Coexistence of $d$-wave superconductivity and antiferromagnetism induced by paramagnetic depairing

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Abstract. It is shown theoretically that, in the superconducting state with $d_{x^2-y^2}$-pairing, a strong Pauli paramagnetic depairing (PD) induces not only the modulated Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) superconducting state but also an incommensurate antiferromagnetic (AFM) (or spin-density wave) ordering with $Q$-vector nearly parallel to a gap node. In this mechanism of field-induced coexistence of the $d$-wave superconducting and AFM orders, a pair-density wave does not have to be assumed. It is argued that this is the common origin of both the coexistent FFLO and AFM phases of CeCoIn$_5$ and the AFM quantum critical behavior around the superconducting $H_{c2}(0)$ seen in several unconventional superconductors.

1. Introduction
At present, we have two intriguing issues on a magnetic order or fluctuation occurring close to $H_{c2}(0)$ in $d$-wave paired superconducting states. One is the antiferromagnetic (AFM) quantum critical behavior reflected in transport measurements around $H_{c2}(0)$ of heavy fermion superconductors CeCoIn$_5$ [1-3], pressured CeRhIn$_5$ [4], NpPd$_3$Al$_2$ [5], and Tl-based cuprates [6]. The other is the AFM order [7] in the high field and low temperature (HFLT) phase [8] of CeCoIn$_5$ which has been identified, based on measurements [9,10] and theoretical explanations [11,12] of elastic properties and doping effects, with a Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) state [8,13]. It is notable that the materials listed above have a couple of common features, such as the $d$-wave pairing and a strong Pauli paramagnetic depairing (PD).

In this report, we point out that, in nodal $d$-wave superconductors, a field-induced enhancement of PD tends to induce an AFM ordering in the superconducting phase just below $H_{c2}(0)$. Conventionally, the AFM ordering is suppressed by the superconducting ordering in zero field [14], and, even in nonzero fields, the quasiparticle damping effect brought by the AFM fluctuation usually suppresses a relatively weak PD effect, suggesting a competition between the two orderings. It is found, however, that a strong PD rather favors coexistence of a $d$-wave superconductivity and an incommensurate AFM order, leading to an enhancement of AFM ordering or fluctuation just below $H_{c2}(0)$.

2. Model and Calculation
We work in a BCS-like electronic Hamiltonian [14] with the superconducting energy gap $\Delta$ and the AFM moment $\mathbf{m}$. By treating $\Delta$ at the mean field level and $m \equiv |\mathbf{m}|$ as a fluctuation,
respectively, the free energy describing the two possible orderings in zero field is described by
\[
\mathcal{F}(\mathbf{H} = 0) = \int d^3r \, g^{-1}|\Delta(r)|^2 - T \ln \text{Tr}_{c,c',m} \exp[-(H_{\Delta,m} - \mu N)/T],
\]
\[
H_{\Delta,m} - \mu N = \sum_{\mathbf{q}} \frac{1}{U} |\mathbf{m}(\mathbf{q})|^2 + \sum_{\mathbf{k},\alpha,\beta} \frac{\hat{S}_\alpha^\beta}{2} \xi(\mathbf{k}) \delta_{\alpha,\beta} \hat{c}_{\mathbf{k}\alpha}
- \sum_{\mathbf{q},\alpha,\beta} \left( \Delta(\mathbf{q}) \hat{\Psi}(\mathbf{q}) + m_\nu(\mathbf{q}) \hat{S}_\nu(\mathbf{q}) + \text{h.c.} \right),
\]
where \( \hat{\Psi}(\mathbf{q}) = -i(\sigma_y)_{\alpha,\beta} \sum_{\mathbf{k}} w_{\mathbf{k}} \hat{c}_{-\mathbf{k} + \mathbf{q}/2,\alpha} \hat{c}_{\mathbf{k} + \mathbf{q}/2,\beta}/2, \hat{S}_\nu(\mathbf{q}) = (\sigma_\nu)_{\alpha,\beta} \sum_{\mathbf{k}} \hat{S}_\alpha^\beta \hat{c}_{\mathbf{k} - \mathbf{q}/2,\alpha} \hat{c}_{\mathbf{k} + \mathbf{q}/2,\beta}/2, \hat{S}_\alpha^\beta \) creates a quasiparticle with spin index \( \alpha \) and momentum \( \mathbf{k} \), \( \sigma_\nu \) are the Pauli matrices, \( \mu \) is the chemical potential, and the positive parameters \( g \) and \( U \) are the attractive and repulsive interaction strengths leading to the superconducting and AFM orderings, respectively.

The gap function \( w_{\mathbf{k}} \) satisfies \( w_{\mathbf{k} + \mathbf{Q}} = -w_{\mathbf{k}} \) for the \( \Delta_{a_{x^2}} \) and \( \Delta_{2y} \)-pairing state, and the dispersion \( \xi(\mathbf{k}) \) satisfies \( \xi(\mathbf{k}) = -\xi(\mathbf{k} + \mathbf{Q}) + T_c \delta_{\mathbf{IC}} \), where \( \mathbf{Q} \) is the commensurate AFM modulation wavevector and is \( (\pi, \pi) \) for the \( \Delta_{a_{x^2}} \)-pairing. A small deviation from the perfect nesting is measured by a small parameter \( \delta_{\mathbf{IC}} \) for a nearly-free electron model. If the tight-binding model with \( IC \) notation is used in examining an AFM ordering, the corresponding incommensurability is measured by the second term of the above \( \xi(\mathbf{k}) \). In a nonzero field \( \mathbf{H} \neq 0 \) of our interest, the Zeeman term \( \gamma_B \hat{H}(\sigma_z)_{\alpha,\beta} \) needs to be added to \( \xi(\mathbf{k}) \delta_{\alpha,\beta} \). At least in the case with a continuous \( H_{c2} \)-transition like Fig.2 (a) below, the orbital depairing needs to be incorporated through the familiar quasiclassical treatment on the quasiparticle Green’s function [13].

To see the position of the AFM ordering, it is convenient to examine the Gaussian AFM fluctuation term \( \mathcal{F}_m \) in the free energy \( \mathcal{F} \), \( \mathcal{F}_m = \sum_\Omega \ln \det[\mathbf{U}^{-1}_\alpha \mathbf{q}_\mathbf{\Omega} - \mathbf{\chi}_{\mathbf{q},\mathbf{q}_\mathbf{\Omega}}(\Omega)] \), where
\[
\mathbf{\chi}_{\mathbf{q},\mathbf{q}_\mathbf{\Omega}}(\Omega) = \int_0^{T-1} d\tau \left( T_\tau \mathbf{\hat{S}}_{\mathbf{q}}(\mathbf{\tau}) \mathbf{\hat{S}}_{\mathbf{q}}(\mathbf{\tau}; 0) \right) e^{i\Omega\tau},
\]
and \( \mathbf{\hat{S}}_{\mathbf{q}}(\mathbf{\tau}) \) denotes \( \mathbf{\hat{S}}_{\mathbf{q}}(\mathbf{\tau}) \) at imaginary time \( \tau \). For the moment, we focus on the Pauli limit with no orbital depairing and with uniform \( \Delta \) in which \( \mathbf{\chi}_{\mathbf{q},\mathbf{q}}(\Omega) = [\chi^{(n)}(\mathbf{q}, \Omega) + \chi^{(an)}(\mathbf{q}, \Omega)] \delta_{\mathbf{q},\mathbf{q}_\mathbf{\Omega}} \), and \( \mathcal{F}_m = -\sum_\Omega T \ln X(\mathbf{q}, \Omega), \) where \( X^{-1}(\mathbf{q}, \Omega) = U^{-1} - \chi^{(n)}(\mathbf{q}, \Omega) - \chi^{(an)}(\mathbf{q}, \Omega). \) A second order AFM ordering occurs when \( X^{-1} = X^{-1}(0,0) = 0 \). The \( O(|\Delta|^2) \) terms in \( \chi^{(n)} \) and \( \chi^{(an)} \) are expressed by Fig.1 (a) and (b), respectively. They have been studied previously [14] in \( H = 0 \) case, where \( \chi_s(\Delta) \equiv \chi^{(n)}(0,0) - \chi^{(an)}(0,0) \Delta = 0 + \chi^{(an)}(0,0) \) taking the form
\[
\chi_s(\Delta) = T \int \frac{d^3p}{(2\pi)^3} \sum_{\epsilon,\sigma} 2w^2 \hat{p}^2 (\mathbf{G}_{\epsilon,\sigma}(\mathbf{p}))^2 \Delta^* \mathbf{G}_{-\epsilon,-\sigma}(-\mathbf{p}) \Delta\mathbf{G}_{\epsilon,\sigma}(\mathbf{p} + \mathbf{Q})
\]

Figure 1. Diagrams describing (a) \( \chi^{(n)} \) and (b) \( \chi^{(an)} \) up to \( O(|\Delta|^2) \), where the cross denotes the particle-hole vertex on the AFM fluctuation, while the filled circle implies the particle-particle vertex on \( \Delta \) or \( \Delta^* \).
behaves like $T^{-2}$ in $T \to 0$ limit and is negative so that the AFM ordering is suppressed by superconductivity [14]. In eq.(3), $\mathcal{G}_{\varepsilon,\sigma}(p) \Delta^* \mathcal{G}_{-\varepsilon,-\sigma}(-p) \mathcal{G}_{\varepsilon,\pi}(p + Q) \Delta \mathcal{G}_{-\varepsilon,-\pi}(-p - Q)$

$$\left(\frac{T}{T_c(0)}\right)^2 \mathcal{G}_{\varepsilon,\sigma}(p) \Delta^* \mathcal{G}_{-\varepsilon,-\sigma}(-p) \mathcal{G}_{\varepsilon,\pi}(p + Q) \Delta \mathcal{G}_{-\varepsilon,-\pi}(-p - Q)$$

To explain effects of strong PD, let us first explain the $m \parallel H$ case in which $\sigma = \sigma$. In this case, the two terms in eq.(3) are found to take the same form as the coefficient of the $O(|\Delta|^4)$ term of the superconducting Ginzburg-Landau (GL) free energy and thus, change their sign upon cooling [13]. Hence, $\chi_s(\Delta)$ becomes positive for stronger PD, leading to a lower $F_m$, i.e., an enhancement of the AFM ordering in the superconducting phase. As well as the corresponding PD-induced sign-change of the $O(|\Delta|^4)$ term which leads to the first order $H_{c2}$-transition [13], the PD-induced positive $\chi_s$ is also unaffected by inclusion of the orbital depairing.

In $m \perp H$ where $\sigma = -\sigma$, a different type of PD-induced AFM ordering occurs in a $d$-wave pairing case with a gap node along $Q$ where $w_{p+Q} = -w_p$: In this case, the first term of eq.(3) arising from $\chi^{(a)}(0,0)$ remains negative as in zero field case and becomes $-N(0)|\Delta|^2/\left[2(\gamma_B H)^2\right]$ in $T \to 0$ limit with no PD-induced sign change, where $N(0)$ is the normal density of states. Instead, the last term of eq.(3) implying $\chi^{(a)}(0,0)$ and thus, $\chi_s$ are divergent like $N(0)|\Delta|/(\gamma_B H)^2 \ln[\text{Max}(t, |\delta|)]$ in $T \to 0$ limit while keeping their positive signs owing to the relation $w_{p+Q} < w_p < 0$, where $t = T/T_c$. This divergence is unaffected by including the orbital depairing. That is, in the $d_x^2-y^2$-wave case with $Q = (\pi, \pi)$, the AFM order tends to occur upon cooling in $m \perp H$. In contrast, $\chi^{(a)}(0,0)$ is also negative in the $d_{x^2-y^2}$-wave case with the same $Q$ satisfying $w_p > 0$ so that the AFM ordering is suppressed with increasing $H$.

3. Examples of Phase Diagrams

In this section, examples of the resulting low temperature phase diagram near $H_{c2}(0)$ will be presented. In the BCS-like model (1) and up to the $O(|\Delta|^2)$ terms (see Fig.1), the $H_{c2}$-transition, i.e., the mean field superconducting transition in $H \neq 0$, is of second order even at lower temperatures for $\alpha \equiv \gamma_B H_{c2}(0)/(2\pi T_c) \leq 0.3$ (see Fig.2(a)), where $\alpha$ is nothing but the Maki parameter except a difference in the numerical factor, while it becomes of first order for larger $\alpha \simeq 1.1$ [13]. It is reasonable to expect the former to correspond to the case of CeRhIn$_5$ under a pressure [4]. Figure 2(a) is one of the phase diagrams in such a case, where the Neel temperature $T_N$ in the normal state with perfect nesting or $U$ was assumed to be the only parameter measuring the pressure dependence. The actual AFM transition temperature in $H > H_{c2}(0)$ for $T_N/T_c = 0.02$ and 0.35 are zero and less than 0.35$T_c$, respectively, because of the finite $\delta_{IC} \simeq 0.6$ used in the calculation. Reflecting the AFM ordering enhanced by PD, the decrease of $T_N$, corresponding to an increase of pressure, results in the shrinkage of the AFM phase just below $H_{c2}(0)$, which reduces to an apparent AFM quantum critical point by a further increase of pressure.

Figure 2(b) is the corresponding result in the tight binding model in the Pauli limit with no orbital depairing (vortices). The $H_{c2}$-transition is of first order in the temperature range shown there. Due to the discontinuous nature of the $H_{c2}$-transition, an apparent AFM quantum critical point is estimated, in $h = H/H_{c2}(0) > 1$, to lie at a lower field than $H_{c2}(0)$ in spite of the PD-induced AFM ordering just below $H_{c2}(0)$. This is consistent with the observations in CeCoIn$_5$ [2,7]. We note that the anomalous doping effect in CeCoIn$_5$ [10] cannot be explained without a spatial modulation of $|\Delta|$ in the HFLT phase [12], implying that both the AFM and FFLO orders coexist in the HFLT phase of CeCoIn$_5$. Calculation results in the case including the FFLO structure will be reported elsewhere [15].

We note that, in the present theory explaining the AFM order just below $H_{c2}(0)$ in CeCoIn$_5$
Figure 2. Typical $t$ ($=T/T_c$) v.s. $h = H/H_{c2}(0)$ phase diagrams (a) following from the use of $\alpha = 0.3$ leading to a second order $H_{c2}$-transition even in low $t$ limit and (b) in the Pauli limit with a first order $H_{c2}$-transition in low $t$, respectively. In both figures, an AFM phase can occur below a solid curve on which $X_0^{-1} = 0$, and each nearly vertical dotted curve is the corresponding $H_{c2}(T)$-curve. Note that, in Fig.2(a), two AFM phase boundaries for $T_N/T_c = 0.35$ and 0.02 are shown in a single figure. Figure 2 (b) was obtained from the corresponding calculation in the tight binding model with the parameters $U = 33$, $t_1 = 100$, and $t_2 = 0.25$ in the unit of $T_c$ and by taking account of the full $\Delta$ dependence with no limitation to the $O(\Delta^2)$ term. The dashed curve denotes the possible upper limit of the AFM transition temperatures at which $\chi_s = 0$. The lower panel of (b) is the $h$-dependence of $X_0^{-1}$ at $t = 0.05$.

with strong PD, the assumption [16] of an additional pairing channel (pair-density wave) is unnecessary, and that both of the AFM order [7] and other observations, such as the anomalous doping effect [10], in the HFLT phase of CeCoIn$_5$ are explained consistently if the FFLO modulation in the HFLT phase is assumed.

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