Antiferromagnetic order in vortex states in paramagnetic and d-wave superconductors

Kazushi Aoyama$^{1,2}$ and Ryusuke Ikeda$^2$

$^1$ Young Researcher Development Center, Kyoto University, Kyoto 606-8302, Japan
$^2$ Department of Physics, Kyoto University, Kyoto 606-8502, Japan

E-mail: bonn@scphys.kyoto-u.ac.jp

Abstract. We theoretically investigate effects of a vortex lattice structure on antiferromagnetic (AFM) ordering induced inside a $d$-wave superconducting (SC) phase due to a strong Pauli-paramagnetic pair-breaking (PPB) effect. It is shown that a PPB-induced AFM order is spatially modulated due to the vortex lattice structure and that, in contrast to the familiar competitive nature of AFM and SC orders, the modulated AFM order is not localized in vortex cores but coexistent with the SC order. Discussion on effects of PPB-induced AFM fluctuation on the spin magnetization is also given.

1. Introduction

The heavy-fermion material CeCoIn$_5$ is a spin singlet and $d$-wave superconductor with a strong Pauli-paramagnetic pair-breaking (PPB) effect. In the case with a magnetic field parallel to the basal plane of this material ($H \parallel ab$), there exists a distinct high field and low temperature (HFLT) superconducting (SC) phase in which a Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) vortex lattice is considered to be realized as a result of the strong PPB effect [1]. Recently, it has been clarified through neutron scattering experiments that, in $H \parallel ab$, an antiferromagnetic (AFM) order with its moment vector oriented in the $c$-direction exists inside the HFLT SC phase in spite of the absence of AFM order in the normal state [2]. Considering that, conventionally, AFM and SC orders are competing with each other in zero field, it is surprising that AFM ordering is rather enhanced inside the SC state. In relation to this, it is natural to expect the AFM critical phenomena observed around $H_{c2}(0)$ in a perpendicular field ($H \parallel c$) to originate from the same mechanism as that of the AFM order in $H \parallel ab$ case.

Previously, we have theoretically shown that the PPB effect enhanced strongly by increasing field and decreasing temperature induces an AFM ordering in a $d$-wave SC state [3]. Then, the problem is how an AFM order resulting from this PPB effect is stabilized in the FFLO vortex lattice, i.e., whether it is localized in the normal-state region such as vortex cores and FFLO nodal planes or not. In this report, we examine the stability of the PPB-induced AFM order in the SC vortex lattice, for brevity, without taking into account the FFLO spatial modulation. In addition, as an example of physical quantities reflecting the PPB-induced AFM fluctuation, we discuss the field dependence of the spin magnetization with the AFM fluctuation included.
2. Model

We start from the following electronic Hamiltonian

\[ \mathcal{H} = \sum_\sigma \int \varphi_\sigma^*(\mathbf{r}) \left[ \varepsilon(-i \nabla + |e|A) - \sigma \mu_B gH \right] \varphi_\sigma(\mathbf{r}), \]

\[ - \sum_{\mathbf{q}, \mathbf{p}, \alpha, \beta} \left[ \Delta^*(\mathbf{q}) (-i \sigma_y)_{\alpha, \beta} \hat{c}_{\mathbf{p}} \hat{c}_{-\mathbf{p}+\mathbf{q}, \alpha} + \frac{\mathbf{q}^2}{2} \hat{c}_{\mathbf{p}+\mathbf{q}, \alpha} \hat{c}_{\mathbf{p}, \beta}/2 + \mathbf{m}(\mathbf{q}) \cdot \sigma_{\alpha, \beta} \hat{c}_{\mathbf{p}}^\dagger \hat{c}_{\mathbf{p}+\mathbf{q}, \alpha} + \text{H.c.} \right] \] (1)

where $\hat{c}_{\mathbf{p}, \alpha}$ is the annihilation operator for a quasiparticle with momentum $\mathbf{p}$ and spin projection $\alpha$, $\varphi_\sigma(\mathbf{r}) = \frac{1}{\sqrt{V}} \sum_{\mathbf{p}} \hat{c}_{\mathbf{p}, \sigma} e^{i \mathbf{p} \cdot \mathbf{r}}$, and $\sigma_i (i = x, y, z)$ are the Pauli matrices. In the first line in eq. (1), $\varepsilon(\mathbf{p})$ is a kinetic energy measured from the Fermi level and satisfies the relation $\varepsilon(\mathbf{p}+\mathbf{Q}_0) = -\varepsilon(\mathbf{p}) + T_c \delta_{\mathbf{IC}}$ with the commensurate nesting vector $\mathbf{Q}_0 = (\pi, \pi, \pi)$ and the $\mathbf{p}$-independent parameter measuring the deviation from the perfect nesting condition $\delta_{\mathbf{IC}}$, and $\mu_B gH$ is the Zeeman energy. On the second line in eq. (1), the SC gap function $\Delta(\mathbf{q})$ and the AFM moment vector $\mathbf{m}(\mathbf{q})$ play roles of the SC and AFM order parameters, respectively.

Throughout this report, the SC transition temperature in zero field is denoted by $T_c$ and the Neel temperature in the nonsuperconducting state with $\delta_{\mathbf{IC}} = 0$ is denoted by $T_N$. Since the pairing symmetry $w_\mathbf{p}$ of $d_{x^2-y^2}$-type in CeCoIn$_5$ of our interest, the identity $w_{\mathbf{p}+\mathbf{Q}_0} = -w_{\mathbf{p}}$ is satisfied.

The free energy functional of this system can be formally written as

\[ \mathcal{F}(\Delta, m) = \mathcal{F}(\Delta, m = 0) + \sum_{\mathbf{q}, \mathbf{q}'} X^{-1}(\mathbf{q}, \mathbf{q}'; \Delta) m(\mathbf{q}) m^*(\mathbf{q}') + O(|m|^4), \] (2)

where the concrete expressions of $\mathcal{F}(\Delta, m = 0)$ and $X^{-1}(\mathbf{q}, \mathbf{q}'; \Delta)$ are derived from the microscopic Hamiltonian (1). First, we determine the $H_{c2}(T)$ curve and the amplitude of the spatially averaged SC gap function $\Delta_0$ from the functional $\mathcal{F}(\Delta, m = 0)$. Next, we examine an AFM instability inside the SC phase by evaluating the second order term in $|m|$, $\sum_{\mathbf{q}, \mathbf{q}'} X^{-1}(\mathbf{q}, \mathbf{q}'; \Delta) m(\mathbf{q}) m^*(\mathbf{q}')$. This procedure in which $\Delta$ and $m$ are separately considered is justified at least near the second order AFM transition. Hereafter, we will restrict our discussion to the case with the configuration $\mathbf{m} \perp \mathbf{H}$ which corresponds to the experimentally observed situation in $\mathbf{H} \parallel ab$. In the expressions which follow, $t$ and $h$ are the temperature and magnetic field which are normalized by $T_c$ and $H_{c2}(0)$, respectively.

3. AFM order in the SC vortex lattice

In the vortex lattice in the parallel field $\mathbf{H} \parallel ab$, the SC gap function can be expressed as $|\Delta(X, Y)|^2 = |\Delta_0|^2 \sum_{\mathbf{K}_\perp} T^{(2)}_{\mathbf{K}_\perp} \exp[i \mathbf{K}_\perp \cdot (X, Y)]$ with a reciprocal lattice vector of the SC vortex lattice $\mathbf{K}_\perp$, where the magnetic field is applied in the $y$-direction and the coordinate $(X, Y)$ denotes $(\gamma_{1/2} \hat{z}, \gamma_{-1/2} \hat{x})$ with the ratio of the SC coherence length in the $ab$ plane to that in the $c$-direction $\gamma$. Then, an AFM order induced in the SC vortex lattice would be expressed with the vector $\mathbf{K}_\perp$ as

\[ m(X, Y) = N \left( 1 + \alpha \sum_{\mathbf{K}_\perp \neq 0} T^{(2)}_{\mathbf{K}_\perp} \exp[i \mathbf{K}_\perp \cdot (X, Y)] \right), \] (3)

where $N$ is a normalization factor which is determined so that the spatial average of $|m(X, Y)|^2$ is equal to 1 and $\alpha$ is a variational parameter which will be determined by minimizing the second order term in $|m|$. Note that positive (negative) values of $\alpha$ indicate AFM orders suppressed (enhanced) at vortex cores. In the evaluation of $\sum_{\mathbf{q}, \mathbf{q}'} X^{-1}(\mathbf{q}, \mathbf{q}'; \Delta) m(\mathbf{q}) m^*(\mathbf{q}')$, the expansion with respect to $|\Delta|$ is performed and the parameters $\gamma = 2.85$ and $\alpha_{\text{Mab}} = \sqrt{2} H_{\text{orb}}^{(ab)}(0)/(1.25 T_c \mu_B g) = 7.5$ are used, where $H_{\text{orb}}^{(ab)}(0)$ is the orbital limiting field in $\mathbf{H} \parallel ab$.
Figure 1. (Color online) (a) Field dependences of the $|m|^2$-term $\sum_{\mathbf{q},\mathbf{q}' } X^{-1}(\mathbf{q},\mathbf{q}' ;\Delta)m(\mathbf{q})m^*(\mathbf{q}')$ (a solid red curve measured by the left vertical axis) and the variational parameter $\alpha$ (a dashed blue one measured by the right axis) at $t = 0.03$ and (b) the obtained phase diagram, where the triangular lattice is assumed and the parameters $\delta_{IC} = 0.001$ and $T_N/T_c = 0.027$ are used. In (a), the $|m|^2$-term becomes negative in the high field region with positive values of $\alpha$, suggesting the occurrence of an AFM order with a spatial modulation commensurate with the vortex lattice structure. An example of the spatial distribution of this AFM order $|m(X,Y)|^2$ is shown in the inset of (b), where dark thick colored regions correspond to vortex cores. As one can see in the main panel of (b), the AFM order is stabilized in the HFLT corner of the SC phase, where a solid red curve and a thick solid one denote the second order transition curve to the AFM order and the first order $H_{c2}$ transition one, respectively.

Our result obtained here for the PPB-induced AFM order in the SC vortex lattice is consistent with recent NMR data suggesting that the AFM order in the HFLT phase of CeCoIn$_5$ is spatially extended without being localized in the normal-state region [7]. Although the FFLO modulation is ignored in the above calculation, the theoretical study taking account of the longitudinal FFLO modulation along $\mathbf{H}$ without in-plane vortex-lattice structures included shows that, at least in the high-field side of the FFLO state, the AFM order is not localized in the FFLO nodal planes but coexistent with the SC order [6]. These results obtained in the two approaches, which are complementary to each other, suggest that the PPB-induced AFM order coexistent with the SC order may be stabilized at least in the high-field side of the longitudinal FFLO vortex lattice state.
Figure 2. (Color online) Field dependence of the spin magnetization at $t = 0.1$ (lower curves) and $t = 0.3$ (upper ones) in the case with (red solid curves) and without (black dashed ones) the AFM fluctuation. The parameters $T_N/T_0 = 0.25975$ and $\delta_{IC} = 0.5$ are used so that the AFM critical point is located at $H_{12}(0)$. The slope of the magnetization curve becomes steeper as the AFM instability is approached.

4. Effects of AFM fluctuation on the spin magnetization

In this section, effects of AFM fluctuation induced by the PPB effect are investigated. We have pointed out that the AFM fluctuation is strongly reflected in the vortex lattice form factor which is a measure of the internal magnetic field [3]. Here, we examine effects of the AFM fluctuation on the magnetization inside the SC phase. Since the magnetization due to the orbital effect is expected to be small compared with the spin magnetization in the case with strong PPB [5], we will ignore the orbital pair-breaking effect, i.e., the vortex lattice for brevity. The spin magnetization can be expressed as

$$M = 2(\mu_B g)^2 N(0)H - \frac{\partial}{\partial H} F(\Delta, m = 0) - \frac{T}{2H} \sum_\mathbf{q} \ln X^{-1}(\mathbf{q}, \mathbf{q}; \Delta),$$

where $N(0)$ is the density of state per spin on the Fermi surface and the third term in the right-hand side corresponds to the contribution from the PPB-induced AFM fluctuation. In the Pauli limiting case without the orbital effect included, the SC gap function will be treated as uniform and the evaluation $X^{-1}(\mathbf{q}, \mathbf{q}; \Delta)$ will be used.

The field dependence of the spin magnetization is shown in Fig. 2, where the AFM instability is located at $H_{12}(0)$. The contribution from the AFM fluctuation is positive and becomes larger as temperature is lowered and field is increased, i.e., as the AFM instability is approached. As a result, the slope of the spin magnetization curve becomes steeper on approaching $H_{12}(0)$. The obtained result is comparable with the experimental data on the magnetization [8], which supports the scenario that the field-induced AFM critical phenomenon observed below $H_{12}(0)$ and in $\mathbf{H} \parallel c$ case is a consequence of the PPB-induced AFM instability. Although we have assumed the configuration $\mathbf{m} \perp \mathbf{H}$ in this example calculation, we believe that the result on the PPB-induced AFM fluctuation is not qualitatively changed even for the configuration $\mathbf{m} \parallel \mathbf{H}$.

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