Magnetism and superconductivity in ferromagnetic heavy-fermion system UCoGe under in-plane magnetic fields

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We study the ferromagnetic superconductor UCoGe at ambient pressure under ab-plane magnetic fields $\boldsymbol{H}$, which are perpendicular to the ferromagnetic easy axis. It is shown that, by taking into account the Dyaloshinskii-Moriya interaction arising from the zigzag chain crystal structure of UCoGe, we can qualitatively explain the experimentally observed in-plane anisotropy for critical magnetic fields of the paramagnetic transition. Because of this strong dependence on the magnetic field direction, upper critical fields of superconductivity, which is mediated by ferromagnetic spin fluctuations, also become strongly anisotropic. The experimental observation of S-shaped $H_{c2} \parallel b$ axis is qualitatively explained as a result of enhancement of the spin fluctuations due to decreased Curie temperature by the b-axis magnetic field. We also show that the S-shaped H_{c2} is accompanied by a rotation of the d vector, which would be a key to understand the experiments not only at ambient pressure but also under pressure.

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I. INTRODUCTION

Since the discovery of a ferromagnetic superconductor UGe_2, a family of ferromagnetic systems, URhGe and UCoGe, has also been found to exhibit superconductivity and they have been extensively studied with special focus on the relationship between ferromagnetism and superconductivity [1–3]. In these compounds, $5f$ electrons are responsible both for the magnetism and the superconductivity, in sharp contrast to the previously found ferromagnetic superconductors, such as $ErRh_4B_4$ and $HoMo_6S_8$, where the magnetism and superconductivity have distinct origins [4].

Among these uranium compounds, UCoGe has the lowest Curie temperature $T_C \sim 2.7$ K and the superconducting transition temperature $T_{sc} \sim 0.6$ K at ambient pressure [3,5–10]. The ferromagnetism is suppressed by applying pressure and T_C seems to approach zero at a critical pressure $p_c \sim 1.3$ GPa. Below this critical pressure $p < p_c$, ferromagnetism and superconductivity coexist in a microscopic way [11,12], while the superconductivity alone survives up to $p > p_c$. The experimental pressure-temperature phase diagram of UCoGe could be understood from theoretical model calculations where Ising spin fluctuations mediate superconductivity [13–17]. Indeed, as revealed by the NMR experiments, spin fluctuations in UCoGe have strong Ising anisotropy and the superconductivity is closely correlated with them especially under magnetic fields [18–20]. The experiments show that the a-axis upper critical field is huge $H_{c2}^{\parallel a} > 25$ T in spite of the low transition temperature $T_{sc} \sim 0.6$ K while H_{c2} for the c axis is merely less than 1 T, which leads to cusplike field angle dependence of H_{c2} in the ac plane. From a theoretical point of view, the anomalous behaviors of the observed ac-plane upper critical fields of the superconductivity can be well understood by taking into account the experimental fact that the Ising spin fluctuations are tuned by a c-axis component of the magnetic fields [19,21]. The successful agreement between the experiments and theories provides strong evidence for a scenario that the pseudospin triplet superconductivity is indeed mediated by the Ising ferromagnetic spin fluctuations in UCoGe.

On the other hand, different characteristic behaviors have been experimentally observed for b-axis magnetic fields in UCoGe [8–10,22]. In the normal (nonsuperconducting) states, the Curie temperature T_C is suppressed by $\boldsymbol{H} \parallel b$ axis and it seems to become zero around $H^* \sim 15$ T, although it is unchanged for $\boldsymbol{H} \parallel a$ axis in the same experiments. The reduction of T_C by $\boldsymbol{H} \parallel b$ axis is accompanied by an enhancement of the spin fluctuations. Accordingly, at low temperatures, H_{c2} is enhanced by the b-axis magnetic field especially around $H = H^*$, resulting in S-shaped H_{c2}. Interestingly, similar behaviors have also been found in the isomorphic compound URhGe, where superconductivity vanishes at a critical $\boldsymbol{H} \parallel b$ axis but it reappears at a high field around which ferromagnetism is suppressed with a tricritical point [23–26].

From a theoretical point of view, based on a scenario of the spin-fluctuations-mediated superconductivity, it is rather natural to expect S-shaped H_{c2} or even reentrant superconductivity, once one simply takes into account enhancement of the spin fluctuations by the reduction of T_C. However, within this theoretical approach, which strongly relies on the experimental observations of anisotropic behavior with the application of in-plane magnetic fields, it is unclear why T_C is unchanged and therefore H_{c2} is not enhanced for a-axis magnetic fields. In order to understand the dependence of H_{c2} on the direction of magnetic field, we should clarify the origin of in-plane magnetic anisotropy. Furthermore, even if one just admits magnetic anisotropy as an experimental fact, the nature of the resulting superconducting state under strong b-axis magnetic field is far from trivial. For small magnetic fields, the superconductivity will coexist with the ferromagnetism as in the zero-field case, and it is robust against the Pauli depairing effect under in-plane magnetic fields due to exchange splitting of the Fermi surface as pointed out by Mineev [27]. On the other hand, for larger magnetic fields

$H \gtrsim H^*$ where the superconductivity survives experimentally, the exchange splitting is small or even vanishing, and therefore the Mineev's mechanism protecting the superconductivity from the Pauli depairing effect does not work. The limitation of the Mineev's mechanism on the Pauli depairing effect should also be recognized for understanding H_{c2} under high pressure where ferromagnetism is suppressed. Even in paramagnetic states where the Pauli depairing effects are expected to be important, experiments obtain large in-plane $H_{c2} \sim 7$–8 T, which is well above the Pauli limiting field estimated from $T_{sc} \sim 1$ K [28]. These values of H_{c2} were obtained without fine tuning of the magnetic field directions and H_{c2} would be further increased by careful tuning of the field directions, since it sensitively depends on a c-axis component of the magnetic fields in UCoGe [8,19]. Theoretically, it is expected that the spin fluctuations are large especially around $p = p_c$ leading to strong coupling superconductivity and the orbital depairing effect would be less relevant there, while the Pauli depairing effect is not suppressed and eventually will break the superconductivity.

In this study, we investigate anisotropy for in-plane critical magnetic fields of paramagnetic transition and superconducting H_{c2} in UCoGe. First, we make an analysis focusing on the zigzag chain crystal structure, which is characteristic in UCoGe. Within a minimal spin model including effects of the zigzag chain structure, we show that the Dyaloshinskii-Moriya (DM) interaction arising from the zigzag structure leads to the in-plane anisotropy for critical magnetic fields of paramagnetic transitions, which shows a qualitative agreement with the experiments. We then examine resulting superconducting H_{c2} phenomenologically considering the suppression of ferromagnetism by application of external fields along the b axis. It is shown that superconductivity can survive above H^* where there is no exchange splitting of the Fermi surface. We find that this robustness of superconductivity stems from the d-vector rotation to reduce magnetic energy cost as the magnetic field is increased. We also touch on the experimental observations based on our calculations.

II. ANISOTROPY FOR CRITICAL MAGNETIC FIELD OF PARAMAGNETIC TRANSITION AND ITS ORIGIN

In this section, we study the origin of strong dependence of critical magnetic field H^* on the field direction in the ab plane. As mentioned in the previous section, the Curie temperature is decreased by magnetic field along the b axis, while it is unchanged by a magnetic field applied parallel to the a axis within the experimental range [8–10,22]. If the magnetic fields are further increased, T_C will be suppressed for a-axis magnetic fields as well. We schematically show an expected magnetic phase diagram of UCoGe in Fig. 1. T_C decreases rapidly by applying magnetic field along the b axis and eventually becomes zero at a critical field H_b^* at zero temperature, while it is robust against the a-axis field and the corresponding critical field H_a^* is much larger than H_b^*. The purpose of this section is to understand qualitatively what causes this anisotropy in the ab plane. Magnetic anisotropy generally arises from spin-orbit interactions, and its details depend on strength of the spin-orbit interactions and crystal structures. In f-electron compounds, basic magnetic properties could be well

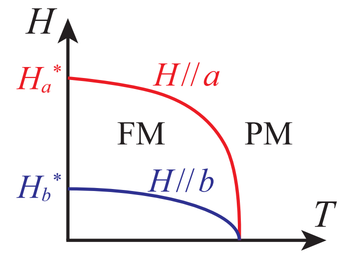

FIG. 1. Expected magnetic phase diagram of UCoGe in temperature (T)-magnetic field (H) plane. FM and PM refer to ferromagnetic phase and paramagnetic phase, respectively. H_a^* and H_b^* are critical magnetic fields at zero temperature.

understood once the local electronic configuration has been fixed by, e.g., neutron scattering experiments. For UCoGe, the experimentally observed Ising magnetic properties may be due to a large weight of $J = 5/2$ states in the single electron state at the U sites. Although precise determination of a level scheme in $5f$-electron systems with low crystal symmetry, such as UGe_2 and UCo(Rh)Ge is very difficult, the resistivity in UCoGe shows rather conventional heavy fermion behaviors with weak anisotropy in effective mass. This implies that UCoGe is well described by effective pseudospin 1/2 quasiparticles corresponding to the observed Ising-like magnetism.

Here, instead of using local electronic structures, we investigate the magnetic anisotropy in UCoGe by focusing on its characteristic crystal structure. As seen in Fig. 2, UCoGe can be viewed as a composition of one-dimensional zigzag chains along the a axis. The point group of UCoGe is $Pnma$ and the zigzag chains do not have local inversion symmetry, although they keep global inversion symmetry. Such a quasi-one-dimensional zigzag structure allows an asymmetric spin-orbit (ASO) interaction [29]

$$H_{\mathrm{ASO}} \sim \sum_{kss'} \sin k_a \sigma^b_{ss'} [a^\dagger_{ks} a_{ks'} - b^\dagger_{ks} b_{ks'}], \tag{1}$$

where $a_{ks}(b_{ks})$ is an annihilation operator of the quasiparticles at the A (B) sublattice of the zigzag chain. In order to understand effects of the ASO interaction qualitatively, we focus only on spin degrees of freedom and introduce a counterpart of the ASO interaction in the spin sector of electrons. Then, in terms of the spin degrees of freedom, the ASO interaction is mapped to a staggered DM interaction,

$$H_{\mathrm{DM}} = \sum_j (-1)^j D_b \left[S^c_j S^a_{j+2} - S^a_j S^c_{j+2} \right], \tag{2}$$

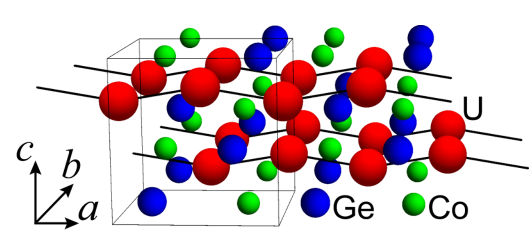

FIG. 2. The crystal structure of UCoGe. Zigzag chains are along the a axis.

where S_j with $j =$ odd (even) corresponds to the pseudospin 1/2 at the A (B) sublattice of the zigzag chain. Note that the direction of the DM vector $\boldsymbol{D} = (0, D_b, 0)$ is consistent with a general symmetry argument for $Pnma$ of UCoGe [30]; there is a mirror symmetry with respect to the $(x, 1/4, z)$ plane [31], which results in $\boldsymbol{D} \parallel b$ axis. In order to elucidate the effect of this DM interaction in the quasi-one-dimensional systems, we investigate a single zigzag chain neglecting interchain interactions. Under this assumption, spin degrees of freedom in UCoGe are described by the following one-dimensional spin Hamiltonian,

$$H_{\rm spin} = -J \sum_j S_j^c S_{j+1}^c - \sum_j \left[h_a S_j^a + h_b S_j^b\right] + H_{\rm DM}. \quad (3)$$

The first term is the Ising ferromagnetic interaction and the second term corresponds to the ab-plane magnetic fields. We have neglected spin-spin interactions of in-plane spin components, since the magnetism of UCoGe has strong Ising nature as verified by the experiments [18–20]. In this section, we use a unit where $J = 1$. This spin model should be considered as a variant of the phenomenological Ginzburg-Landau theory developed by Mineev, where the free energy is written in terms of magnetic degrees of freedom only [32]. In the present study, we use the above spin model as an effective phenomenological description to capture essential physics behind the complicated experimental results with a special focus on the DM interaction. Although the spin model is oversimplified for discussing quantitative properties of UCoGe, it is useful for qualitative discussions as a minimal model. Indeed, as will be discussed in the following, the physical mechanism leading to magnetic anisotropy under in-plane magnetic fields revealed within the spin model analysis is applicable also for more realistic models of UCoGe. We also note that, since the Landé g factors have not been determined in UCoGe, the parameters h_a, h_b should be regarded as a renormalized magnetic fields, which include g factors. Anisotropy of diagonal components of the g factors in a,b directions is expected to be small, $g_{aa} \simeq g_{bb}$, since M-H curves show weak anisotropy between M_a and M_b for small magnetic fields [5]. Although there may be off-diagonal components of the g factor we simply neglected them. If g_{ca} or g_{cb} is large, the ferromagnetic phase transitions are smeared out and become crossover under in-plane magnetic fields. In the present model without such off-diagonal components, there is $\mathbb{Z}_2$ symmetry for general $\boldsymbol{h} = (h_a, h_b, 0)$ with the operation (translation) × (time-reversal) × $\exp[i\pi \sum_j S_j^c]$, which transforms spins as

$$\begin{aligned} S_j^a &\to S_{j+1}^a, \\ S_j^b &\to S_{j+1}^b, \\ S_j^c &\to -S_{j+1}^c. \end{aligned} \quad (4)$$

This symmetry is spontaneously broken in the ferromagnetic phase.

In order to understand the anisotropy of the critical fields H^*, we investigate the Hamiltonian (3) at $T = 0$ by use of infinite density matrix renormalization group (iDMRG) [33–35]. In the present one-dimensional model, we find that the calculated ground state preserves the translational symmetry and the system undergoes a quantum phase transition from a uniform ferromagnetic state with $\langle S_j^c \rangle \neq 0$ to a disordered state

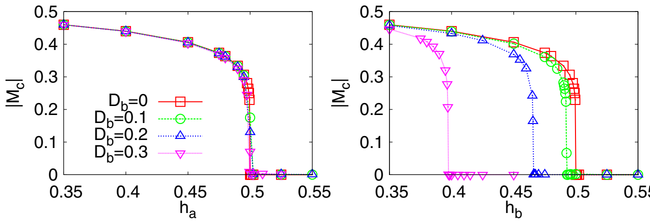

FIG. 3. The c-axis magnetization $|M_c|$ for different values of the DM interaction under the a-axis magnetic field (left) and b-axis magnetic field (right).

with $\langle S_j^c \rangle = 0$ as h is increased. We have confirmed absence of a nonuniform magnetic structure by increasing sizes of assumed sublattice structures in the numerical calculations. This is essentially due to strong Ising anisotropy, which favors the colinear ferromagnetic structure, and coplanar magnetic states might be stabilized if one appropriately includes interchain coupling and the DM interaction is sufficiently large. We note that, indeed, such a coplanar state with a-axis weak antiferromagnetism has been predicted within the Ginzburg-Landau theory [32].

In Fig. 3, we show magnetization as a function of magnetic fields for different values of the DM interaction within our model. For small magnetic fields, the magnetization does not change from that without the DM interaction, since the ground state of the Ising Hamiltonian at $h = 0$ is at the same time an eigenstate of the DM interaction, $H_{\rm DM}|\uparrow\uparrow\cdots\uparrow\rangle = 0$. For large magnetic fields, all the spins are aligned so that they become parallel to the applied fields. Interestingly, the magnetization is not changed by the DM interaction for a-axis magnetic fields even at $h \sim J/2$, while it is rapidly suppressed by b-axis magnetic fields as the DM interaction is increased. This anisotropic behavior can be understood as a result of a competition between the DM interaction and the applied fields; The DM interaction can be rewritten as [36]

$$H_{\rm DM} = \frac{D_b}{2} \sum_{j:{\rm odd}} [\tilde{S}_j^+ \tilde{S}_{j+2}^- + \tilde{S}_j^- \tilde{S}_{j+2}^+] - (j : {\rm even}), \quad (5)$$

$$\tilde{S}_j^\pm = e^{\pm i\pi j/4}\left(S_j^c \pm i S_j^a\right). \quad (6)$$

The DM interaction alone describes decoupled two copies of XY chains in the $\tilde{S}$ basis and it increases quantum fluctuations of spins in the ac plane. Classically, the DM interaction tends to rotate the spins and it frustrates with the Ising interaction. However, once strong a-axis magnetic fields are applied, these ac-plane quantum fluctuations are pinned and effects of the DM interactions get suppressed. Therefore, the calculated magnetization is almost independent of the DM interaction, and in particular, the transition point almost does not change. On the other hand, for b-axis magnetic fields h_b, the DM interaction is not suppressed and the ferromagnetic state is destabilized by the quantum fluctuations, resulting in smaller critical fields h_b^*.

We summarize stability of the Ising ferromagnetism against the DM interaction in Fig. 4. For $h \parallel a$ axis, the critical field h_a^* is almost unchanged from $h_a^* \simeq 0.5\ J$ as D_b is introduced as explained above. It is noted that the system is dominated by the DM interaction for large values of D_b. Around $D_b \simeq$

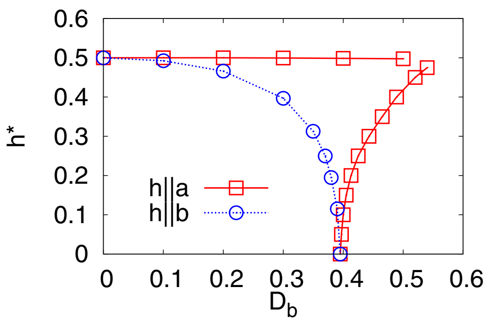

FIG. 4. The critical magnetic fields for a axis (red squares) and b axis (blue circles). D_b is strength of the DM interaction in unit of J.

0.39 J, there is a first-order phase transition between the Ising ferromagnetic phase and a paramagnetic phase at $h = 0$. The latter state is adiabatically connected to the paramagnetic state with large h_a and small D_b. On the other hand, for $h \parallel b$ axis, the critical field h^*_b is suppressed by D_b. If the DM interaction is sufficiently strong, the ferromagnetism is more fragile against h_b than h_a at zero temperature. This suggests that, at finite temperature, the Curie temperature is quickly suppressed by h_b compared with h_a. Therefore, the Hamiltonian (3) qualitatively explains the expected phase diagram Fig. 1 of UCoGe. Although these results are based on the simple spin model (3), we believe that the mechanism due to the DM interaction basically applies to more realistic models. In general, it is possible that strong magnetic anisotropy remains intact even when one includes itinerant nature of electrons into a spin model, although it may be weakened to some extent. Indeed, UCoGe is an itinerant ferromagnet with strong Ising anisotropy as verified in experiments [18–20]. In order to understand the quantitative features of the magnetic anisotropy in UCoGe, one needs to fully include the on-site electron level scheme together with the ASO interaction. This issue is left for a future study.

III. SUPERCONDUCTING UPPER CRITICAL FIELD

In this section, we consider how the reduced Curie temperature affects superconducting transition temperature, based on the scenario that the superconductivity is mediated by the Ising spin fluctuations in UCoGe. Similar problems were theoretically studied by several authors [25,26]. Here, we will focus on qualitative properties and use a simple model to demonstrate effects of the enhanced spin fluctuations on the superconductivity. As was discussed in the previous sections, low-energy properties in UCoGe can be described by quasiparticles interacting through the Ising pseudospin fluctuations. Therefore, we can approximate our kinetic term as

$$S_{\rm kin} = \sum[i\omega - \varepsilon'_k + \tilde{\boldsymbol{h}}\boldsymbol{\sigma}_{ss'}](a^\dagger_{ks}a_{ks'} + b^\dagger_{ks}b_{ks'}) - \sum \varepsilon_k[a^\dagger_{ks}b_{ks'} + (\text{H.c.})] + S_{\rm ASO}, \quad (7)$$

where $\varepsilon_k(\varepsilon'_k)$ corresponds to intersublattice (intrasublattice) hopping energy. The action includes spin-dependent terms described by $\tilde{\boldsymbol{h}} = \boldsymbol{h} + \boldsymbol{h}_{\rm ex}$, where $\boldsymbol{h} = \mu_B \boldsymbol{H}$ is the applied Zeeman field and g factor is simply taken to be $g = 2$, and $\boldsymbol{h}_{\rm ex}$ is the exchange splitting energy of the Fermi surface in the ferromagnetic state. From the experiments [8,22] and the previous sections, it is reasonable to assume that the exchange splitting at zero temperature $\boldsymbol{h}_{\rm ex} \parallel c$ axis depends only on b-axis applied fields. It is phenomenologically approximated as

$$h^c_{\rm ex}(h_b) = \begin{cases} h_{\rm ex}(0)\tanh(1.74\sqrt{h^*_b/h_b - 1}), & (h_b \leqslant h^*_b), \\ 0, & (h_b > h^*_b). \end{cases} \quad (8)$$

This functional form describes a mean-field behavior, $M_c \sim (h^*_b - h_b)^{1/2}$, near the quantum critical point. Note that we have neglected a-axis applied field dependence of $h^c_{\rm ex}$, since it is weak as discussed in the previous sections. One can improve the present model by appropriately modifying $h_{\rm ex}$, e.g., using the critical exponents of the three-dimensional Ising ferromagnets or introducing temperature dependence. The kinetic term also includes the ASO interaction Eq. (1) between the intrasublattices. As in the globally noncentrosymmetric superconductors, the ASO interaction term tends to fix directions of d vectors for spin-triplet superconductivity [37,38]. In UCoGe, however, Cooper pairing between the nearest-neighbor uranium sites along the zigzag chain is expected to be stronger than that between the second-nearest-neighbor sites. The former is intersublattice pairing, while the latter is intrasublattice pairing. This suggests that the ASO interaction between the intrasublattices will affect the subdominant gap functions only, while its effects on the dominant intersublattice gap functions would be negligible in UCoGe. Therefore, we neglect the ASO interaction and do not explicitly take the sublattice structure into account in the following calculations, which allows us to replace a_{ks},b_{ks} with a single operator c_{ks}. Then, we use a simple isotropic dispersion $\varepsilon_k = -2t\sum_{j=a,b,c}\cos k_j, \varepsilon'_k = -\mu$ where μ is the chemical potential. The model parameters are taken to be the same as those in the previous study [19,21], and in particular, the exchange splitting is $h_{\rm ex}(h_b = 0) = 0.5t$, which is large enough to suppress Pauli depairing effects for small h_b. It should be stressed that the ASO is less important for determining directions of d vector of the pseudospin triplet pairing between the nearest-neighbor sites, but still relevant to understand the magnetic anisotropy. The latter effect has already been incorporated in Eq. (8) within the present model for discussing superconductivity, by neglecting h_a dependence of the exchange splitting.

The fermions interact through the Ising spin fluctuations, which is described by

$$S_{\rm int} = -\frac{2g^2}{3}\sum_q \int_0^{1/T} d\tau d\tau' \chi^c(q,\tau - \tau')S^c_q(\tau)S^c_{-q}(\tau'), \quad (9)$$

$$\chi^c(q,i\Omega_n) = \frac{\chi_0}{\delta + q^2 + |\Omega_n|/\gamma_q}, \quad (10)$$

where $\gamma_q = vq$ with $v = 4t$ is the conventional Landau damping factor and $\boldsymbol{S}_q = (1/2)\sum_k c^\dagger_{k-q,s}\boldsymbol{\sigma}_{ss'}c_{ks'}$. We have neglected interactions arising from in-plane spin components, since the Ising spin fluctuations are the dominant fluctuations in UCoGe [18–20]. Zero-temperature mass of the Ising spin fluctuations is described by $\delta(h_b)$, and a mean-field functional form of δ is used for simplicity [13],

$$\delta(h_b) = \begin{cases} \left(h^c_{\rm ex}(h_b)\right)^2 & (h_b \leqslant h^*_b), \\ \left(h^c_{\rm ex}(2h^*_b - h_b)\right)^2 & (h_b > h^*_b). \end{cases} \tag{11}$$

Since the h_b dependence of $\delta(h_b)$ has not been clarified experimentally, we have assumed that it is symmetric about $h_b = h^*_b$. Details of calculation results depend on functional forms of δ, but their overall behaviors are well captured by this simple function.

In order to calculate H_{c2}, we solve the Eliashberg equation within the lowest order in the Ising interaction. The linearized Eliashberg equation reads [21,39]

$$\Delta_{ss}(k) = -\frac{T}{2N}\sum_{k'} V(k,k')[G_{ss'}(k+\Pi)G_{ss'}(-k) + G_{ss'}(k)G_{ss'}(-k-\Pi)]\Delta_{s's'}(k'), \tag{12}$$

where $\mathbf{\Pi} = -i\nabla_R - 2e\boldsymbol{A}(\boldsymbol{R})$ and $\boldsymbol{A}$ is the vector potential giving a uniform magnetic field. The pairing interaction V and the self-energy in the Green's function G are evaluated as

$$V(k,k') = -\frac{g^2}{6}\chi^c(k-k') + \frac{g^2}{6}\chi^c(k+k'), \tag{13}$$

$$\Sigma(k) = \frac{T}{6N}\sum_{qs} g^2\chi^c(q)G^0_{ss}(k+q), \tag{14}$$

where G^0 is the noninteracting Green's function and N is the number of k-point mesh in the Brillouin zone. We have neglected self-energies, which are off-diagonal in spin space, since they are much smaller than the diagonal components when $h \ll$ (band width). In numerical calculations, the lowest Landau level is taken into account for the orbital depairing effect. We focus on the superconducting symmetry for which the d vector is expressed as $\boldsymbol{d} \sim (c_1k_a + ic_2k_b, c_3k_b + ic_4k_a, 0)$ with real coefficients $\{c_j\}$ near the Γ point in the Brillouin zone, and the gap function is calculated self-consistently by solving the Eliashberg equation. We use the same set of model parameters as in the previous studies [19,21], which gives a superconducting transition temperature $T_{sc0} = 0.020t$ at $h = 0$.

In Fig. 5, we show the upper critical field $H^{\parallel b}_{c2}$ together with the previous results for $H^{\parallel a}_{c2}$ [19,21]. The horizontal light blue line indicates the critical applied field h^*_b below (above) which the system is ferromagnetic (paramagnetic). In our numerical calculations, we cannot accurately compute $H^{\parallel b}_{c2}$ near the critical field $h_b \simeq h^*_b$, since strength of the spin fluctuations diverges as $\sim 1/\delta$. As expected, calculated $H^{\parallel b}_{c2}$ is enhanced around $h_b = h^*_b$, which is qualitatively consistent with the experiments on UCoGe [8]. Although the superconducting transition temperature $T_{sc}(h_b = h^*_b)$ seems to exceed $T_{sc}(h_b = 0)$ for the present model parameters in contrast to the experiments, $T_{sc}(h^*_b)/T_{sc}(0)$ strongly depends on $\delta(h_b = 0)$ in our model. If $\delta(0)$ is sufficiently small and the system at zero field is already very close to the criticality $\delta = 0$, enhancement of superconductivity due to reduction of $\delta(h_b)$ would be moderate [14–17]. On the other hand, if $\delta(0)$ is rather away from criticality, enhancement of T_{sc} would be drastic

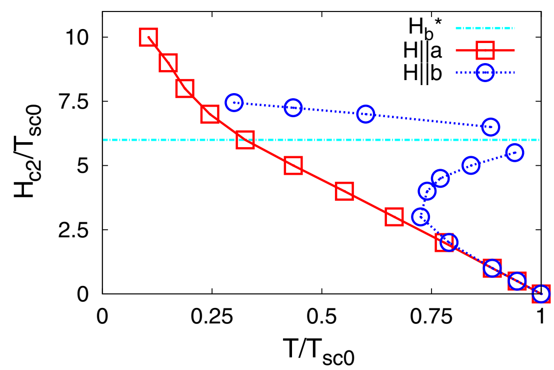

FIG. 5. Temperature dependence of H_{c2} for a axis (red curve) and b axis (blue curve). The dashed line indicates the critical magnetic field H^*_b. $T_{sc0} = 0.02t$ is the superconducting transition temperature at $h = 0$.

when $\delta(h_b)$ is tuned. $T_{sc}(h^*_b)/T_{sc}(0)$ also directly depends on the value of h^*_b, because b-axis magnetic fields not only tune the magnetic criticality but also break the superconductivity at the same time. However, it is noted that enhancement of T_{sc} due to the field-induced criticality is a common qualitative behavior, which is independent of the details.

It is interesting to see that the superconductivity still survives above the critical magnetic field, $h_b > h^*_b$, where the system is paramagnetic. As was discussed by Mineev [27], a large exchange field $h_{\rm ex} \gg T_{sc}$ is essentially important to suppress the Pauli depairing effect for equal-spin pairing states. Since the equal-spin pairing state is realized and $\Delta_{\uparrow\downarrow} = \Delta_{\downarrow\uparrow} = 0$ in the present Ising spin fluctuations model, one might expect that the superconductivity is easily destroyed due to the Pauli depairing effect if the system reaches the paramagnetic state with increasing the magnetic field along b axis. To understand the origin of the robust superconductivity under b-axis magnetic fields, we compare in-plane components of the d vector, d_a and d_b, by calculating

$$\langle|d_a|\rangle = \sqrt{\frac{1}{N}\sum_k \frac{|\Delta_{\uparrow\uparrow}(k) - \Delta_{\downarrow\downarrow}(k)|^2}{4}}, \tag{15}$$

$$\langle|d_b|\rangle = \sqrt{\frac{1}{N}\sum_k \frac{|\Delta_{\uparrow\uparrow}(k) + \Delta_{\downarrow\downarrow}(k)|^2}{4}}. \tag{16}$$

Note that absolute values of the d vector cannot be determined within the present calculations of the linearized Eliashberg equation, but its direction can be self-consistently computed. We show calculation results in Fig. 6 together with $h_{\rm ex}(h_b)$ defined in Eq. (8). The calculation results show that $\langle|d_b|\rangle/\langle|d_a|\rangle \simeq 1$ around $h_b \simeq 0$ and it goes up when small h_b is introduced. This is because Cooper pairing only for the Fermi surface of the major spin takes place at $h_b = 0$, and that for the minor spin is induced at finite $h_b > 0$. By further increasing h_b, the ratio $\langle|d_b|\rangle/\langle|d_a|\rangle$ sharply decreases around $h_b \simeq h^*_b$ and it becomes nearly zero for $h_b > h^*_b$. This means that the d vector at $h_b = 0$ is $\boldsymbol{d} \propto (1,i,0)$ and it rotates to $\boldsymbol{d} \propto (1,0,0)$ for large applied fields, which is perpendicular to the applied b-axis magnetic field. The rotation of d vector from the nonunitary state with $\langle|d_a|\rangle \simeq \langle|d_b|\rangle$ at zero field to the nearly unitary state with $\langle|d_a|\rangle \gg \langle|d_b|\rangle$ at large H_b is due

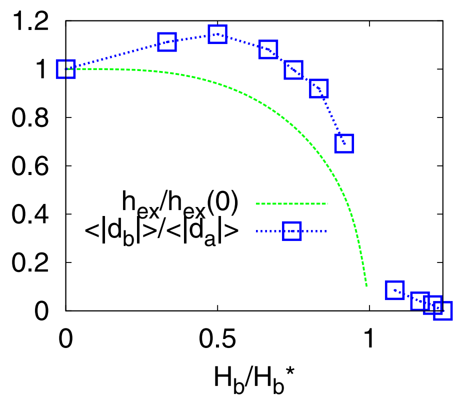

FIG. 6. In-plane components of the d vector as a function of H_b. The green curve is the exchange field $h_{\rm ex}$, which characterizes Fermi surface splitting in the ferromagnetic state.

to reduction of the exchange splitting of the Fermi surface and the Pauli depairing effect. As H_b is increased, the exchange splitting Eq. (8) gets smaller, which weakens the nonunitarity of d vector. At the same time, in order to reduce Zeeman energy cost, the d vector favors a configuration $\boldsymbol{d} \perp \boldsymbol{H}$. The resulting d vector for $h_b > h_b^*$ allows a large Pauli limiting field $H_P^{\parallel b}$ at $T = 0$, which is given by

$$H_P^{\parallel b} = \Delta_0 \sqrt{\frac{\rho(0)}{\chi_N^b - \chi_{sc}^b}}, \tag{17}$$

where Δ_0 and $\rho(0)$ are the gap amplitude and the density of states at the Fermi energy, respectively. χ_N^b is the static susceptibility in normal states and χ_{sc}^b is that in superconducting states given by $\chi_{sc}^b = \chi_N^b[1 - \langle \hat{d}_b^2 \rangle_{\rm FS}]$ within mean-field approximations. When the d vector is perpendicular to b axis, the susceptibility is $\chi_{sc}^b \simeq \chi_N^b$ and the Pauli limiting field becomes large. Therefore, the superconductivity can survive up to large b-axis magnetic fields $h_b \simeq h_b^* \gg T_{sc}(h_b = 0)$ in UCoGe. However, we note that the high field superconductivity is numerically stable only for $H_b \gtrsim H_b^*$ and $H_{c2}^{\parallel b}$ is relatively smaller than $H_{c2}^{\parallel a}$ in the present model. Similar changes of pairing states have been discussed in the previous study for URhGe [25].

We think that this mechanism for suppressing Pauli depairing effects under in-plane magnetic fields is important also for the superconductivity under high pressure. The superconductivity extends over a wide range of pressure and it survives in the paramagnetic phase [3,8] experimentally. Although the Mineev's mechanism of suppressing the Pauli depairing effect does not work in the paramagnetic phase, observed H_{c2} for in-plane magnetic fields are large, $H_{c2} \gtrsim$ 7–8 T, and they well exceed the Pauli limiting field ~ 1 T, which is naively expected for the equal-spin triplet pairing with $T_{sc} \lesssim 1$ K [9]. H_{c2} near the magnetic phase transition point $p_c \simeq 1.3$ GPa is especially nontrivial, since there is a competition between enhanced spin fluctuations and Pauli depairing effect. If the d vector rotates to suppress Pauli depairing effect, the large spin fluctuations lead to strong coupling superconductivity around the critical pressure and it can be robust against in-plane magnetic fields. This mechanism would be relevant for understanding the observed large H_{c2} in UCoGe under pressure.

IV. SUMMARY

We have investigated ferromagnetism and superconductivity in the heavy fermion compound UCoGe under in-plane magnetic fields. For the magnetic properties, we focused on roles of the DM interaction arising from the zigzag chain crystal structure of UCoGe, and qualitatively explained the experimentally observed anisotropy for the critical field of the paramagnetic transition. Then we incorporated this magnetic anisotropy into a simple single-band model for the discussion of superconductivity, where magnetism is tuned by b-axis magnetic fields but is independent of a-axis magnetic fields. Based on the scenario of the ferromagnetic spin fluctuations mediated superconductivity, we demonstrated that $H_{c2}^{\parallel b}$ shows S-shaped behaviors in qualitative agreement with the experiments, while $H_{c2}^{\parallel a}$ is monotonic in temperature. It was also numerically found that the superconductivity survives even for large b-axis magnetic fields for which the system is paramagnetic and Pauli depairing effect is expected to be relevant. We showed that the superconductivity survives robustly due to a rotation of the d vector, which reduces the Zeeman energy cost and suppresses the Pauli depairing effect. The rotation of the d vector would also be important for understanding large H_{c2} under pressure where the Pauli depairing effect is not suppressed by the exchange splitting of the Fermi surface.

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[1] S. S. Saxena, P. Agarwal, K. Ahilan, F. M. Grosche, R. K. W. Haselwimmer, M. J. Steiner, E. Pugh, I. R. Walker, S. R. Julian, P. Monthoux, G. G. Lonzarich, A. Huxley, I. Sheikin, D. Braithwaite, and J. Flouquet, Nature (London) **406**, 587 (2000).

[2] D. Aoki, A. Huxley, E. Ressouche, D. Braithwaite, J. Flouquet, J. P. Brison, E. Lhotel, and C. Paulsen, Nature (London) **413**, 613 (2001).

[3] N. T. Huy, A. Gasparini, D. E. de Nijs, Y. Huang, J. C. P. Klaasse, T. Gortenmulder, A. de Visser, A. Hamann, T.

Görlach, and H. v. Löhneysen, Phys. Rev. Lett. **99**, 067006 (2007).
[4] M. L. Kulić and A. I. Buzdin, in *Superconductivity* (Springer, Berlin, 2008), Chap. 4.
[5] N. T. Huy,, D. E. de Nijs, Y. K. Huang,, and A. de Visser, Phys. Rev. Lett. **100**, 077002 (2008).
[6] E. Slooten, T. Naka, A. Gasparini, Y. K. Huang, and A. de Visser, Phys. Rev. Lett. **103**, 097003 (2009).
[7] A. Gasparini, Y. K. Huang, N. T. Huy, J. C. P. Klaasse, T. Naka, E. Slooten, and A. de Visser, J. Low Temp. Phys. **161**, 134 (2010).
[8] D. Aoki, T. D. Matsuda, V. Taufour, E. Hassinger, G. Knebel, and J. Flouquet, J. Phys. Soc. Jpn. **78**, 113709 (2009).
[9] D. Aoki, M. Taupin, C. Paulsen, F. Hardy, V. Taufour, H. Kotegawa, E. Hassinger, L. Malone, T. D. Matsuda, A. Miyake, I. Sheikin, W. Knafo, G. Knebel, L. Howald, J. P. Brison, and J. Flouquet, J. Phys. Soc. Jpn. **81**, SB002 (2012).
[10] D. Aoki and J. Flouquet, J. Phys. Soc. Jpn. **83**, 061011 (2014).
[11] A. de Visser, N. T. Huy, A. Gasparini, D. E. de Nijs, D. Andreica, C. Baines, and A. Amato, Phys. Rev. Lett. **102**, 167003 (2009).
[12] T. Ohta, T. Hattori, K. Ishida, Y. Nakai, E. Osaki, K. Deguchi, N. K. Sato, and I. Satoh, J. Phys. Soc. Jpn. **79**, 023707 (2010).
[13] D. Fay and J. Appel, Phys. Rev. B **22**, 3173 (1980).
[14] P. Monthoux and G. G. Lonzarich, Phys. Rev. B **59**, 14598 (1999).
[15] Z. Wang, W. Mao, and K. Bedell, Phys. Rev. Lett. **87**, 257001 (2001).
[16] R. Roussev and A. J. Millis, Phys. Rev. B **63**, 140504 (2001).
[17] S. Fujimoto, J. Phys. Soc. Jpn. **73**, 2061 (2004).
[18] Y. Ihara, T. Hattori, K. Ishida, Y. Nakai, E. Osaki, K. Deguchi, N. K. Sato, and I. Satoh, Phys. Rev. Lett. **105**, 206403 (2010).
[19] T. Hattori, Y. Ihara, Y. Nakai, K. Ishida, Y. Tada, S. Fujimoto, N. Kawakami, E. Osaki, K. Deguchi, N. K. Sato, and I. Satoh, Phys. Rev. Lett. **108**, 066403 (2012).
[20] T. Hattori, Y. Ihara, K. Karube, D. Sugimoto, K. Ishida, K. Deguchi, N. K. Sato, and T. Yamamura, J. Phys. Soc. Jpn. **83**, 061012 (2014).
[21] Y. Tada, S. Fujimoto, N. Kawakami, T. Hattori, Y. Ihara, K. Ishida, K. Deguchi, N. K. Sato, and I. Satoh, J. Phys.: Conf. Ser. **449**, 012029 (2013).
[22] T. Hattori, K. Karube, K. Ishida, K. Deguchi, N. K. Sato, and T. Yamamura, J. Phys. Soc. Jpn. **83**, 073708 (2014).
[23] F. Lévy, I. Sheikin, B. Grenier, and A. D. Huxley, Science **309**, 1343 (2005).
[24] Y. Tokunaga, D. Aoki, H. Mayaffre, S. Krämer, M. H. Julien, C. Berthier, M. Horvatić, H. Sakai, S. Kambe, and S. Araki, Phys. Rev. Lett. **114**, 216401 (2015).
[25] K. Hattori and H. Tsunetsugu, Phys. Rev. B **87**, 064501 (2013).
[26] V. P. Mineev, Phys. Rev. B **90**, 064506 (2014).
[27] V. P. Mineev, Phys. Rev. B **81**, 180504 (2010).
[28] D. Aoki and J. Flouquet, J. Phys. Soc. Jpn. **81**, 011003 (2012).
[29] Y. Yanase, J. Phys. Soc. Jpn. **83**, 014703 (2014).
[30] T. Moriya, Phys. Rev. **120**, 91 (1960).
[31] M. Samsel-Czekala, S. Elgazzar, P. M. Oppeneer, E. Talik, W. Walerczyk, and R. Troć, J. Phys.: Condens. Matter **22**, 015503 (2009).
[32] V. P. Mineev, C. R. Phys. **7**, 35 (2006).
[33] U. Schollwöck, Rev. Mod. Phys. **77**, 259 (2005).
[34] U. Schollwöck, Ann. Phys. (N.Y.) **326**, 96 (2011).
[35] I. P. McCulloch, arXiv:0804.2509.
[36] M. Oshikawa and I. Affleck, Phys. Rev. Lett. **79**, 2883 (1997).
[37] *Non-Centrosymmetric Superconductors*, edited by E. Bauer and M. Sigrist (Springer, Berlin, 2012).
[38] M. H. Fischer, F. Loder, and M. Sigrist, Phys. Rev. B **84**, 184533 (2011).
[39] Y. Tada, N. Kawakami, and S. Fujimoto, Phys. Rev. B **81**, 104506 (2010).