Flux line lattice form factor and paramagnetic effects in type II superconductors

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Abstract. Based on the quasiclassical Eilenberger theory, we investigate the vortex structure in type II superconductors with strong Pauli-paramagnetic contributions due to the Zeeman effect. We quantitatively study how the paramagnetic effect suppresses the superconductivity, and evaluate the flux line lattice (FLL) form factor from the calculated internal field distribution both in the s-wave and d-wave pairings. When the paramagnetic effects are strong, the intensity of the FLL form factor increases toward \( H_{c2} \) as a function of an applied field, instead of exponential decay. This anomalous field dependence is due to the induced paramagnetic moments around the vortex core. We discuss the anomalous field-dependence of the FLL form factor observed by the small angle neutron scattering in CeCoIn\(_5\).

1. Introduction
There are two mechanisms for pair-breaking of superconductivity by magnetic fields. One is the diamagnetic pair breaking due to the screening current around vortices from the contribution of the vector potential. The other is the Pauli-paramagnetic pair breaking due to the mismatched Fermi surface of up and down spin electrons by the Zeeman shift. A heavy Fermion compound CeCoIn\(_5\) is a prime candidate of a superconductor with strong Pauli-paramagnetic effect in the vortex states, since at higher fields the upper critical field \( H_{c2} \) changes to the first order phase transition and new Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) state appears [1, 2, 3]. It is expected that, in the presence of strong paramagnetic effect, behaviors of vortex states are different from those of the conventional vortex states, even when the vortex states do not enter to the FFLO state yet. For example, the small angle neutron scattering (SANS) experiment reported anomalous field-dependence of the flux line lattice (FLL) form factor in CeCoIn\(_5\) [4, 5]. While the FLL form factor exponentially decreases as a function of an applied field \( H \), it increases toward \( H_{c2} \) in CeCoIn\(_5\). Therefore, it is important to quantitatively evaluate the paramagnetic contributions in order to understand the anomalous behaviors in the vortex states.

The purpose of this paper is to evaluate the paramagnetic contributions on the vortex states, mainly investigating the FLL form factor, based on the selfconsistent microscopic calculation of the quasiclassical Eilenberger theory. In our previous studies [6, 7], we quantitatively evaluate the paramagnetic effect on the \( H \)-dependence of low temperature specific heat, Knight shift, and magnetization, which show rapid increases near \( H_{c2} \) by the paramagnetic pair breaking. There, we also studied the FLL form factor and found that in the presence of paramagnetic contributions the FLL form factor does not show the exponential decay as a function of \( H \), and can be a increasing function at lower fields [6, 8]. However, there we could not reproduce
the increasing behaviors towards $H_{c2}$ in CeCoIn$_5$ observed by the SANS experiment. Therefore in this paper, we study the case of further strong paramagnetic contribution to reproduce the experimental results. We also discuss differences of the paramagnetic effects between the $s$- and $d$-wave pairings. In the following, after explaining our formulation in Sec. 2, we investigate the differences of the paramagnetic vortex structure between the $s$- and $d$-wave pairings in Sec. 3, and the $H$-dependence of the FLL form factor in Sec. 4. The last section is devoted to the summary.

2. Eilenberger theory with paramagnetic effect

We calculate the spatial structure of the vortex lattice state by the quasiclassical Eilenberger theory in the clean limit, including the paramagnetic effects due to the Zeeman term $\mu_B B(\mathbf{r})$, where $B(\mathbf{r})$ is the flux density of the internal field and $\mu_B$ is a renormalized Bohr magneton [3, 6]. The quasiclassical Green’s functions $g(\omega_n + i\mu B, \mathbf{k}, \mathbf{r})$, $f(\omega_n + i\mu B, \mathbf{k}, \mathbf{r})$, and $f^\dagger(\omega_n + i\mu B, \mathbf{k}, \mathbf{r})$ are calculated in the vortex lattice state by the Eilenberger equation

$$\begin{align*}
\{ \omega_n + i\mu B + \mathbf{v} \cdot (\nabla + i \mathbf{A}) \} f &= \Delta \phi g, \\
\{ \omega_n + i\mu B - \mathbf{v} \cdot (\nabla - i \mathbf{A}) \} f^\dagger &= \Delta^* \phi^* g,
\end{align*}
$$

(1)

where $g = (1 - f f^\dagger)^{1/2}$, $\text{Reg} \geq 0$, and $\mu = \mu_B B_0/\pi k_B T_c$. We consider two cases of the pairing; $s$-wave pairing $\phi(\mathbf{k}) = 1$, and $d$-wave pairing $\phi(\mathbf{k}) \propto \cos 2\psi$. There $\mathbf{k}$ is the relative momentum of the Cooper pair on the spherical Fermi surface, and $\mathbf{r}$ is the center of mass coordinate of the pair. The normalized Fermi velocity $\mathbf{v} = (\sin \theta \cos \psi, \sin \theta \sin \psi, \cos \theta) \propto \mathbf{k}$. Throughout this paper, length, temperature, magnetic field, and energies are scaled by $R_0$, $T_c$, $B_0$, and $\pi k_B T_c$, respectively [3, 6]. Here, $R_0 = \hbar v_F / 2 \pi k_B T_c$, $B_0 = \hbar c / 2 e R_0^2$. As magnetic fields are applied to the $z$-axis direction, in the symmetric gauge the vector potential $\mathbf{A}(\mathbf{r}) = \frac{\mathbf{B}}{\mu} \times \mathbf{r} + \mathbf{a} (\mathbf{r})$, where $\mathbf{B} = (0, 0, H)$ is a uniform flux density and $\mathbf{a} (\mathbf{r})$ is related to the internal field $\mathbf{B}(\mathbf{r}) = \mathbf{B} + \nabla \times \mathbf{a} (\mathbf{r})$. The unit cell of the vortex lattice for $\Delta(\mathbf{r})$ is given by $\mathbf{r} = s_1 (\mathbf{u}_1 - \mathbf{u}_2) + s_2 \mathbf{u}_2$ with $-0.5 \leq s_i \leq 0.5$ ($i = 1, 2$), $\mathbf{u}_1 = (a, 0, 0)$ and $\mathbf{u}_2 = (a/2, a_y, 0)$. In the $d$-wave pairing, we consider both cases of the square vortex lattice ($a_y/a = 1/2$), and the triangular vortex lattice ($a_y/a = \sqrt{3}/2$), since in CeCoIn$_5$ vortex lattice changes between the triangular lattice and the square lattice depending on fields [4, 5].

The pair potential is selfconsistently calculated by

$$\Delta(\mathbf{r}) = g_0 N_0 T \sum_{0 < \omega_n \leq \omega_{\text{cut}}} \langle \phi^* (\mathbf{k}) (f + f^\dagger) \rangle_k$$

(2)

with $(g_0 N_0)^{-1} = \ln T + 2T \sum_{0 < \omega_n \leq \omega_{\text{cut}}} \omega_n^{-1}$. $\langle \cdots \rangle_k$ indicates the Fermi surface average. We use $\omega_{\text{cut}} = 20 k_B T_c$. The vector potential for the internal magnetic field is selfconsistently determined by

$$\nabla \times (\nabla \times \mathbf{A}) = \nabla \times \mathbf{M}_{\text{para}} (\mathbf{r}) - \frac{2T}{\kappa} \sum_{0 < \omega_n} \langle \mathbf{v} \text{ Im} g \rangle_k,$$

(3)

where in addition to the diamagnetic contribution of supercurrent in the last term we include the contribution of the paramagnetic moment $\mathbf{M}_{\text{para}} (\mathbf{r}) = (0, 0, M_{\text{para}} (\mathbf{r}))$ with

$$M_{\text{para}} (\mathbf{r}) = M_0 \left( \frac{B(\mathbf{r})}{H} - \frac{2T}{\mu H} \sum_{0 < \omega_n} \langle \text{Im} \{ g \} \rangle_k \right).$$

(4)

The normal state paramagnetic moment $M_0 = (\mu/\kappa)^2 H$, $\kappa = B_0 / \pi k_B T_c \sqrt{8\pi N_0}$ and $N_0$ is the density of states at the Fermi energy in the normal state.
Figure 1. Field dependence of the spatial-averaged $|\Delta|$ (a) and the FLL form factor $|F_{1,0}|^2$ (b) at $T = 0.2T_c$. In addition to the s-wave pairing case of the triangular vortex lattice (solid triangle), we show the d wave pairing cases of triangular vortex lattice (open triangle) and square vortex lattice (open square).

In our calculation, $\kappa = 17$, and the paramagnetic parameter $\mu = 5$. In this case of the strong paramagnetic effect, the $H$-dependence of the spatial-averaged $|\Delta|$ at $T = 0.2T_c$ is presented in Fig. 1(a). There, $H_{c2}$ is the first order phase transition, since the free energy becomes positive at $H_{c2}$ without approaching $\Delta \to 0$. $H_{c2} \sim 0.075B_0$ in the s-wave pairing. The difference of $|\Delta|$ between the s-wave and d-wave pairings comes from the different ratio $\Delta/k_BT_c$ of the s- and d-wave pairings.

3. Vortex core structure
In Fig. 2, we show the spatial structure of the vortex states at $H = 0.05B_0$ in the presence of strong paramagnetic effect both for the s-wave and d-wave pairings. As shown in Fig. 2(b), outside vortex core the paramagnetic moment $M_{\text{para}}$ is suppressed as expected in bulk of the spin-singlet superconductivity. However, $M_{\text{para}}$ is enhanced around the normal-state-like region of the vortex core. The reason of the enhancement was discussed in Ref. [6] in the relation to the low energy electronic states around the vortex core. In the d-wave pairing, since the low energy states extend outside the vortex core due to the node of the superconducting gap, $M_{\text{para}}(r)$ outside the core is larger compared to that of the s-wave pairing. Instead, at the vortex center, $M_{\text{para}}(r)$ in the d-wave pairing is smaller than that of the s-wave pairing.

In Fig. 2(c) we present the internal field $B(r)$, which consists of diamagnetic and paramagnetic contributions. There $B(r)$ is further enhanced around the vortex core by the enhanced paramagnetic moment at the core, compared to the case of weak paramagnetic effect [6]. Since the paramagnetic contribution at the vortex center is larger in the s-wave paring, enhancement of $B(r)$ is larger in the s-wave pairing than that in the d-wave pairing.

4. Flux line lattice form factor
One of the experimental method to directly see the contribution of the enhanced paramagnetic moment around the vortex core is to observe the Bragg scattering intensity of the FLL form factor in the SANS experiment. The intensity of the $(h,k)$-diffraction peak is given by $I_{h,k} = |F_{h,k}|^2/|q_{h,k}|$ with the wave vector $q_{h,k} = h\mathbf{q}_1 + k\mathbf{q}_2$, $\mathbf{q}_1 = (2\pi/a_x, -\pi/a_y, 0)$ and $\mathbf{q}_2 = (2\pi/a_x, \pi/a_y, 0)$. The form factor $F_{h,k}$ is given by the Fourier transformation of the internal field as $B(r) = \sum_{h,k} F_{h,k} \exp(iq_{h,k} \cdot r)$. The SANS intensity of the main peak at $(h,k) = (1,0)$ probes the magnetic field contrast between the vortex cores and the surrounding. We show the field dependence of $|F_{1,0}|^2$ in Fig. 1(b). In superconductors with weak paramagnetic effect, $|F_{1,0}|^2$ shows exponential decay as a function of $H$, because the variation of $B(r)$ decreases with increasing $H$. However, in the case of strong paramagnetic effect, $|F_{1,0}|^2$ increases toward $H_{c2}$.
because the variation of $B(r)$ rather increases due to the enhanced paramagnetic moment at the vortex core. The amplitude of the paramagnetic moment roughly proportional to $H$.

The SANS experiment in CeCoIn$_5$ reported that $|F_{1,0}|^2$ is almost constant as a function of $H$ at low fields ($0.4 \, \text{T} \leq H \leq 2.0 \, \text{T}$) [4], and increases toward $H_{c2}$, contrary to the conventional superconductors. This behavior, as reproduced by our calculation in Fig. 1(b), indicates that the superconductivity in CeCoIn$_5$ includes very strong paramagnetic effect, which is also an origin of new FFLO phase and the first order $H_{c2}$ phase transition at higher fields.

5. Summary
We have studied the vortex states in the presence of strong paramagnetic effect by the quasiclassical Eilenberger theory. We have quantitatively investigated the suppression of the superconductivity by the paramagnetic effect, and estimated the $H$-dependence of the FLL form factor. The anomalous $H$-dependences of the FLL form factor of the SANS experiment in CeCoIn$_5$ are explained by the strong paramagnetic effect. This is due to the paramagnetic moment around the vortex core. These are important to properly understand the quantitative behavior of the vortex states in strong-paramagnetic superconductors.

Acknowledgments
We are grateful for useful discussions and communications with T. Mizushima, H. Adachi, N. Nakai, K. Suzuki, K. Kumagai, and M.R. Eskildsen.

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