Microscopic picture on antiferromagnetic order induced by paramagnetic pair-breaking in \( d \)-wave superconductor

Y Hatakeyama and R Ikeda
Department of Physics, Kyoto University, Kyoto 606-8502, Japan
E-mail: hatakeyama@scphys.kyoto-u.ac.jp

Abstract. We theoretically investigate possible antiferromagnetic (AFM) orders in Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) superconducting phase with \( d_{x^2-y^2} \)-wave paring induced by the paramagnetic pair-breaking effect. The AFM \( \mathbf{Q} \) vector whose incommensurate part \( \mathbf{q}_{\text{AFM}} \) is parallel to \([1,1,0]\) direction and independent of the field strength is obtained with the dispersion relation which have a remarkably inflected Fermi surface and the largest DOS along \([1,1,0]\) direction. It is shown that, in a field parallel to \([1,1,0]\), \( \mathbf{q}_{\text{AFM}} \) perpendicular to the field direction is stabilized as a result of the coupling between \( \mathbf{Q} \) vector and the wavevector of FFLO modulation. These results are consistent with the observations in the high-field low-temperature phase of CeCoIn\(_5\).

1. Introduction
The discovery of antiferromagnetic (AFM) order in the high field corner of the \( d \)-wave superconducting (SC) phase of CeCoIn\(_5\) [1] has led to a tremendous interest in the genuine picture of the high-field and low-temperature (HFLT) superconducting phase of this compound in fields parallel to the basal plane, which has been identified earlier [2, 3] with the long-sought Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) phase. The detected field-induced AFM order is peculiar in the sense that it is absent outside the HFLT phase, and this feature has been discussed theoretically from different viewpoints so far [4, 5, 6]. Besides this, doping [7] and NMR [8] experiments have given strong support on the picture [6] identifying the HFLT phase with a FFLO state.

The incommensurate \( \mathbf{Q} \) vector of the AFM order observed in the neutron scattering experiments [1, 9] has exhibited the following three features: (i) the incommensurate part \( \mathbf{q}_{\text{AFM}} \) of the \( \mathbf{Q} \) vector \( (\mathbf{q}_{\text{AFM}} = \mathbf{Q} - (\pi, \pi, \pi)) \) is fixed in \([1,1,0]\) or \([1,-1,0]\) direction regardless of the direction of a field \( \mathbf{H} \) (Note that these directions are equivalent due to the tetragonal crystal symmetry of CeCoIn\(_5\)); (ii) \( \mathbf{q}_{\text{AFM}} \) is independent of the field strength; (iii) A \( \mathbf{q}_{\text{AFM}} \) perpendicular to \( \mathbf{H} \parallel [1,1,0] \) is preferred. However, these features have not been successfully explained so far.

In this work, we extend our theory [6, 10] identifying the HFLT phase of CeCoIn\(_5\) with the coexistent phase of AFM and FFLO orders in a \( d_{x^2-y^2} \)-wave superconductor with strong paramagnetic pair-breaking (PPB) in order to study the detailed structures of the AFM order. It is found that the \( \mathbf{Q} \) vector of the AFM order is determined by the nesting vector of the Fermi surface, and that \( \mathbf{q}_{\text{AFM}} \) parallel to \([1,1,0]\) (or \([1,-1,0]\) ) direction reflects the fact that the principal
Fermi surface of CeCoIn$_5$ is remarkably inflected and has the largest density of state along [1,1,0] direction. It is also found that $q_{\text{AFM}}$ is independent of the field strength. Moreover, it is shown that, for $H \parallel [1,1,0]$, $q_{\text{AFM}}$ perpendicular to $H$ is stabilized by the coupling between $Q$ vector of the AFM order and the wavevector of the FFLO modulation parallel to $H$. Therefore, the features of the observed $Q$ vector of the AFM order in CeCoIn$_5$ are explained by the picture that the HFLT phase of CeCoIn$_5$ is the coexistent phase of AFM and FFLO orders induced by strong PPB.

2. Model and calculation

We start with a weak-coupling BCS-like Hamiltonian including the effect of PPB and the mean fields of FFLO SC and AFM orders:

$$\mathcal{H} = \mathcal{H}_{\text{kin}} + \mathcal{H}_{\text{SC}} + \mathcal{H}_{\text{AFM}}$$

(1)

$$\mathcal{H}_{\text{kin}} = \sum_{k,\sigma} \left[ \varepsilon_k - \mu_B H \sigma \right] c_{k,\sigma}^\dagger c_{k,\sigma}$$

(2)

$$\mathcal{H}_{\text{SC}} = \sum_{q} \left\{ \frac{1}{g} |\Delta_q|^2 - \frac{1}{2} \sum_{k,\alpha,\beta} \left[ \Delta_q w_k (i\sigma_y)_{\alpha,\beta} c_{k,\alpha}^\dagger c_{-k+q,\beta} + \text{h.c.} \right] \right\}$$

(3)

$$\mathcal{H}_{\text{AFM}} = \sum_{Q} \left\{ \frac{1}{U} |m_Q|^2 - \frac{1}{2} \sum_{k,\alpha,\beta} \left[ m_Q (\sigma_x)_{\alpha,\beta} c_{k+Q,\alpha}^\dagger c_{k,\beta} + \text{h.c.} \right] \right\}.$$  

(4)

Here, $\mathcal{H}_{\text{kin}}, \mathcal{H}_{\text{SC}}, \text{and } \mathcal{H}_{\text{AFM}}$ are the kinetic energy term with the PPB effect, SC-interaction term, and AFM-interaction one of the Hamiltonian, respectively. Further, $\xi_k$ is the dispersion relation of quasiparticles measured from the Fermi energy, $H$ is the magnetic field parallel to the basal plane, $\Delta_q$ is a FFLO SC order parameter with momentum $q$, and $m_Q$ is an AFM staggered moment with wavevector $Q$ of the AFM modulation. On the basis of observations in CeCoIn$_5$ [1], we have assumed that the AFM staggered moment is perpendicular to the basal plane and the pairing symmetry of SC order is $d_{x^2-y^2}$ [11]: $w_k = \cos(k_x a) - \cos(k_y a)$ where $a$ is the lattice spacing of the basal plane. Based on the recent NMR measurement [8] suggesting the existence of nodal planes of SC order parameter in the HFLT phase, the FFLO modulation of the SC order parameter have been assumed to be of Larkin-Ovchinikov (LO) type: $\Delta(r) = \sqrt{2} \cos(q_{\text{FFLO}} \cdot r)$, where $q_{\text{FFLO}}$ is the wavevector of the FFLO modulation.

From the Hamiltonian (1), we have calculated a AFM ordering in FFLO state in Pauli-limit and have found the most optimal $Q$-vector of the AFM order. The dispersion relation of 2D tight-binding model has been used in order to incorporate the tetragonal crystal symmetry of CeCoIn$_5$:

$$\xi_k = \mu + 2t_1 (\cos(k_x a) + \cos(k_y a)) + 4t_2 \cos(k_x a) \cos(k_y a) + 2t_3 (\cos(2k_x a) + \cos(2k_y a)),$$

(5)

where $\mu$ is the chemical potential, and $t_1, t_2, t_3$ are the hopping integrals. In order to investigate the AFM ordering in a FFLO state, we have focused on the $|m_Q|^2$ term in the free energy. Since the coefficient of the $|m_Q|^2$ term is proportional to the inverse of the AFM susceptibility, the most optimal $Q$ vector has been found by the numerical minimization of the coefficient of the $|m_Q|^2$ term with respect to $Q$. The detail of our calculation is discussed in [10].

Moreover, we have investigated the coupling between the $Q$ vector of the AFM order and the wavevector $q_{\text{FFLO}}$ of the FFLO modulation. The dispersion relation has been assumed to have a quasi-2D cylindrical Fermi surface and satisfy the following relation for the nesting condition: $\xi_{k+Q} = -\xi_k - v_F \cdot q_{\text{AFM}} - \delta_{\text{IC}} T_c$, where $v_F$ is the Fermi velocity, $\delta_{\text{IC}}$ is the parameter representing the deviation from the perfect nesting, and $T_c$ is the SC transition temperature.
We have calculated the free energy expanded in powers of $\Delta$ and $m = mQ$:

$$F(\Delta, m, q_{\text{FFLO}}, q_{\text{AFM}}) = f_{\Delta^2}(q_{\text{FFLO}}) + f_{\Delta^4}(q_{\text{FFLO}}) + f_{\Delta^6} + f_{m^2}(q_{\text{AFM}}) + f_{m^4} + f_{\Delta^2m^2}(q_{\text{FFLO}}, q_{\text{AFM}})$$

(6)

In the calculation of these terms, the orbital depairing effect and the spatial modulation of $\Delta$ in a FFLO state are incorporated using the familiar quasi-classical approximation for the orbital depairing [3, 12]. We have focused on the $m^2$ part of the expanded free energy (6): $F_m = f_{m^2} + f_{\Delta^2m^2}$. We have examined the dependence of $F_m$ on the angle $\theta$ between $q_{\text{AFM}}$ and $q_{\text{FFLO}}$ in order to find the most optimal $\theta$.

3. Results

![Fermi surface and density of states](image)

Figure 1. Fermi surface (solid curve) and the density of states (colormap) of the dispersion relation (5) with the parameter values $t_1 = 20T_c$, $\mu/t_1 = 1.85$, $t_2/t_1 = -1.25$, $t_3/t_1 = 0.65$. The broken curve is the Fermi surface shifted by the nesting vector $(\pi + 0.37, \pi + 0.37)$ in k-space, and the dotted curve is the Fermi surface obtained by using the result of the band calculation [13].

We have numerically investigated the most optimal $q_{\text{AFM}}$. It is found that $q_{\text{AFM}}$ is determined by the nesting vector of the Fermi surface in this model. For example, from the solid and the broken curves in Fig. 1, we can see that the nesting vector of the Fermi surface depicted in Fig 1 is $(\pi + 0.37, \pi + 0.37)$, and the $Q$ vector obtained from the numerical minimization coincides with the nesting vector. As shown below, the $Q$ vector consistent with the observation [1] can be reproduced in this model; therefore it is suggested that the origin of the incommensurate AFM order in the HFLT phase of CeCoIn$_5$ consists in the electronic band structure.

We have examined how the direction of the most optimal $q_{\text{AFM}}$ depends on the dispersion relation. In the simplest case $t_3 = 0$, where the nesting condition of the Fermi surface is relatively kept, $q_{\text{AFM}}$ parallel to $[1,0,0]$ direction is stabilized, which is inconsistent with the experimental $q_{\text{AFM}}$. On the other hand, in the case where $t_3$ is finite, it is possible to have a remarkably inflected Fermi surface and the largest DOS along $[1,1,0]$ direction, as depicted in Fig. 1. These conditions of the Fermi surface correspond to the band 14-electron one obtained from the band calculation [14]. When these conditions are satisfied, we obtain $q_{\text{AFM}}$ parallel to $[1,1,0]$ direction, which is consistent with the observed feature (i) of the $Q$ vector indicated in Sec. 1.

We have investigated the temperature and the field dependence of $q_{\text{AFM}}$. It is found that $q_{\text{AFM}}$ is almost independent of the temperature and the field strength, as shown in Fig. 2. This results reproduce the observed feature (ii) of the $Q$ vector. The reason for the field-independent $q_{\text{AFM}}$ is that the nesting vector, and thus $q_{\text{AFM}}$ are not affected by the Zeeman splitting of the...
Figure 2. (a) Field dependence and (b) temperature dependence of $q_{AFM}$ obtained by a numerical minimization. The same dispersion relation as Fig. 1 is used.

Figure 3. Coupling energy $\Delta F_m$ of the AFM modulation and the FFLO modulation as a function of the angle $\theta$ between $q_{AFM}$ and $q_{FFLO}$.

Fermi surface when the AFM staggered moment $m$ is perpendicular to the field. In this case, the nesting between the up-spin Fermi surface and the down-spin Fermi surface is relevant for the AFM ordering. Because the volume changes of these Fermi surfaces induced by the Zeeman splitting cancels out, the nesting vector is not affected by the Zeeman splitting.

We have examined the interaction between the AFM $Q$ vector and the wavevector $q_{FFLO}$ of the FFLO modulation. Figure 3 shows the coupling energy $\Delta F_m$ as a function of $\theta$, where $\Delta F_m = F_m(\theta) - F_m(0)$. The parameter values used in our calculation are, $\alpha_M = 1.2, \delta IC = 0.4, T/T_c = 0.1, H/H_{orb} = 0.2$, where $\alpha_M = \sqrt{2}H_{orb}/H_P$ is Maki parameter, $H_{orb}$ and $H_P$ are the depairing fields in the orbital limit and in Pauli-limit, respectively. From Fig. 3, we can see that $\Delta F_m$ is minimized when $q_{AFM}$ is perpendicular to $q_{FFLO}$. The experiments such as the ultrasound measurement [15] and NMR measurement [8] are also consistent with the FFLO order in which $q_{FFLO}$ is parallel to $H$. Therefore, this result means that $q_{AFM}$ perpendicular to $H$ is stabilized, which is consistent with the observed feature (iii) of the $Q$ vector.

Acknowledgments

This work was supported by the Grant-in-Aid for the Global COE Program "The Next Generation of Physics, Spun from Universality and Emergence" from the Ministry of Education, Culture, Sports, Science and Technology (MEXT) of Japan.

References

[1] Kenzelmann M et al. 2008 Science 321 1652
[2] Bianchi A, Movshovich R, Capan C, Pagliuso P G and Sarrao J L 2003 Phys. Rev. Lett. 91 187004
[3] Adachi H and Ikeda R 2003 Phys. Rev. B 68 184510
[4] Aperis A, Varelogiannis G and Littlewood P B 2010 Phys. Rev. Lett. 104 216403
[5] Yanase Y and Sigrist M 2011 J. Phys.: Condens. Matter 23 094219
[6] Ikeda R, Hatakeyama Y and Aoyama K 2010 Phys. Rev. B 82 060510
[7] Tokiwa Y et al. 2010 Phys. Rev. B 82 220502; Ikeda R 2010 Phys. Rev. B 81 060510(R)
[8] Kumagai K, Shishido H, Shibauchi T and Matsuda Y 2011 Phys. Rev. Lett. 106 137004
[9] Kenzelmann M et al. 2010 Phys. Rev. Lett. 104 127001
[10] Hatakeyama Y and Ikeda R 2011 Phys. Rev. B 83 224518
[11] Izawa K et al. 2001 Phys. Rev. Lett. 87 057002; Hiasa N and Ikeda R 2008 Phys. Rev. Lett. 101 027001
[12] Ikeda R 2007 Phys. Rev. B 76 134504
[13] Tanaka K, Ikeda H, Nisikawa Y and Yamada K 2006 J. Phys. Soc. Jpn. 75 024713
[14] Onuki Y et al. 2004 J. Phys. Soc. Jpn. 73 769
[15] Watanabe T et al. 2004 Phys. Rev. B 70 020506; Ikeda R 2007 Phys. Rev. B 76 054517