Magnetic field induced pattern of coexisting condensates in the superconducting state of CeCoIn$_5$

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In usual superconductors the carriers form Cooper pairs [1] that have zero total momentum meaning that the superfluid density is homogeneous. We know for decades that it is a priori possible to observe at high fields the Fulde-Ferrel-Larkin-Ovchinnikov (FFLO) [2, 3] state in which the superfluid density exhibits a field dependent modulation. The search for such inhomogeneous condensates in real materials is the subject of tremendous excitement especially after the discovery of a promising high-field superconducting (HFSC) phase in CeCoIn$_5$ [4]. However, subsequent neutron [5] and NMR [6, 7] experiments contradicted the FFLO picture in CeCoIn$_5$ establishing a puzzling coupling of the distinct HFSC state with a magnetic modulation [8]. Here we show that, a novel type of exotic state is observed at high fields in CeCoIn$_5$ in which a pattern of coexisting condensates manifests. The specific pattern includes the d-wave singlet SC state, the staggered $\pi$-triplet SC state, and Spin Density Waves (SDW). Because of particle-hole asymmetry these three condensates may either appear separately or all three together providing a new perspective on antiferromagnetic superconductors that may include high-$T_c$ cuprates and pnictides. The field induced transition to the pattern state in CeCoIn$_5$ is only a paradigm of a generic mechanism that prevents the elimination of the dominating condensate by the field via the formation of a pattern of condensates. This opens new avenues for the search of exotic states not only in electronic systems, but also in other systems where inhomogeneous condensates are actively discussed like trapped atomic fermi gases [8] and dense quark matter.

Among the CeMIn$_5$ class of heavy-fermion superconductors (M=Ir,Rh,Co), CeCoIn$_5$ exhibits the highest superconducting $T_c$ at ambient pressure (2.3K) [10]. The zero field SC gap symmetry is established to be of $d_{x^2-y^2}$-wave type [11]. A distinct HFSC state is observed initially thought to be a realization of the FFLO state. Recent neutron diffraction data in the HFSC state of CeCoIn$_5$ show clearly that an almost commensurate SDW at $Q=(q,q,0.5)$ develops at the onset of the HFSC region and disappears at the same upper critical field with SC in a first order transition. Moreover, the modulation wavevector is not coupled to the magnitude of the external magnetic field ruling out the FFLO mechanism that produces superfluid density modulations that scale with the field. The neutron results agree with previous NMR results [6, 7] that reported SDW ordering in the HFSC state and find no signature of normal state regions required by the FFLO picture. Finally, in conflict with the FFLO expectations, the critical fields for entering the HFSC phase grow with temperature and this behavior becomes more pronounced as we apply pressure [12].

The above facts signal the field induced coexistence of staggered $\pi$–triplet SC with d-wave singlet SC and SDW. The staggered $\pi$–triplet SC component has some similarity with the FFLO state in the sense that the pairs have a finite momentum and therefore the superfluid density is modulated as well. However, it is fundamentally different on basic points. Firstly, it is a spin triplet SC state meaning that the paired quasiparticles have antiparallel spin as in usual Cooper pairs. Secondly, the wavevector $Q$ of the superfluid modulation is driven by the nesting properties of the dispersion and is common with that of the SDW modulation while in the FFLO picture the wavevector is driven by the field. Finally, our staggered triplet SC state coexists with the d-wave singlet SC state and the SDW state, whereas the FFLO state is in fact a coexistence between singlet SC and normal state regions on different portions of the Fermi surface.

The possibility of a dynamically generated $\pi$-triplet order parameter when singlet SC coexists with SDW has already been considered [13, 14, 15, 16, 17]. It has been shown [13, 19] that particle-hole asymmetry is enough to induce the third order parameter whenever the other two are present and in this respect the three condensates form a pattern [19]. Clearly, our findings may be relevant for any antiferromagnetic superconductor and this includes high-$T_c$ cuprates and iron pnictides. Moreover, the staggered $\pi$-triplet SC state may also manifest in the ferromagnetic superconductor UGe$_2$ [20].

Our analysis is absolutely generic, free of any model assumption. We consider the simplest hamiltonian mean field scheme that includes the relevant order parameters and the Zeeman field. The orbital effect of the field is irrelevant for the phenomena that we report, and like for the FFLO states, results concern Pauli limited superconductors where orbital effects are not dominating. Our only requirement is to treat the involved order parameters on the same footing. This is obtained using an eight component spinor that leads to an $8 \times 8$ matrix Green’s function formalism treated elsewhere [13]. The poles of...
The letters $M$, $\Delta_k$ and $\Pi_k$ refer to the order parameters for the Spin Density Wave, d-wave singlet SC and $\pi$-triplet SC, respectively. The $\pi$-triplet order parameter corresponds to Cooper pairs having a finite total momentum equal to the nesting wavevector $Q$. It has the attributes: $\Pi_k = -\Pi_{k+Q} = \Pi_{k'} = \Pi_{-k}$ and because $Q$ is commensurate this triplet SC order parameter is even in Parity. Indeed, our d-wave singlet and staggered $\pi$-triplet SC states share the same nodal structure and therefore, their coexistence is not contradicting the inversion symmetry. The kinetic energy is decomposed into a sum of periodic $\delta_k + Q = \delta_k$ and antiperiodic $\gamma_k + Q = -\gamma_k$ terms on $Q$ translations which is also the commensurate nesting wavevector for the SDW. When $\delta_k = 0$ there is perfect nesting and particle-hole symmetry. Finally $H$ is the Zeeman field where we have set $\mu_B = 1$.

The resulting system of coupled self-consistent gap equations is rather cumbersome exhibiting a peculiar general structure:

$$M = \sum_{k} \sum_{k'} V^{SDW}_{kk'} \left\{ \left\{ \frac{M'}{...} + \delta_k' \Delta_k \Pi_k' \{ ... \} \right\} \right\}$$

$$\Delta_k = \sum_{k} \sum_{k'} V^{dSC}_{kk'} \left\{ \Delta_k' \{ ... \} + \delta_k' M k \Pi_k' \{ ... \} \right\}$$

$$\Pi_k = \sum_{k} \sum_{k'} V^{tr}_{kk'} \left\{ \Pi_k' \{ ... \} + \delta_k' M k \Delta_k' \{ ... \} \right\}$$

where the $n$ sum is on the Matsubara frequencies and $V^{SDW}$, $V^{SC}_{kk'}$, $V^{tr}_{kk'}$ are the effective pairing potentials in the respective symmetry channels. If the dispersion is particle-hole asymmetric where $\delta_k \neq 0$, in none of the above equations we have zero as a self-consistent solution if the other two order parameters are non-zero and naturally the potentials are non-zero as well. In such a system we may either have one or all three order parameters simultaneously present. This is a generic result of relevance for all antiferromagnetic superconductors. The three order parameters, constitute a pattern of condensates. Note that there are numerous other patterns of different order parameters that behave similarly \[19\]. For example, SDW, CDW and FM form a similar pattern suggested as a possible explanation for the CMR phenomenon in manganites \[23\].

The system of self-consistent gap equations is solved numerically on a square lattice with $\gamma_k = \frac{35}{2}$ whereas that in the particle-hole symmetric case \[t' = 0\]. Note that in the particle-hole symmetric case there is no SDW order induced and the critical field of the step-like transition is rather temperature independent or even reduced with temperature. In the inset is shown the corresponding phase diagram in the particle-hole symmetric case ($t' = 0$).
the external field in the particle-hole symmetric case \( t' = 0 \) (dashed lines) and in a particle-hole asymmetric case \( t' = 0.35 \) (full lines). With green, red and blue color we discern the d-wave singlet SC, the \( \pi \)-triplet SC and the SDW gap amplitude respectively. Notice how the coexistent regime is largely expanded with \( t' \). To illustrate this effect we plot in the inset the \( \pi \)-triplet gap as a function of field for \( t' = (0, 0.15, 0.25, 0.35) \).

\[-t (\cos k_x + \cos k_y)\] and \( \delta_k = -t' \cos k_x \cos k_y \) where \( Q = (\pi, \pi) \). For convenience, separable pairing potentials of the form \( V_{k'k} = V_{fkk'} \) have been used, where in our case \( f_k \) are d-wave form factors, \( f_k = \cos k_x - \cos k_y \). A thorough exploration of the combinations of potentials has been done numerically and we have found that there is a fairly big parameter space where the system is a d-wave singlet superconductor in the ground state. At a sufficiently high field, remarkable transitions to a mixed phase of all three order parameters are triggered. As a paradigm, we present in Fig. 1 results obtained with \( V^{WDW} = V^{SC} = V^{\pi tr} = 1.5t \) and particle-hole asymmetry \( t' = 0.35 \). At low temperatures we observe two successive first order transitions with the field. The first of them is from a high value of \( \Delta \) to a smaller value of \( \Delta \). In this step-like regime the staggered triplet \( \Pi \) gap and the SDW M gap appear simultaneously. At a higher field we have the second first order transition at which all three order parameters are eliminated simultaneously.

The resulting H-T phase diagram is reported in the main panel of Fig. 2. The HFSC region in which the full pattern of coexisting condensates is present corresponds to the \( Q \)-phase in CeCoIn$_5$. At the highest critical field the three order parameters are simultaneously eliminated in a first order transition as observed by neutrons.

Remarkably, in the absence of particle-hole asymmetry \( t' = 0 \) (inset of Fig. 2) the SDW order is absent from the field-induced state. The SDW order is induced only because of particle-hole asymmetry given the peculiar structure of the coupled self-consistent gap equations discussed above. The mechanism that drives the \( Q \)-phase in CeCoIn$_5$ is, therefore, the following: to survive at the highest possible magnetic fields the d-wave singlet SC condensate, develops an even in Parity, staggered in \( Q \) and odd in translation triplet superconducting component with the same nodal structure (i.e. the \( \pi \)-triplet component) with which it coexists. Particle-hole asymmetry forces the presence of the third order parameter, the SDW condensate. The full pattern of condensates appears at high fields when the dominating condensate, the d-wave singlet, is "weakened" sufficiently by the Zeeman field. Therefore, the emergence of the pattern of condensates can be viewed as an escapeway from the formation of a magnetic quantum critical point associated with the elimination of the dominant condensate.

Comparing the phase diagrams in Fig. 2 we note that the coexistence "dome" expands with \( t' \) as shown explicitly in Fig. 3. The poles of the Green’s function provide a straightforward explanation for this behavior. When

\( V_{fkk'} = 0 \) (full lines). With green, red and blue color we discern the d-wave singlet SC, the \( \pi \)-triplet SC and the SDW gap amplitude respectively. Notice how the coexistent regime is largely expanded with \( t' \). To illustrate this effect we plot in the inset the \( \pi \)-triplet gap as a function of field for \( t' = (0, 0.15, 0.25, 0.35) \).

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$E_-(k) = 0$ the superconductor reaches its Clogston limit \cite{Clogston1957} and the transition to the multicomponent state is triggered. For higher $\delta_k$, smaller critical fields $H_c$ are necessary for reaching $E_-(k) = 0$ as confirmed by our numerical calculations. This behavior has been observed by applying pressure in CeCoIn$_5$ \cite{Kotetes2006} and we may naturally simulate the effect of pressure as creating more deviations from nesting and therefore more particle-hole asymmetry $\delta_k$.

Tedious calculations led to self-consistent NMR Knight shift and relaxation rates as a function of temperature and field. Characteristic results reported in Fig. 4 are for the same parameters as in Fig. 1 for three characteristic fields ($H = 0.21$, $H = 0.41$ and $H = 0.51$). There is a remarkable agreement with the experimental results \cite{Kotetes2005, Kotetes2006} depicted in the inset of the upper panel. Note the signature of the triplet component and the signature of the first order transition to the Q-phase in the self-consistent calculation and in the experiment. The coexistence of singlet and triplet components evident in the NMR data would be a priori excluded by the inversion symmetry. Only because $Q$ is commensurate the staggered $\pi$-triplet condensate can coexist with the d-wave singlet condensate with which it shares the same nodal structure.

The field induced transition to the pattern state is obtained through an absolutely generic mean field scheme. Therefore, field induced patterns have a generic character and should be viewed as potential alternatives to the FFLO picture not only in superconductors. Complexity in electronic matter is proven to be crucially important. Our findings provide a new perspective in research areas as diverse as the trapped Fermi gases \cite{Coleman2008} and situations of dense quark matter in QCD \cite{Giorgini2008} where inhomogeneous condensates are very actively investigated.

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