum_{\alpha, \beta} \psi_{k, \alpha, \beta}^\dagger \mathcal{F}_{k, \alpha, \beta} \psi_{k, \alpha, \beta}$$

where $\alpha, \beta$ are spin indices, $M_k, \Delta_k$ and $\Pi_k$ are the SDW, the d-wave singlet SC and the $\pi$-triplet SC order parameters respectively, $\mu_B H$ is the Zeeman term for a static uniform field and $n$ is the polarization of the SDW which is taken parallel to that of the $\pi$-triplet SC spins and the external magnetic field.

We have chosen the $z$-axis components for our calculations.

For the odd in momentum spin triplet OP we have

$$\Pi^Q_k = -\Pi^{\bar{Q}}_k = \Pi_k$$

and $\Pi^{\bar{Q}}_k = \Pi_k$. Note that the triplet SC component that we consider is staggered, meaning that the SC pairs have a finite momentum. Similar $\pi$ operators were introduced in the past, i.e. by Yang Sun et al in an SU(4) model for HTC superconductivity [20], but, to our knowledge were first discussed by Psaltakis et al [10].

In the 2D tetragonal system that we consider here, the transformations with respect to $Q = (\pi, \pi)$ are fundamental. The wavevector $Q$ is commensurate meaning that translations from $k$ to $k + 2Q$ bring us back to the same place of the BZ. The electronic dispersion can be generally decomposed into periodic and antiperiodic terms with respect to $Q$: $\xi_k = \gamma_k + \delta_k$, where $\gamma_{k+Q} = -\gamma_k$ and $\delta_{k+Q} = \delta_k$. Here, as an example, we assume a single band tight-binding dispersion where $\gamma_k = -t_1 \cos k_x + \cos k_y$ and $\delta_k = -t_2 \cos k_x \cos k_y$. For $\delta_k = 0$ the system is particle–hole symmetric and perfectly nested at the wavevector $Q$. When $\delta_k < 0$ the system is considered (h)-doped and deviates from perfect nesting.

In order to treat all order parameters on the same footing we adopt an eight component spinor space formalism defined by the following spinor [10, 21]:

$$\psi_k^\dagger = (c_{k\uparrow}, c_{k\downarrow}, c_{-k\uparrow}, c_{-k\downarrow}, c^\dagger_{k+Q\uparrow}, c^\dagger_{k+Q\downarrow}, c_{-k-Q\uparrow}, c_{-k-Q\downarrow})$$

(2)

the following tensor products

$$\hspace{1cm}$$

with $\hat{\sigma}$ being the Pauli matrices, form a convenient basis for the projection of the Hamiltonian in this eight component spinor space.

In the above formalism and assuming all OPs real, our mean-field Hamiltonian is rewritten in the compact form:

$$\mathcal{H} = \sum_k \Psi_k^\dagger \tilde{H}_k \Psi_k$$

(4)

where

$$\tilde{H}_k = \gamma_k \hat{\tau}_3 \hat{\rho}_3 + \delta_k \hat{\rho}_3 - M_k \hat{\tau}_1 \hat{\rho}_3 + \Pi_k \hat{\tau}_2 \hat{\rho}_2 \hat{\rho}_1 + \Delta_k \hat{\tau}_2 \hat{\rho}_2 - \mu_B H \hat{\rho}_3 \hat{\sigma}_3$$

(5)

is the matrix of the system eigenenergies. The corresponding propagator reads:

$$\hat{G}_p(k, i\omega_n) = (-i\omega_n - \tilde{E}_k) \otimes [A(k', \omega_n) \hat{\tau}_2$$

$$+ 2i(\gamma_k(\delta_k - H \mu_B \hat{\rho}_3) \hat{\tau}_1$$

$$+ (\delta_k^2 + H^2 \mu_B^2 - H^2 \mu_B \hat{\rho}_3) \hat{\tau}_3)$$

$$\times \{B(k', \omega_n) + 4H \mu_B (-M_k \delta_k \hat{\rho}_3$$

$$+ \delta_k (\Delta_k + \Pi_k + \omega_n^2) \hat{\sigma}_3 \hat{\tau}_3)$$

$$+ 8 \mu_B \mu_B \hat{\rho}_3 \hat{\sigma}_3 [2M_k \delta_k \hat{\rho}_3 (\gamma_k^2 - \delta_k^2 + \Delta_k^2 - H^2 \mu_B^2) \Pi_k$$

$$- H \mu_B (\delta_k \Delta_k - M_k \Pi_k) \hat{\tau}_1 - \gamma_k (\delta_k \Delta_k - M_k \Pi_k) \hat{\sigma}_3 \hat{\tau}_2$$

$$- 4 A(k', \omega_n) H \mu_B (\delta_k \hat{\sigma}_3 \hat{\tau}_2 - \hat{\rho}_1 \hat{\tau}_2) \times D(k', \omega_n)$$

(6)

where

$$A(k', \omega_n) = M_k^2 + \gamma_k^2 - \delta_k^2 + \Delta_k^2 - H^2 \mu_B^2 + \Pi_k^2 + \omega_n^2$$

$$B(k', \omega_n) = A(k', \omega_n)^2$$

$$D(k', \omega_n) = (\omega_n^2 + E_{+}^2(k'))(\omega_n^2 + E_{-}^2(k'))$$

The poles of the Green function are the following:

$$E_{\pm}(k) = \mu_B H + \sqrt{M_k^2 + \gamma_k^2 + \delta_k^2 + \Delta_k^2 + \Pi_k^2 \pm \Gamma(k)}$$

$$E_{\pm}(k) = \mu_B H - \sqrt{M_k^2 + \gamma_k^2 + \delta_k^2 + \Delta_k^2 + \Pi_k^2 \pm \Gamma(k)}$$

$$\Gamma(k) = 2 \sqrt{(M_k^2 + \gamma_k^2) \delta_k^2 + 2 \delta_k M_k \Delta_k \Pi_k + (\gamma_k^2 + \Delta_k^2) \Pi_k^2}$$

\]
From the above we see that the $\delta_k$ term, when non-zero, induces additional terms that may help in the formation of new Fermi sheets when one of the branches goes to zero.

After projecting the above propagator on the different particle–hole and particle–particle channels, we arrive at the following system of coupled self-consistent equations obeyed by the three OPs:

$$M_k = T \sum_k \sum_n V_{kk}^{SDW} \times \{ M_k(C(k', \omega_n) + 2\Lambda(k', \omega_n)^2 \delta_k^2
- 4A(k', \omega_n)\delta_k^2(M_k^2 + \gamma_k^2 - \delta_k^2)
+ 16\delta_k^2(\Delta_k \Pi_k + \mu_h^2 H^2 \omega_n^2)
- 2\delta_k^2 \sum_\Pi_k k_\Pi (A(k', \omega_n)^2
- f 4(\gamma_k^2 + \Delta_k \Pi_k + \mu_h^2 H^2 \omega_n^2
- \delta_k^2(\Delta_k - \mu_h^2 H^2 + \Pi_k + \omega_n^2)) \times D(k', \omega_n) \}
$$

$$\Delta_k = T \sum_k \sum_n V_{kk}^{SC} \{ \Delta_k \{ C(k', \omega_n) + 2\Lambda(k', \omega_n)^2 \Pi_k^2
- 4A(k', \omega_n)\Delta_k^2 - H^2 \mu_h^2 + 5\Pi_k^2 + \omega_n^2
+ 8[3M_k^2 \delta_k^2 \Delta_k \Pi_k - 3M_k \delta_k \Delta_k \Pi_k
+ (\gamma_k^2 + \Delta_k \Pi_k + \delta_k^2)(3\gamma_k^2 + 4\Delta_k^2)
- 3H^2 \mu_h^2 + 3\Pi_k^2 - \delta_k^2(\Delta_k - H^2 \mu_h^2 + 3\Pi_k^2)
- (\delta_k^2 + H^2 \mu_h^2 \Pi_k + \delta_k^2(\Delta_k^2 - 3H^2 \mu_h^2 - 3\Pi_k^2))\omega_n^2)
+ 2\delta_k^2 M_k \sum_\Pi_k \{ A(k', \omega_n)^2 - 4(\gamma_k^2 + \Delta_k \Pi_k
+ H^2 \mu_h^2(\delta_k^2 - \delta_k^2(\Pi_k + \omega_n^2))\times D(k', \omega_n) \}
$$

$$\Pi_k = T \sum_k \sum_n V_{kk}^{Or} \{ \Pi_k \{ C(k', \omega_n) + 2\Lambda(k', \omega_n)^2 \Pi_k
- 8\delta_k^2 M_k \sum_\Pi_k \{ A(k', \omega_n)^2 - 4\Pi_k^2
+ 2\delta_k^2 \Delta_k \Pi_k - 4H^2 \mu_h^2 \omega_n^2
+ 4\delta_k^2(\Delta_k - H^2 \mu_h^2 + 3\Pi_k^2)\omega_n^2) \times D(k', \omega_n) \}
$$

Where

$$C(k', \omega_n) = \Lambda(k', \omega_n)A(k', \omega_n)^2 + 2\Lambda(k', \omega_n)^2 (\gamma_k^2 + \Delta_k \Pi_k + 4\mu_h^2 H^2 \omega_n^2),$$

Close inspection of the above equations reveals that they have the following structure:

$$M_k = \sum_n \sum_k V_{kk}^{SDW} [M_k \{ \cdots \delta_k \Delta_k \Pi_k \{ \cdots \} \}
$$

$$\Delta_k = \sum_n \sum_k V_{kk}^{SC} [\Delta_k \{ \cdots \delta_k M_k \Pi_k \{ \cdots \} \}
$$

$$\Pi_k = \sum_n \sum_k V_{kk}^{Or} [\Pi_k \{ \cdots \delta_k M_k \Delta_k \{ \cdots \} \}
$$

On the right-hand side of each of the gap equations, there are terms which are not proportional to the gap of the left-hand side. When there is particle–hole asymmetry, then if two of the order parameters are non-zero, zero is not a trivial self-consistent solution for the third order parameter which has to be non-zero as well. Furthermore, the induced term by p–h asymmetry is even in frequency, so we expect it not to vanish after the summation on the Matsubara frequencies. Therefore, in the presence of both SDW and d-wave singlet SC orderings, particle–hole asymmetry would imply the presence of a staggered $\pi$-triplet SC component. Similar arguments are presented in [13] in a slightly different context. Here we stress that particle–hole asymmetry or the $\delta_k$ term does the mixing.

The summations on the Matsubara frequencies are done analytically and the self-consistent gap equations on the real axis were solved numerically to illustrate the mixing of the three order parameters.

3. Numerical results—discussion

We assume a tight-binding dispersion relation on a 2D square lattice up to the next nearest (n.n.) neighbors. We set the nearest neighbors hopping term $t_1 = 1.0$ and vary the n.n. term $t_2$ which is the relevant parameter for particle–hole asymmetry or doping. The value of $t_1$ sets the energy scale in our calculations. The effective potentials are generally decomposed into a momentum dependent part, which includes any proper form factors, and a constant part which sets the amplitude of the coupling strength. We emphasize that in this study the SDW component is taken to be isotropic and the SC components anisotropic assuming a d-wave pairing. As an interesting example, we report our results for the case when the above OPs have potentials of equal amplitude that cause a moderate coupling, favoring a ground state of coexisting d-wave SC and SDW components. Such a situation is realized when $V^{SDW} = V^{SC} = V^{Or} = 3$. This scenario resembles the case where $T_c > T_N$ in [22]. Notice that we have chosen blue, green and red coloring to discern the SDW, d-wave singlet SC and SDW components. As an interesting example, we report our results for the case when the above OPs have potentials of equal amplitude that cause a moderate coupling, favoring a ground state of coexisting d-wave SC and SDW components. Such a situation is realized when $V^{SDW} = V^{SC} = V^{Or} = 3$. This scenario resembles the case where $T_c > T_N$ in [22]. Notice that we have chosen blue, green and red coloring to discern the SDW, d-wave singlet SC and SDW components.
Figure 1. (a) An example of how p–h asymmetry induces a staggered $\pi$-triplet SC component (red or the lower surface). No external field is assumed here ($\mu_B H = 0$). We note that when we have perfect nesting (i.e. $t_2 = 0$) there is at low temperatures coexistence of SDWs with d-wave singlet SC (blue and green respectively or the surface that takes the higher values and the one that develops at higher temperatures, respectively) and above a given temperature we have a transition to a state where only d-wave singlet SC is present. We note that the staggered $\pi$-triplet SC component (red or the lower surface) appears for $t_2 \neq 0$. In fact with $t_2 \neq 0$ it is impossible to obtain any of the two order parameters coexisting without the third one, whatever the choice of the effective potentials or the exact electronic dispersions. (b) We present two different 2D cuts on the previous 3D figure, one for $t_2 = 0$ (full lines) and the other one for $t_2 = 0.5$ (dashed lines). Note that while particle–hole asymmetry has negligible influence on the temperature behavior, it induces the staggered $\pi$-triplet component almost at the same temperature at which the d-SC–SDW coexistence would arise.

Figure 2. (a) We illustrate the influence of a uniform magnetic field in a particle–hole asymmetric system ($t_2 = 0.5$). With no external field (full lines) the system exhibits the coexistence of the three OPs below a given temperature. At a finite external field (dashed lines), the three order parameters arise simultaneously in a first order transition at the same temperature. The field reduces drastically the SDW (blue or the curve that takes the higher values at low-T) producing a dominant $\pi$-triplet SC component (red) in the low-T regime. (b) The field dependence of the OPs at the ground state ($T = 0$) and half-filling ($t_2 = 0$). Varying the magnetic field we induce a first order transition from the SDW + d-SC state to a mixed singlet–triplet SC order. This transition exhibits many similarities to the transitions to an FFLO state. In the FFLO state is considered to be a singlet state, whereas our staggered state is triplet. Moreover, in the FFLO state there are regions of the Fermi surface (FS) which are superconducting and regions of the FS which are not gapped etc (they are normal). In our case, all regions of the FS are gapped. This is in fact a transition to a novel SC state in which singlet and triplet staggered components coexist. Note that this last coexistence does not require the presence of particle–hole asymmetry. If the system was particle–hole asymmetric, the high field state would involve a weak SDW component as well since, as we have noticed, it is impossible to observe any pair of the above components without the third one.

4. Conclusions

In conclusion, we have shown that particle–hole asymmetry mixes d-wave singlet SC with $\pi$-triplet staggered SC and SDWs. We may either observe one of them, or else all three of them. As a result, in any SDW superconductor there are both singlet and staggered triplet superconducting components. This may be behind the unsettled controversies about the parity of the order parameter in many of the SDW superconducting systems. Moreover, we have shown that the application of a uniform external magnetic field induces new transitions that exhibit remarkable similarities with the Fulde–Ferrel phases.
We believe that our new SC states, where basically d-wave singlet SC and staggered $\pi$-triplet SC coexist, the latter being dominant, may be in fact behind the signatures of FFLO phases that are reported in Ce based heavy-fermion compounds.

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