UPt$_3$ as a Topological Crystalline Superconductor

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We investigate the topological aspect of the spin-triplet $f$-wave superconductor UPt$_3$ through microscopic calculations of edge- and vortex-bound states based on the quasiclassical Eilenberger and Bogoliubov-de Gennes theories. It is shown that a gapless and linear dispersion exists at the edge of the $ab$-plane. This forms a Majorana valley, protected by the mirror chiral symmetry. We also demonstrate that, with increasing magnetic field, vortex-bound quasiparticles undergo a topological phase transition from topologically trivial states in the double-core vortex to zero-energy states in the normal-core vortex. As long as the $d$-vector is locked into the $ab$-plane, the mirror symmetry holds the Majorana property of the zero-energy states, and thus UPt$_3$ preserves topological crystalline superconductivity that is robust against the crystal field and spin-orbit interaction.

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Introduction.— The unconventional aspect of the heavy-fermion superconductor UPt$_3$ emerges as a multiple phase diagram in the temperature $T$ vs magnetic field $H$ plane, which is unique among a handful of strongly correlated superconductors. In low fields, UPt$_3$ undergoes a double superconducting transition from a normal phase to the A-phase at $T_{c2} \approx 550$ mK and from the A-phase to the B-phase at $T_{c2} \approx 500$ mK. The C-phase appears in the regime of low $T$’s and high $H$’s. In spite of numerous works on UPt$_3$ over the past three decades following the discovery of superconductivity, the pairing mechanism and gap function have not been fully elucidated yet.

A recent experiment has clarified the remarkable twofold symmetry breaking of the angle-resolved thermal conductivity in the $ab$-plane of the C-phase. This convincingly suggests a spin-triplet $f$-wave function belonging to the $E_{1u}$ representation, where the gap function in the B-phase is described by the two-component $d$-vector and in the C-phase it reduces to a single component with the twofold symmetry breaking. Even within the B-phase, the $d$-vector rotates from $d(k) \propto \lambda_a b + \lambda_b a$ to $\lambda_a b + \lambda_b a$ with increasing $H \parallel c$ at the critical magnetic field $H_{c1} \approx 2$ kG, where $\lambda_{a,b}(k) = k_a (5k_b^2 - k^2)$ and $a$, $b$, and $c$ are the unit vectors in a hexagonal crystal. Most bulk thermodynamic experiments are understandable with the $E_{1u}$ scenario and another candidate based on the $E_{2u}$ representation, described by $d' \propto c (k_a + i k_b) k_b$, because both have point and line nodes in the B-phase. The latter scenario gives rise to the spontaneous breaking of the time-reversal symmetry in the B-phase and the fourfold symmetry breaking in the C-phase. These two scenarios differ in that the multi-component order parameters originate from the multiple $d$-vector in the $E_{1u}$ scenario and from the orbital degrees of freedom for the $E_{2u}$ representation.

In this Letter, we examine topological crystalline superconductivity in the B-phase of UPt$_3$ appropriate for the $E_{1u}$ scenario with multiple $d$-vectors. On the basis of a recent idea of Majorana fermions protected by crystal point group symmetries, it is demonstrated that the nontrivial topological property is directly linked to the orientation of the $d$-vector, and thus the field-induced rotation of the $d$-vector is accompanied by the topological phase transition of vortex-bound states, which is not observed in the $E_{2u}$ scenario. Here, the topological aspects are unveiled through the microscopic calculations of edge and vortex core states. It is shown that zero-energy states exist at the edge of the $ab$-plane, which form the topological “Majorana valley”. Furthermore, employing numerical calculations of the Bogoliubov-de Gennes (BdG) equation, we examine the discretized quantum structure of quasiparticles (QP’s) bound at a double-core vortex and a normal-core vortex. It is found that increasing the magnetic field $H \parallel c$ induces a topological phase transition from topologically trivial states in the double-core vortex to symmetry-protected Majorana fermions in a normal-core vortex with $d \perp c$ via nontopological Dirac fermions.

The purposes of this Letter are to help identify the pairing symmetry of UPt$_3$ and to place this material in the proper position of topological crystalline superconductors.

Formulation.— Here, we utilize both the quasiclassical Eilenberger theory and the BdG theory. The former is valid for $\Delta \ll E_F$, which is well satisfied for most superconductors including UPt$_3$, where $\Delta$ and $E_F$ denote the pair potential and Fermi energy, respectively. The vortex-bound QP state is, however, discretized at $\Delta^2/E_F$...
by (the amplitudes of the two pair potentials, $\Delta_1$, $\Delta_2$) self-consistently solve Eqs. (1) and (3) at $\lambda$ which is typically fixed at the field, the quasiclassical Green’s function is described in particle-hole space by

$$\tilde{g}(\mathbf{k}, \mathbf{r}, \omega_n) = \frac{1}{\pi} \left( \frac{\tilde{g}(\mathbf{k}, \mathbf{r}, \omega_n) - i \tilde{f}(\mathbf{k}, \mathbf{r}, \omega_n)}{\tilde{g}(\mathbf{k}, \mathbf{r}, \omega_n) + i \tilde{f}(\mathbf{k}, \mathbf{r}, \omega_n)} \right),$$

(2)

with the momentum on the Fermi surface $\mathbf{k} = k_F$, $\mathbf{r} = (k_x, k_y, k_z)/k_F$, the center-of-mass coordinate $\mathbf{r}$, and the Matsubara frequency $\omega_n = (2n + 1)\pi k_B T/\hbar$ with $n \in \mathbb{Z}$. The Fermi velocity is assumed as $v_F(\mathbf{k}) = v_F \mathbf{k}$ on a three-dimensional Fermi sphere.

The spin-triplet order parameter is expressed with the $\mathbf{d}$-vector as $\Delta(\mathbf{k}, \mathbf{r}) = i\mathbf{d}(\mathbf{k}) \cdot \hat{\mathbf{r}}$ $\mathbf{r}$, where $\hat{\mathbf{r}}$ is the Pauli matrix. The self-consistent condition for $\Delta$ is given as

$$\Delta(\mathbf{k}, \mathbf{r}) = N_0 \pi k_B T \sum_{|\omega_n| \leq \omega_c} \langle \mathcal{V}(\mathbf{k}, \mathbf{k}^{\prime}) \tilde{f}(\mathbf{k}^{\prime}, \mathbf{r}, \omega_n) \rangle_{\mathbf{k}^{\prime}},$$

(3)

where $N_0$ is the density of states in the normal state. The cutoff energy $\omega_c$ is set to be $\hbar \omega_c = 20k_B T_c$ with the transition temperature $T_c$ and $\langle \cdots \rangle_{\mathbf{k}}$ indicates the Fermi surface average. In the B-phase without a magnetic field, the $\mathbf{d}$-vector is described by $\mathbf{d} = \Delta_1 \lambda_0 \mathbf{b} + \Delta_2 \lambda_0 \mathbf{c}$. We neglect the splitting of $T_c$ into $T_{c1}$ and $T_{c2}$ because the amplitudes of the two potential, $\Delta_1$ and $\Delta_2$, are nearly equal at low temperatures in the B-phase. The pairing interaction is $\mathcal{V}(\mathbf{k}, \mathbf{k}^{\prime}) = g(\lambda_0(\mathbf{k}) \lambda_0(\mathbf{k}^{\prime}) + \lambda_0(\mathbf{k}^{\prime}) \lambda_0(\mathbf{k}))$, where the coupling constant $g$ is determined by $(g N_0)^{-1} = \ln(T/T_c) + \pi k_B T \sum_{|\omega_n| \leq \omega_c} |\hbar \omega_n|^{-1}$. We self-consistently solve Eqs. (1) and (3) at $T = 0.5 T_c$.

By using the self-consistent solution of $\tilde{g}$ in Eqs. (1), (2), and (3), the spin current is calculated as

$$\mathbf{j}_\mu(\mathbf{r}) = \frac{\hbar}{2} N_0 \pi k_B T \sum_{|\omega_n| \leq \omega_c} \langle \mathbf{v}(\mathbf{k}) \text{Im}[g_\mu(\mathbf{k}, \mathbf{r}, \omega_n)] \rangle_{\mathbf{k}},$$

(4)

where $g_\mu$ is defined as $g_\mu = g_0 \mathbf{1} + g \cdot \hat{\mathbf{r}}$. The local density of states (LDOS) for the energy $E$ is given by $N(\mathbf{r}, E) = \langle N(\mathbf{k}, \mathbf{r}, E) \rangle_{\mathbf{k}}$, where the angle-resolved LDOS is

$$N(\mathbf{k}, \mathbf{r}, E) = N_0 \text{Re} \left[ g_0(\mathbf{k}, \mathbf{r}, \omega_n) |i\hbar \omega_n \rightarrow E + i\eta| \right].$$

(5)

We here introduce a positive infinitesimal constant $\eta$, which is typically fixed at $\eta = 0.007\pi k_B T_c$. To obtain $g_0(\mathbf{k}, \mathbf{r}, \omega_n)|i\hbar \omega_n \rightarrow E + i\eta|$, we solve Eq. (1) with $\eta = -i E$ instead of $i\hbar \omega_n$ under $\Delta$ obtained self-consistently.

To obtain the discretized nature of vortex-bound states, we calculate the BdG equation. Since we here consider a straight vortex line along the $c$-axis ($F \parallel \mathbf{c}$), the wave number $k_c$ is a well-defined quantum number. The BdG equation with a definite $k_c$ is given as

$$\int d\rho_2 \left( \hat{h}_k(\rho_1, \rho_2) - \Delta_{k_c}(\rho_1, \rho_2) \right) = E_{\rho_1, \rho_2},$$

(6)

where $\hat{h}_k(\rho_1, \rho_2) = \delta(\rho_1 - 2\pi^2 \nu^2_{2D}/2m - E_{2D}(k_c))$ with $\nu^2_{2D} = \hbar^2 / (2m)(k_{c1}^2 - k_{c2}^2)$ reflects the $k_c$-cross section of the Fermi surface. The order parameter in Eq. (6) is obtained from the self-consistent solution of the quasiclassical theory and the relation $\Delta_{k_c}(\rho_1, \rho_2) = (2\pi)^{-2} \int dk_{c}^2 \Delta(\mathbf{k}, \rho) e^{i k_{c}^2 \rho_{12}}$, where $\rho = (\rho_1 + \rho_2)/2$, $\rho_{12} = \rho_1 - \rho_2$, and $k_{c}^2$ are in the $ab$-plane. Equation (6) describes QPs with the energy $E_{\rho_1, \rho_2}$ and the wave function $\tilde{u}_{\nu, k_c}(\rho_1, \rho_2) = \langle \tilde{u}_{\nu, k_c}, \rho_1, \rho_2 | \tilde{u}_{\nu, k_c}, \rho_1, \rho_2 \rangle$, where the index $\nu \in \mathbb{Z}$ denotes the $\nu$-th excited state of Eq. (6).

Edge states.---First, using the quasiclassical theory, we consider the edge state at the surface perpendicular to the $ab$-plane. We here set a surface at $a = 0$ and impose the specular boundary condition on $\tilde{g}$ as $\tilde{g}(\mathbf{k}, \mathbf{r}, \omega_n) = \tilde{g}(\mathbf{k}, \mathbf{r}, \omega_n)$ at $a = 0$, where $\mathbf{k} = \mathbf{k} - 2a \mathbf{e}_k$. In the B-phase without a magnetic field, the $\mathbf{d}$-vector is described by $\mathbf{d}(\mathbf{k}, a) = \Delta_\perp(\mathbf{a}) \lambda_0(\mathbf{k}) \mathbf{b} + \Delta_\parallel(\mathbf{a}) \lambda_0(\mathbf{k}) \mathbf{c}$.

The spatial profile of the order parameter along the $a$-axis is shown in Fig. (1a). At $a = 0$, the specular boundary condition suppresses $\Delta_\perp$ coupled with a momentum $\mathbf{k}_0$ perpendicular to the surface. In contrast, $\Delta_\parallel$ coupled to a parallel momentum $\mathbf{k}_0$ is enhanced by compensating for the loss of $\Delta_\perp$ at the surface. Away from the surface, $\Delta_\perp$ increases and $\Delta_\parallel$ decreases toward the order parameter in the bulk B-phase $\Delta_0 = \Delta_\perp = \Delta_\parallel$. Figure (1a) also shows the spin current $j_{\mu}(a)$, implying that the $a$-component of the spin flows along the $b$-axis on the surface.

Figure (1b) shows LDOS at the surface ($a = 0$) and bulk ($a/a_0 = 40$), where $R_0 = \hbar v_F / (2 \pi k_B T_c)$. The two peaks at $E = \Delta_0$ and $E = (16 \sqrt{5}/45) \Delta_0$ in the bulk LDOS are shifted to higher energies in the surface LDOS as a result of the enhancement of $\Delta_\parallel$ at the surface. It is clearly seen that the zero-energy LDOS at the surface has substantial weight (about half of the normal state), owing to the dispersionless zero-energy state connecting point nodes at the north and south poles of the Fermi sphere, similarly to that in the superfluid $^3$He-A.

We can separate the spin states by rotating the spin quantization axis to the $a$-axis as $\mathbf{d} = \Delta_0(\lambda_0 \mathbf{b} + \lambda_0 \mathbf{c}) = \Delta_0(\lambda_+ \mathbf{a}_+ - \lambda_- \mathbf{a}_-)$, where $\lambda_\pm = \mp(\lambda_0 \pm i \lambda_b) / \sqrt{2}$. $\mathbf{a}_+ = (\mathbf{b} + i \mathbf{c}) / \sqrt{2}$, and $\mathbf{a}_- = -(\mathbf{b} - i \mathbf{c}) / \sqrt{2}$. In Figs. (1c) and
FIG. 1. (Color online) (a) Spatial profiles of order parameters and spin current $j_{\alpha b}^s$ along the $a$-axis. (b) LDOSs $N(E)$ at the surface and bulk. (c) Angle-resolved LDOS $N(\mathbf{k}, E)$ at the surface as a function of $k_b$ for $\mathbf{k}_c = 0$. (d) Stereographic view of the dispersion of the surface bound state in $\rightarrow$ and $\leftarrow$-spin sectors.

FIG. 2. (Color online) Energy spectra of QPs classified with the azimuthal angular momentum $L_c$ at $k_b = 0$: (a) double-core vortex and (b) normal-core vortex. (c) Phase profiles of $d_{\text{bulk}}$ and $d_{\text{core}}$ and quasiclassical trajectories with $k_b = 0$ (white arrow) and $k_b \neq 0$ (black arrow).

tex, as seen in Fig. 2(c), the phases of $d_{\text{bulk}}(\varphi = 0)$ and $d_{\text{core}}$ are the same.

Figure 2(a) shows the energy spectrum of low-lying QPs in the double-core vortex with $k_b = 0$, obtained from the numerical diagonalization of Eq. (10). All the eigenvalues are classified in terms of the angular momentum along the $c$-axis, $L_c = -i\hbar \int d\mathbf{p} \mathbf{u}_{\nu,k_{c}}^\dagger (a_d \mathbf{b} - b_d \mathbf{a}) \mathbf{u}_{\nu,k_{c}}$. It is seen from Fig. 2(a) that zero-energy eigenstates are absent even in the vicinity of $L_c = 0$. To clarify the absence in the double-core vortex, let us consider the quasiclassical trajectories across the vortex core, as shown in Fig. 2(c). The quasiclassical trajectory with the momentum $k_b = 0$ effectively feels the $\pi$-phase shift of the pair potential, because the induced pair potential $d_{\text{core}} = \Delta_c \lambda_b a$ becomes zero for $k_b = 0$, where the $\pi$-phase shift is necessary for the zero-energy state. In contrast, the trajectory with $k_b \neq 0$ feels $d_{\text{core}}$ interrupting the $\pi$-phase shift, which prevents the formation of the zero-energy state. Since the QP state at the vortex core is obtained as the superposition of all the contributions of the quasiclassical trajectories with various $k_b$’s, the zero-energy state is absent in the double-core vortex.

The normal-core vortex with $d_{\text{core}} = 0$ is accompanied by the spin-degenerate zero-energy modes with $L_c = 0$, as shown in Fig. 2(b). Within our model, the zero-energy states form the flat band along $k_c$. Note that, in a magnetic field $H \sim H_{\text{rot}}$, the normal-core vortex lattice with a hexagonal symmetry is observed in the small-angle neutron scattering experiment [21]. In the regime of $H < H_{\text{rot}}$, the normal-core vortex is described by $d(|\rho| \rightarrow \infty) = \Delta_0 e^{i\varphi} (\lambda_b b + \lambda_c c)$. The zero-energy state is found to be fragile against the Zeeman field $H \parallel c$ and lifted to finite energies. In the regime of $H > H_{\text{rot}}$ where $d(|\rho| \rightarrow \infty) = \Delta_0 e^{i\varphi} (\lambda_b b + \lambda_c c)$, however, the zero-energy states with $L_c = 0$ remain robust against the magnetic field along the $c$-axis, because the $\uparrow$- and $\downarrow$-spin sectors of the $\mathbf{d}$-vector can be regarded as a spinless
chiral superconductor. Hence, in the normal-core vortex, the excitation energy of the low-lying QP jumps to a zero-energy at the critical field where the $d$-vector is locked in the $ab$-plane. As described below, at $H = H_{\text{rot}}$, the vortex-bound states undergo the topological phase transition associated with the mirror Chern number.

**Majorana fermions protected by mirror symmetries.**—Finally, we clarify the symmetry protection and the Majorana nature of zero-energy edge- and vortex-bound states in the B-phase of UPt$_3$. We start with the BdG Hamiltonian,

$$\hat{H}(k) = \begin{pmatrix} \hat{\epsilon}(k) & \hat{\Delta}(k) \\ \hat{\Delta}^\dagger(k) & -\hat{\epsilon}^\dagger(k) \end{pmatrix}. \tag{7}$$

Here, $\hat{\epsilon}(k)$ is the Hamiltonian in the normal state of UPt$_3$, which holds the $D_{6h}$ hexagonal symmetry. We find that two different mirror symmetries protect Majorana fermions in the B-phase: One is the mirror reflection $\mathcal{M}_a$ with respect to the $ca$-plane, which protects the Majorana valley on a surface normal to the $c$-axis. The other is the mirror reflection $\mathcal{M}_b$ with respect to the $ab$-plane, which protects the Majorana zero mode in a vortex along the $c$-axis. Below we show that the difference in symmetry gives rise to a difference in Majorana nature between the edge- and vortex-bound states. Note that UPt$_3$ shows an antiferromagnetic order in the normal state below about 5 K. Even if the antiferromagnetic order coexists with the superconducting order, the mirror symmetries are preserved macroscopically beyond the scale of the coherence length.

First, we consider the symmetry protection of the surface states. Because the gap function in the B-phase is invariant under the mirror reflection $\mathcal{M}_a \cong i \sigma_b$, the BdG Hamiltonian $\hat{H}(k)$ satisfies $\hat{\mathcal{M}}_a \hat{H}(k) \hat{\mathcal{M}}_a^\dagger = \hat{H}(ka, -kb, kc)$ with $\hat{\mathcal{M}}_a \equiv \text{diag}(\mathcal{M}_a, \mathcal{M}_a^*)$. Therefore, combining the mirror symmetry with the time-reversal symmetry $\mathcal{T}$ and the particle hole symmetry $\mathcal{C}$, we have “mirror chiral symmetry” $\{\mathcal{T}, \hat{H}(k)\} = 0$ with $\mathcal{T} = \mathcal{C} \hat{\mathcal{M}}_a$ at $k_0 = 0$ [22]. The mirror chiral symmetry enables us to define the one-dimensional winding number $w(k_c) = -(4\pi i)^{-1} \int_{-\infty}^{\infty} \text{d}k_a \text{tr} [\mathcal{T} \hat{H}^{-1} \partial_{k_c} \hat{H}]$ [23, 24], which is evaluated as $|w(k_c)| = 2$ for $k_b = 0, |k_c| < k_F$ and $w(k_c) = 0$ for other $k_b$’s and $k_c$’s. Thus, the system is topologically non-trivial and the bulk-edge correspondence ensures the existence of the Majorana valley in Fig. 1(d) with a flat dispersion connecting the point nodes as $E = 0$ at $k_b = 0$ and $|k_c| < k_F$. In addition, owing to the mirror chiral symmetry, the Majorana valley shows the Majorana Ising anisotropy that the surface bound states are gapped only by a magnetic field along the $b$-axis [25]. A magnetic field in the $ca$-plane or the $d$-vector rotation in the high-field phase in the B-phase does not obscure the topological protection since the combination of the mirror reflection $\mathcal{M}_a$ and the time-reversal is not broken, but each of them is broken. Here, note that, while the Majorana valley has a close similarity to the topological Fermi arcs in $^3$He-A [26, 27], the arcs’ topological origins are totally different: The time-reversal breaking is essential for the topological Fermi arcs, but not for the Majorana valley.

For the topological protection of zero-energy states in a vortex, the mirror reflection $\mathcal{M}_b \propto i \sigma_a$ with respect to the $ab$-plane is essential. Following Ref [11] one can show that, if the gap function is odd under the mirror reflection $\mathcal{M}_b$, $\mathcal{M}_b \hat{\Delta}(k) \mathcal{M}_b^\dagger = -\hat{\Delta}(ka, kb, -kc)$, a normal-core vortex may support the Majorana zero mode protected by the mirror symmetry: In this case, $\hat{H}(k)$ commutes with the mirror operator $\hat{\mathcal{M}}_b^{(-)} \equiv \text{diag}(\mathcal{M}_b, -\mathcal{M}_b^*)$. On the mirror reflection invariant plane $k_c = 0$, the system splits into two subsectors with two different eigenvalues of $\hat{\mathcal{M}}_b^{(-)}$, and because of the minus sign in front of $\mathcal{M}_b$ in the mirror operator $\hat{\mathcal{M}}_b^{(-)}$, each mirror subsector supports its own particle-hole symmetry. This means that the mirror subsectors are topologically equivalent to class D of the table in Ref. [28] and thus the nontrivial Chern number in each subsector ensures non-Abelian Majorana fermions [11, 29].

Since $d(k) \propto \lambda_c b + \lambda_c c$ does not have a definite mirror parity under $\mathcal{M}_b$, the spin-orbit interaction or crystal field, which is ignored in the numerical calculations above, lifts zero-energy states, implying that the B-phase with the configuration of such a $d$-vector is topologically trivial for vortex-bound states. On the other hand, for $d(k) \propto \lambda_c a$ rotated by a high magnetic field $H \parallel c$, the gap function is odd under the mirror reflection $\mathcal{M}_b$, and Majorana vortex-bound states protected by the mirror symmetry are possible. Actually, for UPt$_3$ with five closed Fermi surfaces [30], the parity of the mirror Chern number at $k_c = 0$ is odd [31]. This ensures that there exist Majorana zero modes in a vortex along the $c$-axis. Hence, the low-lying QPs bound at the normal-core vortex undergo the topological phase transition from non-topological zero modes to symmetry protected Majorana fermions with increasing magnetic field. The topological phase transition without closing the bulk gap but accompanied by symmetry breaking has also been discussed in Refs. [23] and [32] recently.

**Concluding remarks.**—We have investigated the topological aspect of edge- and vortex-bound states for the recently identified gap function of the UPt$_3$ B-phase. In the edge state, Majorana fermions with linear dispersion are bound and their zero-energy states form the Majorana valley. The Majorana valley is protected by the mirror chiral symmetry, responsible for Ising anisotropy.

Note that the symmetry-protected Majorana valley at the surface can be detected by tunneling spectroscopy [33, 34]. The flat dispersion gives rise to a finite zero bias tunneling conductance, where the tunneling conductance is related to the surface LDOS [Fig. 1(b)] in the low transparent limit. The Majorana Ising anisotropy results in a decrease in the zero bias conductance under a magnetic field only along the $b$-axis. In contrast, the
surface states in the $E_{2u}$ scenario are not coupled with a magnetic field along the $b$-axis.

We have also demonstrated that the double-core vortex is not accompanied by the zero-energy state. As $H$ increases, the finite energy excitations in a double-core vortex undergo the topological transition to symmetry-protected Majorana fermions via topologically trivial zero modes in a normal-core vortex. The Majorana fermions are protected by a mirror symmetry against perturbations, such as a magnetic field, a crystal field, and a spin-orbit interaction, when the $d$-vector is locked in the $ab$-plane, $d(k) \propto \lambda_a b + \lambda_b a$. Hence, the B-phase of UPt$_3$ offers a promising platform for studying topological crystalline superconductors.

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