Magnetic structure of the antiferromagnetic Fulde–Ferrell–Larkin–Ovchinnikov state

Youichi Yanase$^{1,2}$ and Manfred Sigrist$^2$

$^1$ Department of Physics, Niigata University, Niigata 950-2041, Japan
$^2$ Theoretische Physik, ETH Zurich, 8093 Zurich, Switzerland

E-mail: yanase@phys.sc.niigata-u.ac.jp

Received 30 July 2010, in final form 11 August 2010
Published 17 February 2011
Online at stacks.iop.org/JPhysCM/23/094219

Abstract

The properties of incommensurate antiferromagnetic (AFM) order in the Fulde–Ferrell–Larkin–Ovchinnikov (FFLO) state are studied by solving the Bogoliubov–de Gennes (BdG) equations. The relationship between the electronic structure and the magnetic structure is clarified. We find that the magnetic structure in the AFM-FFLO state includes three cases. (I) In the strongly localized case, the AFM staggered moment is confined into the FFLO nodal planes where the superconducting order parameter vanishes. (II) In the weakly localized case, the AFM staggered moment appears in the whole spatial region, and its magnitude is enhanced around the FFLO nodal planes. (III) In the extended case, the AFM staggered moment is nearly homogeneous and slightly suppressed in the vicinity of the FFLO nodal planes. The structure of Bragg peaks in the momentum resolved structure factor is studied in each case. We discuss the possibility of an AFM-FFLO state in the heavy fermion superconductor CeCoIn$_5$ by comparing these results with the neutron scattering data of CeCoIn$_5$. Experimentally the magnetic structure and its dependence on the magnetic field orientation in the high-field superconducting phase of CeCoIn$_5$ are consistent with case (II).

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

1. Introduction

The possible presence of a spatially modulated state in superconductors in a high magnetic field was predicted by Fulde and Ferrell [1], and by Larkin and Ovchinnikov [2] more than 40 years ago. While the Bardeen–Cooper–Schrieffer (BCS) theory assumes Cooper pairs with vanishing total momentum, the Fulde–Ferrell–Larkin–Ovchinnikov (FFLO) superconducting state represents a condensate of Cooper pairs with a finite total momentum. Since the FFLO state has an internal degree of freedom arising from the reflection or inversion symmetry, a spontaneous breaking of the spatial symmetry occurs. Although this novel superconducting state with an exotic symmetry has been attracting much interest, the FFLO state has not been observed in superconductors for nearly 40 years. Under these circumstances, the discovery of a new superconducting phase in CeCoIn$_5$ at high magnetic fields and low temperatures [3, 4] triggered many theoretical and experimental studies because this high-field superconducting (HFSC) phase is a likely candidate for the FFLO state [5]. The recent interest in the FFLO superconductivity/superfluidity extends further into various related fields, such as organic superconductors [6–10], cold atom gases [11, 12], astrophysics, and nuclear physics [13].

The HFSC phase of CeCoIn$_5$ has been interpreted widely within the concept of the FFLO state [5, 14–23]. However, recent observations of the magnetic order in the HFSC phase call for a reexamination of this conclusion [24, 25]. It is not unlikely that this order will be closely connected with an antiferromagnetic (AFM) quantum critical point observed in CeCoIn$_5$ [26, 27]. Moreover, the nuclear magnetic resonance (NMR) [24, 28, 29] and neutron scattering [25, 30] measurements may have uncovered a novel superconducting state in this strongly correlated electron system.

Neutron scattering measurements have found that the wavevector of the AFM order is incommensurate $\vec{q}_{AF} = \vec{Q} + \vec{q}_{inc}$ with $\vec{Q} = (\pi, \pi)$ and the AFM staggered moment $\vec{M}_{AF}$ is oriented along the c-axis [25]. Recent
experiments have shown that the incommensurability \( q_{\text{inc}} \) is fixed along \([1, -1, 0]\) irrespective of whether the magnetic field is directed along \([1, 1, 0]\) or \([1, 0, 0]\) in the tetragonal lattice [30]. These magnetic structures are consistent with the NMR measurements [31].

Some theoretical scenarios have been proposed to explain the AFM order in the HFSC phase of CeCoIn\(_5\). We have analyzed the possibility that AFM order arises from the inhomogeneous Larkin–Ovchinnikov (LO) state [32, 33]. The AFM order triggered by the emergence of \( \pi \)-triplet pairing or pair density wave (PDW) has been investigated in the BCS state [34–36] and in the homogeneous Fulde–Ferrell (FF) state [37]. In order to identify the HFSC phase of CeCoIn\(_5\), it is highly desirable to examine these possible phases by comparing their properties with the experimental results. In this study, we investigate the magnetic structure of the AFM-FFLO state, in which the AFM order appears in the inhomogeneous LO state, and discuss the recent neutron scattering measurements.

### 2. Formulation

Our theoretical analysis is based on the microscopic model,

\[
H = -t \sum_{\langle \langle i,j \rangle \rangle, \sigma} n_i c_i^{\dagger} c_j^{\sigma} + t' \sum_{\langle i,j \rangle, \sigma} n_i c_i^{\dagger} c_{j+}^{\sigma} + J' \sum_{i,\sigma} n_{i+} n_i \quad \text{in the tetragonal phase approximation,}
\]

\[
+ U \sum_i n_i n_i - V \sum_{\langle i,j \rangle} n_i n_j + J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j - g_B H \sum_i \vec{S}_i, \tag{1}
\]

where \( \vec{S}_i \) is the spin operator and \( n_i \) is the number operator at site \( i = (m, n) \). To describe the quasi-two-dimensional electronic structure of CeCoIn\(_5\), we assume a square lattice, in which the brackets \( \langle \langle i,j \rangle \rangle \), \( \langle i,j \rangle \), and \( \langle \langle i,j \rangle \rangle \) denote the summation over the nearest-neighbor sites, next-nearest-neighbor sites, and third nearest-neighbor sites, respectively.

The on-site repulsive interaction is given by \( U \), and \( V \) and \( J \) stand for the attractive and AFM exchange interactions, respectively, between nearest-neighbor sites. We introduce \( V \) to stabilize the d-wave superconducting state within the mean field Bogoliubov–de Gennes (BdG) equations and choose \( J > 0 \) favoring AFM correlation in CeCoIn\(_5\). The effective interaction leading to the d-wave superconductivity near the AFM instability arises from the simple Hubbard model or periodic Anderson model beyond the mean field theory [38, 39], but we here assume the interactions \( V \) and \( J \) to describe these features in the inhomogeneous LO phase on the basis of mean field BdG equations. Although the BdG equations neglect the AFM spin fluctuation beyond the mean field approximation, they are suitable for studying the qualitative features of the inhomogeneous superconducting and/or magnetic state. The roles of AFM spin fluctuation have been discussed in [33].

With the last term in equation (1), we include the Zeeman coupling due to the applied magnetic field. The g-factor is assumed to be \( g_B = 2 \). The magnetic field lies in the ab-plane of the tetragonal lattice and the superconducting vortices are neglected for simplicity. We choose the unit of energy such that \( t = 1 \) and \( t' / t = 0.25 \), \( t'' / t = 0.05 \). The chemical potential enters as \( \mu = \mu_0 + (\frac{1}{2} U + 4V) n_0 \), where \( n_0 \) is the number density for \( U = V = J = H = 0 \). We vary the bare chemical potential from \( \mu_0 = -1.25 \) to \(-1.15 \) to investigate the possible magnetic structures in the AFM-FFLO state. Then, we obtain the number density \( n = 0.72 \pm 0.82 \).

We study the magnetic structure in the AFM-FFLO state in the following way. First, the BdG equations are self-consistently solved for the mean fields of the spin \( \langle \vec{S}_i \rangle \), charge \( \langle n_i \rangle \), and superconductivity \( \Delta_{\alpha \beta}^{\sigma} = \langle c_{i, \sigma} c_{j, \rho}^\alpha \rangle \), where \( \vec{S}_i \) is the spin operator parallel to the magnetic field. We take into account the Hartree term arising from \( U, V, \) and \( J \).

Since the spin singlet d-wave state is stable in this model, the superconducting order parameter is described as

\[
\Delta_{\alpha \beta}^{d}(\vec{q}) = \Delta_{\alpha \beta}^{\uparrow \downarrow}(\vec{q}) + \Delta_{\alpha \beta}^{\downarrow \uparrow}(\vec{q}) - \Delta_{\alpha \beta}^{\uparrow \downarrow}(\vec{q}) - \Delta_{\alpha \beta}^{\downarrow \uparrow}(\vec{q}), \tag{2}
\]

with \( \vec{a} \) and \( \vec{b} \) being the unit vector along the \( a \)- and \( b \)-axes, respectively. As for the spatial dependence of \( \Delta_{\alpha \beta}^{d}(\vec{q}) \), we find that the inhomogeneous LO state is stable against the uniform FF state. Then, the order parameter is real and oscillates in the space. We assume the single-q spatial modulation along the magnetic field in which the order parameter is approximately described as \( \Delta_{\alpha \beta}^{d}(\vec{q}) \sim \Delta \cos(q_{\text{FFLO}}^\theta \cdot \vec{q}) \) with \( q_{\text{FFLO}}^\theta \parallel \vec{H} \) except for the vicinity of the BCS–FFLO transition. This is the most stable FFLO state in the presence of superconducting vortices when the Fermi surface is nearly isotropic. We determine the stable superconducting state by comparing the condensation energy of BCS, FFLO and normal states. The orientation of magnetic field is taken into account in the direction of \( q_{\text{FFLO}}^\theta \) in our formulation. The case of \( q_{\text{FFLO}}^\theta \) not parallel to \( \vec{H} \) will be discussed at the end of this paper.

Second, we determine the magnetic instability by calculating the transverse spin susceptibility using the random phase approximation,

\[
\chi_{\alpha \beta}^{\pm}(\vec{q}, \vec{q}') = \frac{\chi_{\alpha \beta}^{\pm}(\vec{q}, \vec{q}')}{1 - \sum_\delta I(\vec{q}, \vec{k}) \chi_{\alpha \beta}^{\pm}(\vec{k}, \vec{q}')} \tag{3}
\]

where \( I(\vec{q}, \vec{k}) = U, I(\vec{q}, \vec{k} \pm \vec{a}) = I(\vec{q}, \vec{k} \pm \vec{b}) = -\frac{4}{\pi}, \) and otherwise \( I(\vec{q}, \vec{k}) = 0 \). The bare spin susceptibility \( \chi_{\alpha \beta}^{\pm}(\vec{q}, \vec{q}') \) is calculated for the mean field Hamiltonian obtained by solving the BdG equations. The magnetic instability is determined by the divergence of transverse spin susceptibility assuming a second order magnetic phase transition. Then, the criterion is \( \lambda_{\max} = 1 \) where \( \lambda_{\max} \) is the maximum eigenvalue of the matrix \( \mathbf{K}(\vec{q}, \vec{k}) = \sum_\delta I(\vec{q}, \vec{k}) \chi_{\alpha \beta}^{\pm}(\vec{k}, \vec{q}') \). The magnetic moment perpendicular to the magnetic field is obtained as

\[
M(\vec{k}) = I^{-1}(\vec{k}, \vec{k}) m(\vec{k}) \tag{4}
\]

near the critical point, where \( m(\vec{k}) \) is the eigenvector of \( \mathbf{K}(\vec{q}, \vec{k}) \) for the eigenvalue \( \lambda_{\max} \) and \( \sum_\delta I^{-1}(\vec{q}, \vec{k}) I(\vec{q}, \vec{k}) = \delta_{\vec{q}, \vec{k}} \). We denote the AFM staggered moment \( M_{\text{AF}}(\vec{i}) = (-1)^{m+n} M(\vec{i}) \) with \( \vec{i} = (m, n) \).
Figure 1. The AFM staggered moment normalized by its maximum value $M_{\text{AF}}(\vec{r})/M_{\text{max}}$ with $\vec{r} = (m, n)$ in the case of $\vec{q}_{\text{FFLO}} \parallel \vec{q}_{\text{inc}}$. This FFLO modulation corresponds to the experimental setup of CeCoIn$_5$ for the magnetic field along the $[1, \pm 1, 0]$ direction [25]. (a), (b), and (c) show (I) the strongly localized case, (II) the weakly localized case, and (III) the extended case, respectively. We solve the BdG equations for $\vec{q}_{\text{FFLO}}$ in the AFM-FFLO state in the following sections. In our (a) the magnetic field. FFLO modulation corresponds to the experimental setup of CeCoIn$_5$ for the magnetic field along the $[1, \pm 1, 0]$ direction. Since the effect of induced PDW order, which plays an important role to stabilize the AFM-FFLO state, is appropriately captured in our calculation.

3. Magnetic structure

Here we show that the magnetic structure in the AFM-FFLO state is classified into three cases. (I) In the strongly localized case, the AFM moment is confined into the FFLO nodal planes where the superconducting order parameter vanishes. The magnitude of AFM moment away from the nodal planes is typically $\sim 0.01$ of that around the nodal planes. (II) In the weakly localized case, the AFM moment appears in the whole spatial region, and its magnitude is enhanced around the FFLO nodal planes, typically twice. (III) In the extended case, the AFM moment is nearly homogeneous and slightly suppressed in the vicinity of the FFLO nodal planes.

Owing to the four fold rotation symmetry of the tetragonal lattice the incommensurate wavevector $\vec{q}_{\text{inc}} = \vec{q}_{\text{inc}}^a \parallel \vec{a}$ or $\vec{b}$ direction and is different from the experimental observation $\vec{q}_{\text{inc}} \parallel [1, \pm 1, 0]$ [25]. However, the relationship between the magnetic structure and relative angle of $\vec{q}_{\text{inc}}$ and $\vec{q}_{\text{FFLO}}$ (and $\vec{H}$) is appropriately captured in our calculation.

4. Neutron scattering

For a comparison with neutron scattering experiments [25, 30], we calculate the magnetic structure factor $|\langle M(\vec{q}) \rangle|^2$, where $M(\vec{q}) = M(\vec{q})$ is the Fourier transformed magnetic moment given as

$$M(\vec{q}) = \sum_i M(\vec{r}_i)e^{i\vec{q}\vec{r}_i}. \quad (5)$$

Here we normalize $M(\vec{r}_i)$ so that $\sum_i |M(\vec{q})|^2 = 1$, to discuss the relative intensity of Bragg peaks. Figures 3 and 4 show the magnetic structure factor in the AFM-FFLO states with $\vec{q}_{\text{FFLO}} \parallel \vec{q}_{\text{inc}}$ and $\vec{q}_{\text{FFLO}} \parallel \vec{q}_{\text{inc}}^a + \vec{q}_{\text{inc}}^b$ respectively. The former corresponds to CeCoIn$_5$ under the magnetic field along the $[1, \pm 1, 0]$ direction, while the latter is realized in the magnetic field along the $[1, 0, 0]$ or $[0, 1, 0]$ direction. We have shown the figures rotated by $45^\circ$ for a comparison with neutron scattering experiments [25, 30].

In addition to the main Bragg peaks at $\vec{q} = \vec{q}_{\text{inc}}^a$, and/or $\vec{q} = \vec{q}_{\text{inc}}^b$, satellite peaks appear along the direction of the
Figure 2. The normalized AFM staggered moment $M_{\text{AF}}(\vec{i}) / M_{\text{max}}$ in the case of $\vec{q}_{\text{FFLO}} \parallel \vec{q}_{\text{inc}} + \vec{q}_{\text{inc}}$. This FFLO modulation corresponds to the CeCoIn$_5$ in the magnetic field along the $[1, 0, 0]$ or $[0, 1, 0]$ direction [24, 30]. We assume the same parameters as in figure 1. The AFM order occurs at (a) $(T, H) = (0.0264, 0.164)$, (b) $(T, H) = (0.0324, 0.155)$, and (c) $(T, H) = (0.035, 0.15)$, respectively. We solve the BdG equations for $56 \times 56$ lattices to keep the amplitude of the FFLO modulation vector $|\vec{q}_{\text{FFLO}}|$ similar to that in figure 1. The arrow shows the direction of the magnetic field.

Figure 3. The magnetic structure factor $|M(\vec{q})|^2$ in the AFM-FFLO state with $\vec{q}_{\text{FFLO}} \parallel \vec{q}_{\text{inc}}$. This AFM-FFLO state can be realized in CeCoIn$_5$ for the magnetic field along the $[1, \pm 1, 0]$ direction [25]. We show the figures rotated by 45 for a comparison with neutron scattering experiments. The center of each figure shows $\vec{q} = \vec{Q} = (\pi, \pi)$, and, therefore, the position from the center shows the incommensurate wavevector $\vec{q}_{\text{inc}}$. We assume the same parameters as in figure 1.

magnetic field from the main peaks. These satellite peaks arise from the broken translational symmetry in the FFLO state, and their amplitude reflects the spatial inhomogeneity of magnetic structure. Therefore, the satellite peaks are pronounced in (I), the strongly localized case, while they are obscure in cases (II) and (III).

We now discuss the possible magnetic structure of CeCoIn$_5$ in the HFSC phase on the basis of figures 3 and 4. The strongly localized case (I) is incompatible with two features of neutron scattering experiments. First, the satellite peaks are absent or have a very weak intensity [25, 30]. Second, the position of the main Bragg peaks is independent of the orientation of the magnetic field in the $ab$-plane [30]. The extended case (III) is incompatible with the neutron scattering measurement for magnetic fields along $[1, \pm 1, 0]$ for which the incommensurate wavevector $\vec{q}_{\text{inc}}$ is perpendicular to the field $\vec{H}$ [25]. On the other hand, the weakly localized case (II) shown in figures 3(b) and 4(b) is consistent with the neutron scattering experiments in which the incommensurate wavevector is perpendicular to the field direction $\vec{q}_{\text{inc}} \perp \vec{H}$ for $\vec{H} \parallel [1, \pm 1, 0]$, and the position of the main Bragg peaks does not change by rotating the magnetic field in the $ab$-plane. The four main Bragg peaks appear in figure 4(b) in contrast to figure 3(b) owing to the symmetry of the system. This change has also been observed in the neutron scattering measurement [30]. According to these discussions, the magnetic structure in the possible AFM-FFLO state in CeCoIn$_5$ should be (II), the weakly localized case. This is the main conclusion of this paper.
5. Discussion

We studied the magnetic structure of AFM order in the FFLO superconducting state. We find that the spatial inhomogeneity of the magnetic moment is reduced by increasing the incommensurability $|\eta_c|, |\eta_b|$ and enhancing the nesting of the Fermi surface. This change of the magnetic structure is realized in our model by decreasing the number density from the half filling. Comparing our results with the neutron scattering experiments in CeCoIn$_5$, the unconventional magnetic order in the HFSC phase of CeCoIn$_5$ is consistent with the AFM-FFLO state proposed by us when the AFM staggered moment is weakly localized around the FFLO nodal planes. This is the `weakly localized case' in our classification of the magnetic structure.

Finally, we discuss two points. (1) In our discussion we assumed that the FFLO modulation vector $\vec{q}_{\text{FFLO}}$ lies parallel to the magnetic field, since this is the most stable FFLO state, unless the anisotropy of the Fermi surface favors another $\vec{q}_{\text{FFLO}}$. On the other hand, if $\vec{q}_{\text{FFLO}}$ is fixed by the anisotropic electronic structure, the position of the Bragg peaks measured by neutron scattering would be independent of the magnetic field orientation, consistent with the experimental observation. This would apply to the AFM-FFLO state in the `weakly localized case' as well as in the `strongly localized case' and the `extended case'. This implies, however, that BCS-to-AFM-FFLO transition would be of first order [21–23]. While this is in contrast to the experimental observation, we cannot exclude a weakly first order transition which is experimentally hard to detect.

(2) The magnetic structure for the magnetic field along $\vec{q}_{\text{inc}}$ is strongly localized $\parallel\vec{q}_{\text{FFLO}}$. This AFM-FFLO state can be realized in CeCoIn$_5$ for the magnetic field along the [1, 0, 0] or [0, 1, 0] direction [30]. We assume the same parameters as in figure 3.

Figure 4. The magnetic structure factor $|M(\vec{q})|^2$ in the AFM-FFLO state with $\vec{q}_{\text{FFLO}} \parallel \vec{q}_{\text{inc}} - \vec{q}_{\text{inc}}$. This AFM-FFLO state can be realized in CeCoIn$_5$ for the magnetic field along the [1, 0, 0] or [0, 1, 0] direction [30]. We assume the same parameters as in figure 3.
