Antiferromagnetic ordering induced by paramagnetic depairing in unconventional superconductors

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Antiferromagnetic (AFM) (or spin-density wave) quantum critical fluctuation enhanced just below \( H_{c2}(0) \) have been often observed in \( d \)-wave superconductors with a strong Pauli paramagnetic depairing (PD) including CeCoIn\(_5\). It is shown here that such a tendency of field-induced AFM ordering is a consequence of strong PD and should appear particularly in superconductors with a gap node along the AFM modulation. Two phenomena seen in CeCoIn\(_5\), the anomalous vortex lattice form factor and the AFM order in the Fulde-Ferrell-Larkin-Ovchinnikov state, are explained based on this peculiar PD effect.

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Recently, the heavy-fermion \( d \)-wave paired superconductor CeCoIn\(_5\) with strong paramagnetic depairing (PD) has been thoroughly studied from the viewpoint of identifying its high field and low temperature (HFLT) phase near the zero temperature depairing field \( H_{c2}(0) \) with a possible Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) state \( ^1 \). On the other hand, this material also shows an antiferromagnetic (AFM) or equivalently, a spin-density wave ordering \( ^2 \) in the HFLT phase and transport phenomena suggestive of an AFM quantum critical point (QCP) lying near \( H_{c2}(0) \) \(^3\). A similar AFM fluctuation enhanced near \( H_{c2}(0) \) has also been detected in other heavy-fermion superconductors \( ^4, ^5 \) and cuprates \( ^6 \), all of which seem to have strong PD and a \( d \)-wave pairing. A conventional wisdom on this issue will be that, in zero field, the nonvanishing superconducting (SC) energy gap suppresses AFM ordering and thus that the field-induced reduction of the gap leads to a recovery of AFM fluctuation. However, it is difficult to explain, based on this picture, why an apparent QCP is realized not above but only just below \( H_{c2}(0) \) \(^7\) in those materials. Rather, the fact that the field-induced AFM ordering or QCP close to \( H_{c2}(0) \) is commonly seen in superconductors with a \( d \)-wave pairing and strong PD suggests a common mechanism peculiar to superconductivity in finite fields and independent of electronic details of those materials such as the band structure.

In this paper, we point out that, in nodal \( d \)-wave superconductors, a field-induced enhancement of PD tends to induce an AFM ordering just below \( H_{c2}(0) \). Although relatively weak PD tends to be suppressed by the quasiparticle damping effect brought by the AFM fluctuation, strong PD rather favor coexistence of a \( d \)-wave superconductivity and an AFM order. Detailed mechanism of this field-induced enhancement of AFM fluctuation or ordering below \( H_{c2} \) depends upon the relative orientation between the moment \( \mathbf{m} \) of the expected AFM order and the applied field \( \mathbf{H} \). In \( \mathbf{m} \parallel \mathbf{H} \) case, strong PD change the sign of the \( O(m^2|\Delta|^2) \) term in the free energy for any pairing symmetry, just like that of its \( O(|\Delta|^4) \) term leading to the first order \( H_{c2} \)-transition \(^2\), where \( m \equiv |\mathbf{m}| \) and \( \Delta \) are order parameters of an expected AFM phase and a spin-singlet SC one. In contrast, the field-induced AFM ordering in \( \mathbf{m} \perp \mathbf{H} \), which is possibly satisfied in CeCoIn\(_5\) in \( \mathbf{H} \perp c \) \(^8\), is a peculiar event to the \( d \)-wave paired case with the momentum (\( k \)) -dependent gap function \( w_k \) satisfying \( w_k = -w_{k+Q} \) and tends to occur irrespective of the presence of the first order \( H_{c2} \)-transition, where \( Q \) is the wave vector of the commensurate AFM modulation. As a consequence of this PD-induced magnetism, two striking phenomena observed in CeCoIn\(_5\), an AFM order \(^9\) stabilized by a FFLO spatial modulation and an anomalous flux density distribution in the vortex lattice \(^{10} \), will be discussed.

First, we start from a BCS-like electronic Hamiltonian \(^{11} \) for a quasi two-dimensional (2D) material with \( \Delta \) and \( m \) introduced as functionals. By treating \( \Delta \) at the mean field level, the free energy expressing the two possible orderings is written in zero field case as

\[
F(\mathbf{H}=0) = \sum_{\mathbf{r}} \frac{1}{g} |\Delta(\mathbf{r})|^2 - T \ln \text{Tr}_{c,\mathbf{r},m} \exp[-H_{\Delta m}/T],
\]

\[
H_{\Delta m} = \sum_{\alpha,\beta=\uparrow,\downarrow} \left( \sum_{\mathbf{k}} \mathbf{c}_{\mathbf{k},\alpha} \mathbf{c}_{\mathbf{k},\beta} \delta_{\alpha,\beta} \mathbf{\hat{c}}_{\mathbf{k},\beta} - \sum_{\mathbf{q}} [\mathbf{m}(\mathbf{q}) \cdot \mathbf{\hat{S}}(\mathbf{q})^\dagger] + \text{h.c.} \right) + \sum_{\mathbf{q}} \left( \frac{1}{U} [\mathbf{m}(\mathbf{q})]^2 + \Delta(\mathbf{q}) \Psi(\mathbf{q})^\dagger \Psi(\mathbf{q}) \right),
\]

where

\[
\Psi(\mathbf{q}) = -\sum_{\mathbf{k}} w_k \hat{c}_{\mathbf{k}+\mathbf{q}/2,\uparrow} \hat{c}_{\mathbf{k}+\mathbf{q}/2,\downarrow}, \quad \hat{S}_\nu(\mathbf{q}) = (\sigma_\nu)_{\alpha,\beta} \sum_{\mathbf{k}} \hat{c}_{\mathbf{k}+\mathbf{Q},\alpha} \hat{c}_{\mathbf{k}+\mathbf{Q},\beta}/2, \quad \hat{c}_{\mathbf{k},\alpha} \text{ creates a quasiparticle with spin index } \alpha \text{ and momentum } \mathbf{k}, \quad \sigma_\nu \text{ are the Pauli matrices, and the positive parameters } g \text{ and } U \text{ are the attractive and repulsive interaction strengths leading to the SC and AFM orderings, respectively. The dispersion } \epsilon_{\mathbf{k}} \text{, measured from the chemical potential, satisfies } \epsilon_{\mathbf{k}} = -\epsilon_{\mathbf{k}+Q} + T_\delta \delta_{\mathbf{k},\alpha,\beta} \text{, where a small parameter } \delta_1 \text{ measuring an incommensurability of the AFM order was introduced. In the case with a nonzero } \mathbf{H} \text{ of our interest, the Zeeman energy } \mu_H \mathbf{H} \cdot (\sigma)_{\alpha,\beta} \text{ needs to be added to } \delta_{\mathbf{k},\alpha,\beta}. \text{ Below, we focus on either the case, } \mathbf{m} \perp \mathbf{H} \text{ or } \mathbf{m} \parallel \mathbf{H} \text{ by choosing the spin quantization axis along } \mathbf{H}. \text{ The orbital field effect will be included later.}
\]

To examine an interplay between the AFM and SC orderings below, let us consider the Gaussian AFM
induced AFM ordering occurs in a

\[ \chi_{q,\Omega}(q) = \int_0^{T-1} d\tau \langle T_\tau \hat{S}_\nu(q;\tau) \hat{S}_\nu(q';0) \rangle e^{i\Omega \tau}, \tag{2} \]

with a fixed \( \nu \), and \( \hat{S}_\nu(q) \) denotes \( \hat{S}_\nu(q) \) at imaginary time \( \tau \). For the moment, we focus on the Pauli limit with no orbital field effect and with uniform \( \Delta \) in which \( \chi_{q,\Omega}(q) = [\chi^{(n)}(q,\Omega) + \chi^{(an)}(q,\Omega)] e^{-\Omega q^2} \), and

\[ \chi^{(n)}(0,\Omega) = -T \sum_{p,\xi,\sigma=\pm 1} \sum_{\xi',\sigma'} \frac{d_{\xi,\sigma}(e_{p+Q}) d_{\xi',\sigma}(e_{p})}{D_{\xi+\Omega,\pi}(p+Q) D_{\xi',\sigma}(p)}, \]

\[ \chi^{(an)}(0,\Omega) = T \sum_{p,\xi,\sigma=\pm 1} \sum_{\xi',\sigma'} \frac{(-w_p w_{p+Q}) |\Delta|^2}{D_{\xi+\Omega,\pi}(p+Q) D_{\xi',\sigma}(p)}, \tag{3} \]

where \( e_p \) is a fermion’s (boson’s) Matsubara frequency, \( d_{\xi,\sigma}(e_p) = i e \pm \sigma \mu B H + e_p \), and \( D_{\xi,\sigma}(p) = d_{\xi,\sigma}(e_p) d_{\xi',\sigma}(e_{-p}) + |\Delta|^2 / |\Delta|^2 \). Main features of \( \chi^{(n)} \) and \( \chi^{(an)} \) are seen in their \( O(|\Delta|^2) \) terms. In zero field, \( \chi_s(\Delta) \equiv \chi_s(0,0) \) behaves like \( T^{-2} \) in \( T \to 0 \) limit and is negative so that the AFM ordering is suppressed by superconductivity.\[10]\]

To explain results in the case of strong PD, let us first focus on \( \mathbf{m} \parallel \mathbf{H} \) case in which \( \sigma = \sigma \). For a near-perfect nesting, the \( O(|\Delta|^2) \) terms of \( \chi^{(n)}(\Delta=0) \) and \( \chi^{(an)}(\Delta=0) \), at \( |q| = \Omega = 0 \), take the same form as the coefficient of the quartic \( O(|\Delta|^4) \) term in the approximate GL energy and thus, change their sign upon cooling.\[12,13]\] Thus, \( \chi_s(\Delta) \) becomes positive for stronger PD, leading to a lower \( \mathcal{F}_m \), i.e., an enhancement of the AFM ordering in the SC phase. As well as the corresponding PD-induced sign-change of the \( O(|\Delta|^2) \) term which leads to the first order \( H_{c2} \) transition,\[2,12]\] the PD-induced positive \( \chi_s \) is also unaffected by inclusion of the orbital depairing.

In \( \mathbf{m} \perp \mathbf{H} \) 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 \( w_{p+Q} w_p < 0 \) : In this case, the \( O(|\Delta|^2) \) term of \( \chi^{(n)}(0,0) \) remains negative and becomes \( -N(0)|\Delta|^2 / [2(\mu_B H)^2] \) in \( T \to 0 \) limit with no PD-induced sign change, where \( N(0) \) is the density of states in the normal state. Instead, the corresponding \( \chi^{(an)}(0,0) \) and thus, \( \chi_s \) are divergent like \( N(0)|\Delta^2 / [2(\mu_B H)^2] \ln[\text{Max}(t,|\delta_1|)] \) in \( T \to 0 \) limit while keeping their positive signs, where \( t = T/T_c \). This divergence is unaffected by including the orbital depairing. That is, in the \( d_{xy}-d_{xy} \)-wave case with \( \mathbf{Q} = (\pi, \pi) \), the AFM order tends to occur upon cooling even in \( \mathbf{m} \perp \mathbf{H} \). In contrast, \( \chi^{(an)}(0,0) \) is also negative in the \( d_{xy}-d_{xy} \)-wave case satisfying \( w_{p+Q} w_p > 0 \) so that the AFM ordering is rather suppressed with increasing \( H \).

A possible AFM phase boundary in \( \mathbf{m} \parallel c \perp \mathbf{H} \) defined as the temperature at which \( X_0^{-1} \equiv |X(0,0)|^{-1} \) vanishes up to \( O(|\Delta|^2) \) is shown in Fig.2(a) together with the corresponding \( \chi_s = 0 \) curve, which is the upper limit of a PD-induced AFM phase to occur and shifts to higher temperature for larger \( |\delta_1| \). Here, the orbital depairing brought by the gauge field \( \mathbf{A} \) has been incorporated through the quasiparticle Green’s function \( G_{\varepsilon,\sigma}(r_1, r_2) \) in real space with its semiclassical replacement \[2,12]\]

\[ G_{\varepsilon,\sigma}(r_1, r_2) \equiv G_{\varepsilon,\sigma}(r_1 - r_2) \exp[i e (hc)^{-1} \int_{r_2} A \cdot dl] \].

In Fig.2(a), we have used \( \alpha_M^{(ab)} \) (Maki parameter in \( \mathbf{H} \perp c \) defined as the temperature at which \( X_0^{-1} \equiv |X(0,0)|^{-1} \) vanishes up to \( O(|\Delta|^2) \) is shown in Fig.2(a) together with the corresponding \( \chi_s = 0 \) curve, which is the upper limit of a PD-induced AFM phase to occur and shifts to higher temperature for larger \( |\delta_1| \). Here, the orbital depairing brought by the gauge field \( \mathbf{A} \) has been incorporated through the quasiparticle Green’s function \( G_{\varepsilon,\sigma}(r_1, r_2) \) in real space with its semiclassical replacement \[2,12]\]

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\[ G_{\varepsilon,\sigma}(r_1, r_2) \equiv G_{\varepsilon,\sigma}(r_1 - r_2) \exp[i e (hc)^{-1} \int_{r_2} A \cdot dl] \].
\[ \frac{\gamma hc}{(2e \xi_0^3)} \] is the \( H_{c2}(0) \)-value in \( H \parallel c \) defined near \( T_c \) with the coherence length \( \xi_0 \). The AFM phase is lost in \( H > H_{c2} \) due to the discontinuous \( H_{c2} \)-transition in \( t < 0.215 \). With a larger \( X_0^{-1} \) in the normal state, the uniform AFM phase boundary in Fig.2(a) is pushed down to \( t = 0 \) to reduce to an AFM-QCP.

The limitation to the \( O(|\Delta|^2) \) term of \( \chi_s \) overestimates the AFM ordering. In fact, using the full expression of \( \chi_s \), the AFM region for \( \delta_t = 0 \) is limited to an invisibly narrow region in the vicinity of \( H_{c2}(0) \). Nevertheless, the PD-induced AF order for nonzero \( \delta_t \) also follows from the full \( \chi_s(\Delta) \). By substituting \( \Delta \) obtained from the gap equation into eq.(3), the lines on which the full \( \chi_s(\Delta) \) vanishes are obtained, in the Pauli limit with uniform \( \Delta \), as the dashed curves in Fig.2(b). The \( \chi_s > 0 \) region becoming wider with increasing \( |\delta_t| \) suggests that, as in CeCoIn\( _5 \), the PD-induced AFM order near \( H_{c2}(0) \) should be incommensurate. Similar results also follow from the direct use of the tight-binding model \( \boxed{16} \).

Interestingly, the AFM ordered region is expanded further by the presence of the FFLO modulation \( \Delta(\zeta) \equiv \sqrt{2} \cos(q_{LO} \zeta) \), where \( \zeta \) is the component parallel to \( H \) of the coordinate. To demonstrate this, the gradient expansion \( \boxed{15} \) will be applied to the \( O(m^2) \) term of the mean field expression of \( \mathcal{F}_m \). Up to the lowest order in the gradient, its \( O(\zeta) \)-dependent part simply becomes

\[
\delta \mathcal{F}^{\text{(MF)}}_m = \int d\zeta m(\zeta) \left[ -(X_0^{-1}(\zeta)^2 \frac{\partial^2}{\partial \zeta^2} - \chi_s(\Delta(\zeta))) \right] m(\zeta),
\]

where \( (X_0^{-1}(\zeta)^2 = \partial^2 X^{-1}(k,0)/\partial k^2)_{k=0} \). and we only have to examine its sign which, for uniform \( \Delta \), corresponds to that of \( -\chi_s \). For simplicity, by using the \( q_{LO} \)-data in Ref.\[14\], we find that \( \delta \mathcal{F}^{\text{(MF)}}_m \) \( < 0 \) below the blue solid curve in Fig.2(b), indicating that the FFLO order can coexist with the AFM order in most temperature range. Close to the FFLO transition (red solid) curve on which \( q_{LO} = 0 \), \( m(\zeta) \) is found to have the modulation \( \sim \sin(q_{LO} \zeta) \), so that this AFM order is continuously lost as the FFLO nodal planes goes away from the system \( \boxed{17} \). Oppositely, the form of \( m(\zeta) \) deep in the FFLO state may not be examined properly in terms of the present gradient expansion and will be reconsidered elsewhere.

Next, we examine the anomalous flux density distribution in the vortex lattice of CeCoIn\( _5 \) in \( H \parallel c \) as another phenomenon suggestive of an AFM fluctuation enhanced just below \( H_{c2} \). The flux distribution is measured by the form factor \( |F| \), which is the Fourier component of the longitudinal magnetization \( M_s(\mathbf{r}) = (B_s(\mathbf{r}) - H)/(4\pi) \) at the shortest reciprocal lattice vector \( \mathbf{K} \) and implies the slope of the flux density \( B_s \) in real space. Here, \( M_s(\mathbf{r}) = \sum_{\mathbf{K} \neq 0} M_s(\mathbf{K}) e^{i \mathbf{K} \cdot \mathbf{r}} \) is given by

\[
M_s(\mathbf{K}) = ic^{-1}K^{-2} \left[ \mathbf{K} \times \mathbf{j}(\mathbf{K}) \right]_c - \frac{\delta \mathcal{F}}{\delta B_{pd}(-\mathbf{K})} \bigg|_{B_{pd} = 0},
\]

where \( \mathbf{j}(\mathbf{K}) \) and \( B_{pd}(\mathbf{K}) \) are Fourier components of the orbital supercurrent density and a Zeeman field \( B_{pd} \) imposed to define \( M_s \), respectively. It is straightforward to, based on the approach in Ref.\[2 \], obtain \( M_s \) in the weak-coupling model with no AFM fluctuation by fully taking account of the PD and the orbital depairing. In our numerical calculations, the \( O(|\Delta|^4) \) contributions to \( M_s \) are also incorporated. Nevertheless, it is instructive to first focus on its \( O(|\Delta|^2) \) terms. In \( H \ll H_{c2}\parallel(0) \), the contribution to \( M_s \) from the spin part (last term) of eq.(5) is given by

\[
M_s(\mathbf{K})^{(pd)} = \frac{\mu_B N(0)}{2\pi T}|\Delta(\mathbf{K})\text{Im} \psi(1) + i \frac{\mu_B H}{2\pi T};
\]

which is negative, where \( \psi(1) \) is the first derivative of the digamma function. Thus, the PD tends to enhance the magnetic screening far from the vortex core. This is one of origins inducing a field-induced increase of \( |F| \). However, such an enhancement of \( |F| \) calculated beyond the \( O(|\Delta|^2) \) terms in the weak coupling model is much weaker in the \( d \)-wave case than in the \( s \)-wave one \( \boxed{18} \), although it is the \( d \)-wave material CeCoIn\( _5 \) which has clearly shown such an enhanced \( |F| \) \( \boxed{9} \). This has motivated us to see how the PD-induced AFM fluctuation is reflected in \( |F| \). For this purpose, let us first consider the \( \mathbf{m} \perp \mathbf{H} \) case and start with the Pauli limit again in which \( M_s \) is determined by the last term of eq.(5). By noting that this term can be obtained as the first derivative of the free energy density with respect to \( \mu_B H \), it is found that the contribution to \( M_s \) from the Gaussian AFM fluctuation is positive and proportional to \( \sim O(|\Delta(\mathbf{r})|^2) \mu_B H \sum_{\mathbf{q}} X(\mathbf{q},0)/T^3 \), implying a suppressed screening due to the AFM fluctuation, for weak PD (\( \mu_B H \ll T \)), while it is negative and given by \( -2\mu_B T|\Delta(\mathbf{r})|^2(\mu_B H)^{-3} |\mu_B| \text{Max}(|\delta_t|,|t|) \sum_{\Omega} \sum_{\mathbf{q}} X(\mathbf{q},\Omega), \) suggesting an enhancement due to the AFM fluctuation of the screening and thus, of \( |F| \), for strong PD (\( \mu_B H \gg T \)), respectively.

In Fig.3, we show \( h \) v.s. \( |F| \) curves obtained by incorporating the orbital depairing for both cases with and without contributions to eq.(5) from the AFM fluctuation through \( \mathcal{F}_m \), where \( |F| \) was normalized by that in the GL region near \( T_c \). Based on the result in Fig.2(a), the familiar phenomenological form of \( X(\mathbf{q},\Omega), N(0)X(\mathbf{q},\Omega) = 1/[m_N(t,h) + (\mathbf{q} \times \mathbf{z})^2 \xi_0^{(N)} + \xi_0^{(N)}] /\mu_B T \) was assumed in calculating the \( \mathcal{F}_m \)-contribution to eq.(5), where \( m_N(t,h) = t + 1 - h/h_{QCP} \), and \( \xi_0^{(N)} = 0.68 \xi_0 \), and \( v^2 \) is the squared Fermi velocity averaged over the Fermi surface. The remarkable peak just below \( H_{c2} \) of the red solid curve is a reflection of the afore-mentioned growth of \( \chi^{(an)} \) in \( \mathbf{m} \perp \mathbf{H} \). A similar \( |F| \)-enhancement also occurs in \( \mathbf{m} \parallel \mathbf{H} \) (dashed) curves with increasing \( H \), reflecting the afore-mentioned sign change of \( \chi_s \) due to large PD. To the best of our knowledge, the favorable direction of the moment in CeCoIn\( _5 \) in \( H \parallel c \) is unclear at present. If, in CeCoIn\( _5 \), the \( \mathbf{m} \parallel \mathbf{H} \) components are dominant in the AFM fluctuation even in \( H \parallel c \), the \( |F(t,h)| \) data \( \boxed{9} \) growing with increasing field and on further cooling is a reflection of the \( d_2-\gamma^2 \)-wave pairing \( \boxed{19} \) accompanied by a strong AFM fluctuation with \( Q \parallel (\pi, \pi) \).
In conclusion, an AFM ordering or fluctuation enhanced close to $H_{c2}(0)$, often seen in unconventional superconductors, is a direct consequence of strong paramagnetic depairing and also of their $d$-wave pairing symmetry with a gap node parallel to the AFM modulation. The AFM ordering enhanced due to the FFLO modulation suggests that the HFLT phase in CeCoIn$_5$ is a coexisting state of the AFM and FFLO orders. Discussing the AFM-QCP issues in systems with a $d$-wave pairing symmetry, the present work is straightforward and will be performed elsewhere.

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