Order parameter and vortices in the superconducting $Q$-phase of CeCoIn$_5$

D.F. Agterberg$^1$, M. Sigrist$^2$, and H. Tsunetsugu$^3$

$^1$ Department of Physics, University of Wisconsin-Milwaukee, Milwaukee, WI 53211
$^2$ Theoretische Physik ETH-Hönggerberg CH-8093 Zürich, Switzerland and
$^3$ Institute for Solid State Physics, University of Tokyo, Kashiwa, Chiba 277-8581, Japan

Recently, it has been reported that the low-temperature high-magnetic field phase in CeCoIn$_5$ ($Q$-phase), has spin-density wave (SDW) order that only exists within this phase. This indicates that the SDW order is the result of the development of pair density wave (PDW) order in the superconducting phase that coexists with $d$-wave superconductivity. Here we develop a phenomenological theory for these coexisting orders. This provides selection rules for the PDW order and further shows that the detailed structure of this order is highly constrained. We then apply our theory to the vortex phase. This reveals vortex phases in which the $d$-wave vortex cores exhibit charge density wave (CDW) order and further reveals that the SDW order provides a unique probe of the vortex phase.

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The low-temperature high-magnetic field phase in CeCoIn$_5$ ($Q$-phase) has been thought to be the best example of a FFLO superconductor [1, 2, 3, 4] and has thus generated a tremendous interest [5, 6]. However, the recent measurements of Kenzelmann et al. [7], is pair density wave (PDW) superconductivity. If the SDW order is associated with a wavevector $Q$, then the PDW order must have the wavevector $-Q$ to be able to induce the SDW order. The SDW order has $Q = (q, q, 0.5)$, which is too large to be a consequence of the long-wavelength modulation of a FFLO phase [2, 3, 4, 8]. The PDW order is more akin to the $\pi$-triplet staggered pairing suggested by Aperis [9] or to the PDW order suggested in La$_{2-x}$Ba$_x$CuO$_4$ at $x = 1/8$ [10]. The ensuing physical picture is then a $d$-wave superconductor at low fields with PDW order appearing through a second order phase transition at high fields. These two types of superconducting order will coexist in the $Q$-phase.

The observation of this PDW order raises a series of deep questions about the origin of this phase. To help address these, we have developed a phenomenological theory for this PDW order. Our approach complements that given by Kenzelmann et al. and is based on irreducible representations of the full space group. We find that this theory strongly constrains the PDW order and provides useful information about the vortex phase.

**PDW superconducting order parameter:** Our approach is to classify the PDW order in terms of irreducible representations of the full space group [13]. For CeCoIn$_5$ this is $P4/mmm$. For order appearing at a wavevector $Q$, the order parameter is defined by the irreducible representations of $G_Q$ (set of elements conserving $Q$) and the star of the wavevector $Q$ (set of wavevectors symmetrically equivalent to $Q$). For $Q = (q, q, 0.5) = (q, q, -0.5)$ $G_Q = \{E, C_{2n}, \sigma_z, \sigma_\ell\}$ with $C_{2n}$ the 180°-rotation around the axis $(1, 1, 0)$, $\sigma_z$ and $\sigma_\ell$ the mirror operations at the basal plane and the plane perpendicular to $(1, -1, 0)$, respectively. Note $(0, 0, 1)$ is a reciprocal lattice vector. In Table I, we give the irreducible representations of $G_Q$ together with representative basis functions for spin-singlet pairing (scalar functions $\psi(k)$ [11]), spin-triplet pairing (vector functions $d(k)$ [11]), and spin density order $(S_j)$.

To define the additional order parameter components at the wavevectors in the star of $Q$ we use the elements $\{E, C_4, C_4^2, C_4^3\}$ (these give the star of $Q$, $\{Q_1, Q_2, Q_3, Q_4\}$ respectively, as shown in Fig. 1). This then defines a superconducting order parameter with four components which we define as $\Delta_{\Gamma} = (\Delta_{\Gamma, Q_1}, \Delta_{\Gamma, Q_2}, \Delta_{\Gamma, Q_3}, \Delta_{\Gamma, Q_4})$. With these definitions, the symmetry properties of the order parameter are given as follows ($D_{\Gamma}(q)$ defined in Table I): translation $T$, $\Delta_{\Gamma, Q_j} \rightarrow e^{iQ_j T} \Delta_{\Gamma, Q_j}$ ($\Delta_{\Gamma, Q_j} \rightarrow e^{-iQ_j T} \Delta_{\Gamma, Q_j}$); time-reversal operation $\Delta_{\Gamma, Q_j} \rightarrow \Delta_{\Gamma, -Q_j}$. Moreover,
TABLE I: Representative spin-singlet, spin-triplet, and spin density basis functions for the different irreducible representations that have momentum $Q_1 = (q, q, 0.5)$.  

| Irrep ($\Gamma_i$) | $D_{\Gamma_i}(E)$ | $D_{\Gamma_i}(\sigma_z)$ | $D_{\Gamma_i}(C_{2q})$ | $D_{\Gamma_i}(\sigma_z)$ | Representative $\psi(k)$ | Representative $d(k)$ | Representative $S_i$ |
|-------------------|------------------|------------------|------------------|------------------|------------------|------------------|------------------|
| $\Gamma_1$       | 1                | 1                | 1                | 1                | $s, k_x k_y$      | $\hat{z}(k_x - k_y), k_z (\hat{x} - \hat{y})$ | $S_z$           |
| $\Gamma_2$       | 1                | 1                | -1               | -1               | $k_x^2 - k_y^2$   | $\hat{z}(k_x + k_y), k_z (\hat{x} + \hat{y})$ | $S_z$           |
| $\Gamma_3$       | 1                | -1               | 1                | -1               | $k_x (k_x + k_y)$ | $\hat{x} k_x - \hat{y} k_y, \hat{x} k_y - \hat{y} k_x$ | $S_x - S_y$    |
| $\Gamma_4$       | 1                | -1               | 1                | -1               | $k_x (k_x - k_y)$ | $\hat{x} k_x + \hat{y} k_y, \hat{x} k_y + \hat{y} k_x$ | $S_x + S_y$    |

The transformations $G_Q$ lead to

$$
C_4 : \quad D_{\Gamma_i}(C_4)(\Delta_{\Gamma_1},Q_1, \Delta_{\Gamma_2},Q_2, \Delta_{\Gamma_1},Q_3, \Delta_{\Gamma_4},Q_4) \\
\sigma_z : \quad D_{\Gamma_i}(\sigma_z)(\Delta_{\Gamma_1},Q_1, \Delta_{\Gamma_2},Q_2, \Delta_{\Gamma_3},Q_3, \Delta_{\Gamma_4},Q_4) \\
C_{2Q} : \quad D_{\Gamma_i}(C_{2Q})(\Delta_{\Gamma_1},Q_1, \Delta_{\Gamma_2},Q_2, \Delta_{\Gamma_3},Q_3, \Delta_{\Gamma_4},Q_4) \\
\sigma_\zeta : \quad D_{\Gamma_i}(\sigma_\zeta)(\Delta_{\Gamma_1},Q_1, \Delta_{\Gamma_2},Q_2, \Delta_{\Gamma_3},Q_3, \Delta_{\Gamma_4},Q_4)
$$

(1)

Table II reveals that both singlet and triplet order parameters belong to the same representation which implies that singlet and triplet superconductivity are mixed. This mixing is due to spin-orbit coupling which cannot be justifiably ignored in CeCoIn$_5$. Formally, this is a consequence of the fact that $G_Q$ does not contain inversion symmetry. Previous studies have examined the development of singlet-triplet mixing in related situations [12-14], often through Lifshitz invariants that appear in the Ginzburg Landau free energy when parity symmetry is broken. We have confirmed that our formalism yields the same results as through the use of Lifshitz invariants.  

**Free Energy and PDW solutions:** We use a Ginzburg Landau theory to describe the PDW and $d$-wave order parameters. While this will not be reliable on a quantitative level, it will allow us to correctly identify the properties of the PDW order and make robust experimental predictions. The PDW Ginzburg Landau free energy density is constructed by imposing invariance under the above symmetries (note that this free energy density is the same for all $\Gamma_i$).

$$
f = \alpha \sum_i [\Delta_{\Gamma_i},Q_i]^2 + \beta_1 (\sum_i |\Delta_{\Gamma_i},Q_i|^2)^2 + \beta_2 \sum_i |\Delta_{\Gamma_i},Q_i|^2 |\Delta_{\Gamma_i},Q_j|^2 + \beta_3 (|\Delta_{\Gamma_i},Q_j|^2 |\Delta_{\Gamma_i},Q_j|^2 + |\Delta_{\Gamma_i},Q_3|^2 |\Delta_{\Gamma_i},Q_4|^2) + \beta_4 |\Delta_{\Gamma_i},Q_1, \Delta_{\Gamma_i},Q_2, \Delta_{\Gamma_i},Q_3, \Delta_{\Gamma_i},Q_4|^2 + \kappa_1 \sum_i [D_{\Delta_{\Gamma_i},Q_i}]^2 + \kappa_2 \sum_i (-1)^i [D_{\Delta_{\Gamma_i},Q_i}]^2 + \kappa_3 \sum_i [D_{\Delta_{\Gamma_i},Q_i}]^2 + \kappa_4 \sum_i [D_{\Delta_{\Gamma_i},Q_i}]^2 + \frac{1}{2} (\nabla \times A)^2
$$

(2)

where $D = -i \nabla - 2 e A$, $B = \nabla \times A$, $D_1$ corresponds to the $(1, 1, 0)$, and $D_2$ to the $(1, -1, 0)$ direction. The free energy density for the $d$-wave order parameter is taken to be:

$$
f_d = \alpha_d |\Delta_d|^2 + \beta_d |\Delta_d|^4 + \kappa D |\Delta_d|^2 + \kappa_c |D_{\Delta_d}|^2
$$

(3)

The coupling between these order parameters is given by (note that this coupling is the same for all $\Gamma_i$):

$$
f_c = \beta_c \sum_i [|\Delta_{\Gamma_i}|^2 |\Delta_{\Gamma_i},Q_i|^2 + \beta_2 [\Delta_{\Gamma_i}^3 (\Delta_{\Gamma_i},Q_1, \Delta_{\Gamma_i},Q_3, \Delta_{\Gamma_i},Q_5, \Delta_{\Gamma_i},Q_4)] + c.c.
$$

(4)

This free energy is similar to one studied earlier in the context of PDW order in Ref. [12]. The "homogeneous" phase in the absence of a magnetic field has five PDW states distinct by symmetry, if we ignore the $d$-wave phase (the phase factors $\phi_1$, $\phi_2$, and $\phi_3$ are not determined by the free energy):

$$
\Delta_{\Gamma_1}^{(1)} = (e^{i \phi_1}, 0, 0, 0) \\
\Delta_{\Gamma_1}^{(2)} = (e^{i \phi_2}, e^{i \phi_1}, 0, 0) \\
\Delta_{\Gamma_1}^{(3)} = (e^{i \phi_3}, 0, e^{i \phi_2}, 0) \\
\Delta_{\Gamma_1}^{(4)} = (e^{i \phi_4}, e^{i \phi_2}, e^{i \phi_3}, e^{i (\phi_1 + \phi_3 - \phi_2)}) \\
\Delta_{\Gamma_1}^{(5)} = (e^{i \phi_5}, e^{i \phi_4}, e^{i \phi_2}, e^{i (\phi_1 + \phi_3 - \phi_2)}).
$$

(5)

This set is reduced to $\Delta_{\Gamma_1}^{(3)}$ and $\Delta_{\Gamma_1}^{(4)}$ in the presence of a $d$-wave order parameter [12]. Finally, a magnetic field in the basal plane along the $(1, 1, 0)$-direction favors the state $\Delta_{\Gamma_1}^{(3)}$ as it removes the degeneracy between the $Q_1$ and $Q_2$ wavevectors (the pairs $Q_1, Q_3$, and $Q_2, Q_4$
remain degenerate). As an example we assume that the field lies along (1,−1,0)-direction and yields the state (0,e^{i\phi_2},0,e^{i\phi_4}). Choosing \(\phi_2 = \phi_4 = 0\), the spatial dependence of the PDW order is given by \(\Delta_{d,R}\cos(Q_2 \cdot R)\). In view of the coupling to the d-wave order parameter the relative phase between \(\Delta_d\) and \(\Delta_{d,R}\) can be either 0 (\(\pi\)) or \(\pm\pi/2\) \([12]\) which are both permitted by the free energy. Generally, the combined PDW and d-wave superconductivity must then take one of two forms when vortices are ignored: \(\Delta_d + |\Delta_{d,R}|\cos(Q_2 \cdot R)\) (time reversal violating phase) or \(\Delta_d + |\Delta_{d,R}|\cos(Q_2 \cdot R)\) (time-reversal invariant phase).

Coupling to spin-density wave: The SDW order can be induced through the combined PDW and d-wave superconductivity \([2]\). We assume here that the SDW is sufficiently weak so as to not alter the free energy significantly. The free energy density for the SDW order is given by \(\Delta_{s1,2}\Gamma\cos(Q_2 \cdot R)\). In view of the coupling to the d-wave vortex cores of the two PDW degrees of freedom \(\Delta_{d,R}\), we find that there exist stable phases where this happens. These phases are defined by the relative displacements \(\tau_i\) of the PDW vortex cores from the d-wave vortex cores. In such phases, the d-wave vortex cores exhibit CDW order. (ii) The SDW order leads to Bragg peaks that are determined by the reciprocal lattice vectors of the vortex lattice and the displacements \(\tau_i\) (see Eq. 14).

For a detailed derivation of the above results, we carry out the simplest realistic analysis. We assume that the correlation length of the spin-density order is much smaller than the coherence length of the superconducting order. We take Eq. 7 as the term driving the SDW order (the same arguments can be applied if Eq. 6 is used). From this we obtain

\[
S_{dR}^z(R) = \frac{\gamma_1 H_1}{\alpha_n} [\Delta_{d(R)}^* \Delta_{d,R}(R) + \Delta_{d}(R) \Delta_{d,R}^*(R)].
\]

The spatial dependence of the PDW and d-wave order parameter can now be determined in the high-field limit for which the field \(H\) may be considered uniform. From Eq. 8 one finds that the d-wave component yields an Abrikosov vortex lattice. Using \(z \) to represent the (0,0,1)- and \(x\) the (1,1,0)-direction, the vortex lattice solution can be given by

\[
\Delta_d(\tilde{x},\tilde{z}) = \Delta_{d0} \sum_n c_n e^{iq(n-1/2)\tilde{x}} e^{-i(z-z_n)^2/\kappa^2}
\]

where \(\tilde{x} = x/\epsilon, \tilde{z} = \epsilon z\), the vortex lattice in the coordinates \(\tilde{x},\tilde{z}\) has the basis vectors \(a = (a,0)\) and \(b = b(\cos \alpha, \sin \alpha)\) \([19]\), \(c_n = e^{i\pi \rho_{n}^2 - i\pi \tau_{n}(n+1)}, q = 2\pi/\alpha, z_n = b \sin \alpha(n + 1/2), \rho = (b/a) \cos \alpha, \) and \(\epsilon = [(\kappa - \kappa_c)/\kappa]^{1/4}\). The parameter \(\epsilon\) scales lengths in the \(x\) and \(z\) directions to take the anisotropy into account. This solution is an \(n = 0\) eigenstate of the operator \(\tilde{D}^2 = D^2 + D_z^2 = (-i\nabla - 2eA)^2\) with eigenvalues \((2n + 1)/\kappa^2\) and \(l^2 = \Phi_0/(2\pi H) (n = 0, 1, 2, \ldots\) is the Landau level (LL) index). The macroscopic degeneracy of the eigenstates of \(\tilde{D}^2\) is exploited to create the Abrikosov vortex lattice solutions and, at the same time, plays a central part in constructing degenerate solutions for the displaced vortex lattice \(\phi_n\) characterized by a vector \(\tau\): \(\phi_n(r + \tau) = e^{-i\tau \phi_n(r + \tau)}\) with \(\phi_0(r)\) being a vortex lattice solution in LL \(n\). The states \(\phi_n\) and \(\phi_0\) are degenerate eigenstates of the operator \(\tilde{D}^2\).

In order to determine the PDW vortex structure it suffices to consider the linear equation for the PDW order parameter, which is found by keeping both Eqs. 3 and 4 and by setting \(\beta_1 = 0\) in Eq. 3. As a technical simplification, we set \(\kappa_1 = |\kappa_2|/\kappa_3 = \kappa/(\kappa + \kappa_c)\) to ensure that the d-wave order and the PDW order share the same \(\tilde{D}^2\) operator and hence have the same eigenstates (results without this simplification will be given elsewhere). Minimization of the free energy yields the following for the two degrees of freedom in the PDW order:

\[
\Pi \Delta_{d,R}(Q_2) = -\beta_1 \Delta_{d,R}^2 \Delta_{d,R}(Q_2) - \beta_2 \Delta_{d,R}^2 \Delta_{d,R}^*(Q_2)
\]
\[ \tilde{\Pi} \Delta_{\tau_4,Q_4} = -\beta_{c1}|\Delta_0|^2 \Delta_{\tau_4,Q_4} - \beta_{c2} \Delta_0^2 \Delta_{\tau_4,Q_2} \]  \\
with \( \tilde{\Pi} = (\alpha + \sqrt{(\kappa_1 - \kappa_2)(\kappa_1 + \kappa_2)} D^2) \). To solve these equations, we expand the PDW order in eigenstates of the \( D^2 \) operator. At sufficiently high fields, the PDW order will lie predominantly in the \( n = 0 \) eigenstate for both \( \Delta_{\tau_4,Q_2} \) and \( \Delta_{\tau_4,Q_4} \), and we ignore the smaller higher \( n \) contributions here. As mentioned above, these solutions are degenerate, implying the use of two displacement vectors \( \tau_2 \) and \( \tau_4 \). At the second order transition where the PDW order appears, the vortex lattice structure is determined entirely by the \( d \)-wave order parameter, so the only undetermined parameters are \( \tau_2 \) and \( \tau_4 \). Solving the resulting linear equation yields the result that the optimal PDW state is found by minimizing \( \beta_{c1}\beta_3(\tau_2) - |\beta_{c2}\tilde{\beta}(\tau_2,\tau_4)| \) with respect to \( \tau_2 \) and \( \tau_4 \) where

\[ \beta_3(\tau) = \sum_G e^{-i2\pi_{G,T}} e^{G \cdot G} \]  \\
\[ \tilde{\beta}(\tau_2,\tau_4) = \sum_G e^{-i2\pi_{G_i,T_i}} e^{G \cdot G_i} \]  \\
where \( G \) are the reciprocal lattice vectors of the vortex lattice, \( G = G + \frac{2\pi B}{\Phi_0} \times \tau_2 \) and \( \tilde{\beta} = 0 \) unless \( \tau_2 + \tau_4 = T \), where \( T \) is a vortex lattice translation vector. For \( \beta_{c1} < 0 \) it follows immediately that \( \tau_2 = \tau_4 = 0 \) while the solution for \( \beta_{c1} > 0 \) requires a numerical minimization to determine \( \tau_2 \). The resulting configurations are shown in Fig. 2, assuming that the \( d \)-wave order forms a hexagonal vortex lattice.

Here we provide a description of the phases in Fig. 2. The phase diagram depends upon \( r = |\beta_{c2}/\beta_{c1}| \) and in all the phases we can choose \( \tau_4 = -\tau_2 \). We find that there are four phases: in Phase 1 \((0 \leq r < 0.07)\), \( \tau_4 = \gamma(a + b) \) and \( \gamma \) evolves continuously from \( 1/3 \) to \( 1/2 \); in Phase 2 \((0.07 \leq r < 0.31)\) \( \gamma \) stays fixed at \( 1/2 \) (Fig. 2 shows \( \tau_4 = a/2 \) which is equivalent solution to \( \tau_4 = (a+b)/2 \)). In Phase 3 \((0.31 \leq r < 0.5)\), \( \tau_4 = \gamma_4 \alpha \) where \( \gamma_4 \) changes continuously from \( 1/2 \) to \( 0 \); finally in Phase 4 \((r > 0.5)\), \( \tau_4 = 0 \). The arguments of Ref. [12] imply that in Phases 1 through 3, the \( d \)-wave vortex cores have charge density wave order at twice the PDW wave-vectors.

The solution of the vortex lattice problem for the PDW order allows the SDW order to be determined which is particularly important as neutron scattering measures the Fourier transform of \( S^2(R) \). Eq. (12) yields the intriguing result that the SDW order will exhibit Bragg peaks at \( k \) positions that depend upon \( \tau_2 \) and \( \tau_4 \):

\[ k = Q_2 + G + \frac{2\pi B}{\Phi_0} \times \tau \]  \\
where \( G \) is a reciprocal lattice vector of the vortex lattice and \( \tau \) is either \( \tau_2 \) or \( \tau_4 \). Consequently, the relative position of the vortex cores of the PDW and \( d \)-wave order can be retrieved from the position of the Bragg peaks in the SDW order.

**Conclusions:** We have developed a phenomenological theory for the \( Q \)-phase of CeCoIn\(_5\) to identify the possible symmetries for the PDW order. This theory is used to determine phases in which the PDW and \( d \)-wave vortex lattice are relatively displaced, leading to CDW order in the \( d \)-wave vortex cores. Interestingly, these structures can be probed by the position of the SDW Bragg peaks.

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**FIG. 2:** Possible vortex configurations for the PDW order. The yellow circles give the zeroes of the \( d \)-wave order parameter, the blue diamonds give the positions of the zeroes of \( \Delta_{\tau_4,Q_4} \), and the red triangles give the positions of the zeroes of \( \Delta_{\tau_4,Q_2} \).