Majorana vortex-bound states in three-dimensional noncentrosymmetric superconductors

Po-Yao Chang,1 Shunji Matsuura,2 Andreas P. Schnyder,3 and Shinsei Ryu1

1Department of Physics, University of Illinois at Urbana-Champaign, Urbana, IL 61801, USA
2Department of Physics and Mathematics, McGill University, Montréal, Québec, Canada
3Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany

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Noncentrosymmetric superconductors (NCSs), characterised by antisymmetric spin-orbit coupling and a mixture of spin-singlet and spin-triplet pairing components, are promising candidate materials for topological superconductivity. An important hallmark of topological superconductors is the existence of protected zero-energy states at surfaces or in vortex cores. Here we investigate Majorana vortex-bound states in three-dimensional nodal and fully gapped NCSs using numerical as well as analytical methods. We show that depending on the crystal point-group symmetries and the topological properties of the bulk Bogoliubov-quasiparticle wave functions, different types of zero-energy Majorana modes can appear inside the vortex core. We find that for nodal NCSs with tetragonal point group $C_{4v}$, the vortex states are dispersionless along the vortex line, forming one-dimensional Majorana flat bands, while for NCSs with $D_4$ point-group symmetry the vortex modes are helical Majorana states with a linear dispersion along the vortex line. NCSs with monoclinic point group $C_2$, on the other hand, do not exhibit any zero-energy vortex bound states. Considering continuous deformations of the quasiparticle spectrum in the presence of vortices, we show that the flat-band vortex bound states of $C_{4v}$ point-group NCSs can be adiabatically connected to the dispersionless vortex-bound states of time-reversal symmetric Weyl superconductors. Experimental implications of our results for thermal transport and tunnelling measurements are discussed.

Introduction.— Topological superconductors have in recent years become a subject of intense research due to their potential use for technical applications in device fabrication and quantum information [1–5]. By the bulk-boundary correspondence, zero-energy Majorana modes appear at the surface or inside the vortex core of topological superconductors. The experimental search for Majorana modes, which can be utilised as basic building blocks (i.e., half a qubit) for topological quantum computers, is the focus of a growing research effort [6–8]. These Majorana modes are robust against symmetry preserving impurity scattering processes and deformations of the superconducting order parameter. While topological superconductivity can be artificially engineered in heterostructures with an ordinary $s$-wave superconductor and, say, a semiconductor [9–11] or a topological insulator [12], it can also occur naturally in certain correlated materials with strong spin-orbit coupling (SOC).

One promising class of materials for topological superconductivity are the noncentrosymmetric superconductors (NCSs) [13]. In these systems, the absence of inversion symmetry together with strong SOC and electronic correlations can give rise to unconventional pairing states with topologically nontrivial characteristics [14–23]. For example, in CePt$_3$Si [24–26], macroscopic as well as microscopic measurements indicate an unconventional superconducting state with a mixture of spin-singlet and spin-triplet pairing components and line nodes in the superconducting gap. Experimental evidence for unconventional pairing symmetries has also been reported for CeIrSi$_3$ [27], CeRhSi$_3$ [28], Y$_2$C$_3$ [29], Li$_2$Pt$_3$B [30–32], and BiPd [33]. Both fully gapped and nodal NCSs with sizeable spin-triplet pairing components exhibit nontrivial topological properties, which manifest themselves in terms of different types of zero-energy surface states. In fully gapped NCSs the surface states are dispersing helical Majorana modes, whereas nodal NCSs exhibit flat-band surface states [15–18,21,34]. and depending on the crystallographic point group, may also support helical Majorana modes or arc surface states [22]. Experimentally, it is possible to distinguish among different types of surface states using Fourier-transform scanning tunnelling spectroscopy [35] or surface transport measurements [36,37].

Most of the candidate materials for noncentrosymmetric topological superconductivity are strong type-II superconductors, with Ginzburg-Landau parameters $\kappa$ of the order of $\sim 100$ [13]. Hence, zero-energy Majorana modes may emerge inside magnetic vortices of these superconducting compounds [23,38,40]. In this paper, we examine vortex-bound states of three-dimensional (3D) NCSs and study how their appearance is related to the crystal point-group symmetries of the superconductor and the nontrivial topological properties of the bulk Bogoliubov-quasiparticle wave functions. Using both numerical and analytical methods, we compute the vortex-bound state spectra of $(s + p)$-wave NCSs with three different point-group symmetries: the two tetragonal point-groups $D_4$ and $C_{4v}$, as well as the monoclinic point-group $C_2$ [41].

One of our primary findings is that $D_4$ point-group NCSs support gapless helical Majorana states inside vortex cores. These subgap states disperse linearly along the vortex line, and are akin to one-dimensional helical Majorana modes that exist at the edge of fully gapped topological NCSs in two dimensions. Remarkably, these vortex-bound states appear both in the fully gapped topological phase and in the nodal phase that separates the fully gapped trivial phase from the topological one (see Figs. [1a] and [2]). While these helical Majorana vortex states exist in an extended region of the phase diagram of Fig. [1a], they are unstable against perturbations that break the $D_4$ point-group symmetry of the superconduc-
tor (SC) $^{42}$ For NCSs with tetragonal point-group symmetry $C_{4v}$, on the other hand, we find that there are zero-energy vortex-bound states which are dispersionless along the vortex line, forming a one-dimensional Majorana flat band (Fig. 3). In contrast, $C_2$ point-group NCSs do not exhibit any zero-energy vortex-bound states neither in the fully gapped nor in the nodal phase (Fig. 4).

Interestingly, the existence of these vortex-bound states in nodal NCSs correlates to some degree with the appearance of extra surface states, that appear in addition to the flat-band surface states. That is, for nodal NCSs with $D_4$ point-group symmetry the helical vortex-bound states always appear together with helical Majorana cones on the surface which are protected by a $Z_2$ topological number $^{18} 22$. (In the following, we refer to these Majorana cone surface states as the “$Z_2$ surface states”). On the other hand, for nodal $C_{4v}$ point-group NCSs the existence of flat-band vortex states is correlated with the appearance of helical arc states on the surface $^{22}$, see Table I. These arc surface states are superconducting analogues of the Fermi arcs that exist on the surface of Weyl semimetals $^{43-45}$. Using translation symmetry in the vortex direction, we fix the momentum along the vortex line and consider adiabatic deformations of the quasiparticle spectrum that do not close the bulk energy gap for this fixed momentum. By use of this procedure, we find that the vortex-bound states (extra surface states) of $D_4$ and $C_{4v}$ point-group NCSs are adiabatically connected to the vortex-bound states (surface states) of fully gapped topological SCs and time-reversal symmetric Weyl SCs, respectively. Conversely, finite-energy vortex-bound states of nodal NCSs with $C_2$ point-group symmetry can be related to finite-energy vortex-bound states of fully gapped trivial SCs (cf. Table I).

*Model Hamiltonian and symmetries.* — To study the appearance of vortex-bound states in nodal NCSs, we consider a generic single-band Bogoliubov-de Gennes (BdG) Hamiltonian $H = \sum_{\mathbf{k} \in \mathbb{BZ}} \Psi_{\mathbf{k}}^\dagger \mathcal{H}(\mathbf{k}) \Psi_{\mathbf{k}}$, with

$$\mathcal{H}(\mathbf{k}) = \begin{pmatrix} \mathcal{H}_0(\mathbf{k}) + \mathcal{H}_1(\mathbf{k}) + \mathcal{H}_2(\mathbf{k}) \end{pmatrix},$$  

and the Nambu spinor $\Psi_{\mathbf{k}} = (c_{\mathbf{k} \uparrow}, c_{\mathbf{k} \downarrow}, c_{-\mathbf{k} \uparrow}^\dagger, c_{-\mathbf{k} \downarrow}^\dagger)^T$, where $c_{\mathbf{k} \sigma}$ ($c_{\mathbf{k} \sigma}^\dagger$) denotes the electron annihilation (creation) operator with momentum $\mathbf{k}$ and spin $\sigma = \uparrow, \downarrow$. The normal-state Hamiltonian $\mathcal{H}_0(\mathbf{k}) = \mathcal{H}_\mu(\mathbf{k})I_{2 \times 2} + a \mathcal{H}_s(\mathbf{k}) \cdot \sigma$ describes electrons on a cubic lattice with nearest-neighbor hopping $t$, chemical potential $\mu$, spin-independent dispersion $\varepsilon(\mathbf{k}) = t(\cos k_x + \cos k_y + \cos k_z) - \mu$, and Rashba-type SOC $a \varepsilon(\mathbf{k}) \cdot \sigma$ with strength $\alpha$. Here, $\sigma = (\sigma_1, \sigma_2, \sigma_3)$ is the vector of Pauli matrices. Due to the absence of inversion symmetry, the superconducting gap $\Delta(\mathbf{k})$ contains in general an admixture of even-parity spin-singlet and odd-parity spin-triplet pairing components, $\Delta(\mathbf{k}) = \Delta_s \mathcal{I} \mathcal{I}_{2 \times 2} + \Delta_t \mathcal{D}(\mathbf{k}) \cdot \sigma(\mathcal{I} \mathcal{I}_{2 \times 2})$, where $\Delta_s$ and $\Delta_t$ represent the spin-singlet and spin-triplet pairing amplitudes, respectively. For the spin-triplet pairing term we assume that the vector $\mathcal{D}(\mathbf{k})$ is oriented parallel to the polarization vector $\mathbf{I}(\mathbf{k})$ of the SOC $^{46}$. For our numerical calculations we will set $(t, \alpha, \Delta_s) = (-1, 1, 1)$ and study the vortex-bound states as a function of $\Delta_s$, $\mu$, and different types of SOC potentials. Different values of $(t, \alpha, \Delta_s)$ do not qualitatively change our results. With $\varepsilon(\mathbf{k}) = \varepsilon(-\mathbf{k})$ and $\mathcal{H}(\mathbf{k}) = -\mathcal{H}(-\mathbf{k})$, Hamiltonian $^{1}$ is invariant under both time-reversal symmetry (TRS) and particle-hole symmetry (PHS), $U_T^{-1} \mathcal{H}(\mathbf{k}) U_T = \mathcal{H}(-\mathbf{k})$ and $U_P^{-1} \mathcal{H}(\mathbf{k}) U_P = -\mathcal{H}(-\mathbf{k})$, with $U_T = I_{2 \times 2} \otimes i \sigma_2$ and $U_P = \sigma_1 \otimes I_{2 \times 2}$, respectively. Hence, since $U_P U_T = -I_{4 \times 4}$ and $U_P U_T = I_{4 \times 4}$, $\mathcal{H}(\mathbf{k})$ belongs to symmetry class DIII.

The specific form of the spin-orbit coupling vector $\mathbf{I}(\mathbf{k})$ is constrained by the lattice symmetries of the superconductor $^{47}$. In the following we consider NCSs with three different crystal point-group symmetries: the tetragonal point groups $D_4$ and $C_{4v}$, as well as the monoclinic point group $C_2$. Within a tight-binding expansion, we obtain for the crystal point group $D_4$ to lowest order

$$\mathbf{I}(\mathbf{k}) = (a_1 \sin k_x, a_1 \sin k_y, a_2 \sin k_z).$$  

(2a)

For the tetragonal point group $C_{4v}$, which is relevant for CePt$_3$Si, CeRhSi$_3$, and CeIrSi$_3$, the vector $\mathbf{I}(\mathbf{k})$ takes the form

$$\mathbf{I}(\mathbf{k}) = (a_1 \sin k_y, -\sin k_x, 0).$$  

(2b)

The lowest order terms compatible with $C_2$ point-group symmetry (represented by BiPd) are given by

$$\mathbf{I}(\mathbf{k}) = (a_1 \sin k_x + a_5 \sin k_y, a_2 \sin k_y + a_4 \sin k_x, a_3 \sin k_z).$$  

(2c)

For a pair of vortex-antivortex lines oriented along the $z$ axis, the spin-singlet and spin-triplet order parameters are modified as $\Delta_{s,t}(x, y) = \Delta_{s,t} \alpha e^{i\phi(x, y)}$, where the phase angle $\phi(x, y)$ is given by $\phi(x, y) = \tan^{-1}[2aby/(x^2 + (by)^2 - a^2)]$. This describes a vortex and antivortex line with winding number $\pm 1$ located at $(a, 0)$ and $(-a, 0)$, respectively. In order to compute the vortex-bound states we set $(a, b) = (8, 2)$ and diagonalize the BdG Hamiltonian $^{1}$ on a $50 \times 50 \times 60$ cubic lattice with periodic boundary conditions (PBCs) in all three directions.

### Table I. Depending on the crystal point-group symmetries (first column), nodal NCSs can exhibit different types of zero-energy vortex-bound states (second column). As indicated in the third column, the appearance of these different vortex states correlates with the existence of extra surface states besides the flat-band states.

| Vortex states | Extra surface states | Adiabatic deformation |
|---------------|----------------------|-----------------------|
| $D_4$ helical states | $Z_2$ Majorana cone | fully gapped top. SC |
| $C_{4v}$ flat bands | helical arc states | Weyl SC with TRS |
| $C_2^a$ none | none | gapped trivial SC |

\(^a\) for phase IV.
Phase diagram.— The phase diagram of Hamiltonian (1) in the absence of vortices is shown in Figs. 1(a)-1(c) as a function of spin-singlet pairing amplitude $\Delta_s$ and chemical potential $\mu$. Two fully gapped phases with trivial and nontrivial topology (phases I and II in Fig. 1) are separated by a nodal superconducting phase (phases III and IV in Fig. 1) \[48\]. Interestingly, for the $\Delta_2$ point-group NCS we find that there are two distinct gapless phases with a Lifshitz transition in between, at which the nodal rings touch each other and recombine in a different manner [see Figs. 1(d) and 3(a)-3(d)]. The topological properties of the fully gapped phases I and II in Fig. 1 are characterized by the 3D winding number $\nu_3$, which is defined as $\nu_3 = \int_{BZ} d^3k e^{i\mu k^\mu} \text{Tr}[(q^{-1} \partial_{q_z} q)(q^{-1} \partial_{q_y} q)(q^{-1} \partial_{q_y} q)]$, where $q$ is the off-diagonal block of the spectral projector \[49\]. We find that phase I is topologically nontrivial with $\nu_3 = -1$, while phase II is trivial with $\nu_3 = 0$. The topological characteristics of the nodal phases III and IV, on the other hand, are described by the one-dimensional winding number $\nu_1 = \frac{i}{2\pi} \int_L d\mu \mu \text{Tr}[(q^{-1} \partial_{\mu} q)]$, where $L$ is a closed path that interlinks with a line node. In both nodal phases III and IV, the winding number $\nu_1$ evaluates to $\pm 1$ for each nodal ring.

Vortex-bound states in $D_4$ point-group NCSs.— Let us now discuss the surface states and vortex-bound states of a nodal NCS with $D_4$ point-group symmetry in phase III of Fig. 1(a). In this region of parameter space the bulk Bogoliubov quasiparticle spectrum exhibits two topologically stable nodal rings, which are centered about the (001) axis [Figs. 2(a) and 2(b)]. The one-dimensional winding number $\nu_1$ (topological charge) of these two nodal rings is $\nu_1 = \pm 1$, which by the bulk-boundary correspondence results in the appearance of flat-band surface states \[18\] \[22\]. In addition to the surface flat bands, nodal $D_4$ NCSs exhibit $Z_2$ Majorana surface states. This is shown in Figs. 2(c) and 2(d) for the (100) surface, where a helical Majorana cone appears at $(k_s, k_z) = (0, 0)$ of the surface Brillouin zone (BZ). As shown in Ref. 18, this Majorana surface state is protected by the one-dimensional $Z_2$ topological invariant $W_L = \prod_{K} \text{Pf} \left[ q^T(K) \right] / \sqrt{\text{det} \left[ q(K) \right]}$, where $L$ is a time-reversal-invariant (TRI) path along the transverse direction (i.e., here along the (100) direction) of the 3D BZ and $K$ denotes the two TRI momenta on the path $L$. Choosing $L$ to be oriented along the $k_z$ axis with $(k_y, k_z) = 0$ we find that $W_L = -1$, which signals the appearance of a zero-energy helical Majorana state at the surface momentum $(k_y, k_z) = 0$. At the other three TRI momenta of the surface BZ there are no surface states, in agreement with $W_L = +1$ for these momenta.

$D_4$ point-group NCSs support zero-energy helical Majorana states not only on the surface but also inside vortex cores. This is illustrated in Fig. 2(e), which shows the energy spectrum in the presence of a pair of vortex and antivortex lines oriented along the $z$ axis. At energies smaller than the bulk gap there appear vortex-bound states which disperse linearly along the vortex lines. These vortex-bound states are similar to the one-dimensional helical Majorana modes that exist at the edge of a fully gapped topological NCS in two dimen-
appearances. The numerical simulations of Fig. 2 are in excellent agreement with an analytical derivation of the vortex-bound states which we present in the Supplemental Material [49, 50].

By employing continuous deformations of the quasiparticle spectrum of Hamiltonian (1), one can show that the $Z_2$ surface states and the helical vortex-bound states of the nodal NCS with $D_4$ point-group symmetry [phase III in Fig. 1(a)] originate from the nontrivial properties of the adjacent fully gapped phase of the $D_4$ NCS [phase I in Fig. 1(a)]. To be more specific, let us fix the momentum along the vortex line (e.g., to $k_z = 0$) and consider adiabatic deformations connecting phase III to phase I that do not close the bulk gap at this particular momentum. During this deformation process, the two nodal rings shrink to nodal points at the north and south poles of the Fermi sphere and vanish, while the zero-energy vortex and surface states at $k_z = 0$ remain unaffected. Moreover, the $Z_2$ invariant $W_2$ of the nodal phase III can be shown to be directly related to the 3D winding number $\nu_3$ of the fully gapped phase I (cf. Ref. 10). Hence, the zero-energy vortex and $Z_2$ surface states of a nodal $D_4$ NCS are adiabatically connected to the vortex and surface states of a fully gapped topological NCS with $D_4$ point-group symmetry. A similar deformation process connecting phase III to phase II, on the other hand, does not exist, since upon crossing the transition line between phase III and phase I, the nodal rings approach each other and pair-annihilate. As a result, the zero-energy $Z_2$ surface states and vortex-bound states disappear as one traverses the transition line.

Vortex-bound states in $C_{4v}$ point-group NCSs.— Next we study surface and vortex-bound states of a nodal $C_{4v}$ point-group NCS in phase III of Fig. 1(b). The bulk quasiparticle spectrum in this nodal phase [Figs. 3(a) and 3(b)] resembles the one of the $D_4$ NCS [Figs. 2(a) and 2(b)] and shows two nodal rings around the poles of the Fermi sphere. These line nodes have a nontrivial topological charge, which, as a consequence of the bulk-boundary correspondence, lead to the appearance of flat-band surface states. In addition, $C_{4v}$ NCSs support helical arc surface states, that connect the projected nodal rings in the surface BZ [see Figs. 3(c) and 3(d)]. These helical arc surface states are protected by a two-dimensional $Z_2$ number, which is defined for each plane perpendicular to the (001) direction, (i.e., for planes with fixed $k_z$). The arc surface states of $C_{4v}$ NCSs can be viewed as superconducting analogues of the Fermi arcs in Weyl semimetals [43–45], or alternatively as time-reversal invariant versions of the arc states in the A phase of superfluid $^3$He [52, 53].

Due to the bulk-vortex correspondence [52], vortex lines in $C_{4v}$ NCSs support zero-energy bound states which are dispersionless along the vortex line. This is illustrated in Figs. 3(e) and 3(f) for a pair of vortex and antivortex lines that are oriented along the $z$ axis. Just as the arc surface states, these flat-band vortex-bound states connect the projected bulk nodes in $k_z$ momentum space. Using an adiabatic deformation of the Bogoliubov quasiparticle spectrum that does not close the bulk energy gap at the momenta $k_z$, in between the two projected nodal rings, we find that the flat-band vortex states and the arc surface states of the $C_{4v}$ NCSs can be related to the vortex states and surface states of a time-reversal symmetric Weyl superconductor. That is, upon approaching the boundary of phase III in Fig. 1(b) where $\Delta_s = 0$ and $\mu > -3$, the nodal rings shrink to points at the north and south poles of the Fermi sphere and the $C_{4v}$ NCSs turns into a time-reversal invariant Weyl superconductor, i.e., a time-reversal symmetric analogue of the A phase of $^3$He.
Vortex-bound states in $C_2$ point-group NCSs.—Lastly, we examine the surface and vortex-bound states of NCSs with $C_2$ point-group symmetry. The phase diagram of $C_2$ NCSs as a function of spin-singlet pairing amplitude $\Delta_s$ and chemical potential $\mu$ displays two distinct nodal phases, which differ in the orientation of the nodal rings [Figs. 1(a), 1(d), and 4(a)-4(d)]. In phase III the nodal rings are oriented along the (001) axis, while in phase IV they are centered about the (110) direction. As in the previous two cases, the topological characteristics of these nodal rings, which is described by the one-dimension winding number $v_1$, leads to the appearance of flat-band surface states. In addition, phase III supports $Z_2$ Majorana surface states, whereas phase IV does not exhibit any additional surface states. This is exemplified in Figs. 1(e) and 4(f), which show the energy spectrum at the (100) surface of a $C_2$ NCS in phase IV. Flat-band surface states appear within regions of the surface BZ that are bounded by the projected bulk nodal rings. But otherwise there exist no additional surface states in phase IV. Indeed, the energy spectrum along the $k_z = 0$ line is fully gapped (Fig. 4(f)). Using the same adiabatic deformations as before, we find that phase III can be connected to phase I, showing that the $Z_2$ surface states of phase III originate from the topological properties of the fully gapped phase I. Phase IV, on the other hand, can be deformed into phase II by shrinking the nodal rings into points at opposite sides of the Fermi surface until they vanish, which corroborates our finding that there are no additional surface states in phase IV.

In contrast to NCSs with $D_4$ or $C_{4v}$ point-group symmetry, NCS with monoclinic point-group $C_2$ do not support any zero-energy vortex-bound states, neither in the fully gapped phases I and II nor in the nodal phases III and IV. This suggests that the symmetries of the tetragonal point groups $D_4$ and $C_{4v}$ play a key role for the stability of the zero-energy vortex-bound states. The absence of zero-energy vortex states in $C_2$ point-group NCSs is demonstrated in Fig. 4(g) for phase IV, which shows the energy spectrum for a vortex-antivortex pair oriented along the (110) axis, and also follows from an analytical argument [49][54].

Summary and discussion.—In summary, we have studied zero-energy vortex-bound states in 3D nodal and fully gapped NCSs. While vortex lines in NCSs with tetragonal point-group $D_4$ and $C_{4v}$ support zero-energy vortex-bound states, $C_2$ point-group NCSs do not exhibit any Majorana vortex-bound states. We have found that the existence of Majorana vortex-bound states in nodal NCSs correlates with the appearance of Majorana cone and arc surface states. Our findings suggest that tetragonal point-group symmetries are important for the stability of zero-energy vortex states in NCSs. This is reminiscent of the zero modes at dislocation lines of band-topological insulators which are stabilized by certain space group symmetries [55].

Our findings have implications for experiments on 3D NCSs and on heterostructures, in which topological superconductivity is induced via the proximity effect of a conventional $s$-wave superconductor [56][57]. Vortex bound-states can be directly observed in ordinary and spin-resolved scanning tunneling microscopy. The helical Majorana vortex states of $D_4$ point-group NCSs can carry currents along the vortex lines, which could in principle be detected using thermal transport measurements [40]. Moreover, the vortex-bound states are expected to be observable in terms of the cross-correlated responses between the orbital angular momentum $L$ and the thermal polarization $P_E$ of a 3D topological SC, which were recently discussed in Ref. [58]. The so-called gravitomagnetoelectric polarizability of a 3D topological SC (i.e., the analogue of the magnetoelectric polarizability of a 3D topological insulator) is given by

$$\chi_{ab}^{E} = \frac{\partial E_{ab}^{s}}{\partial E_{g}^{s}} = \frac{\partial P_{E}^{a}}{\partial \Omega^{b}}, \quad a, b = x, y, z,$$

where $\Omega$ is the (external) angular velocity of the SC and $E_{g}^{s} = -T^{-1} \nabla T$ represents the temperature gradient. Note that the thermal polarization $P_{E}$ is related to the distribution of the induced heat $\Delta Q$ via $\Delta Q = -\nabla \cdot P_{E}$. According to Eq. (3) a thermal polarization (entropy polarization) $\chi_{ab}^{s}$ can be generated by rotating the system with angular velocity $\Omega^{p}$. The presence of vortex lines leads to an additional contribution to the angular momentum and hence to an additional accumulation of entropy (heat) at the top and bottom surfaces of the 3D SC. Vortex bound-states, on the other hand, can carry a thermal current connecting top and bottom surfaces.

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lation.
[50] Following Ref. [38], we consider the normal state band struc-
ture $h = (-\frac{\Delta^2}{2\mu} - \mu)\varepsilon_{2x2} + \alpha I(k) \cdot \sigma$ and the pairing term $\Delta = (\Delta_s + \frac{i}{2} \nabla \cdot D + i \nabla \cdot (i\sigma_2)$, where $m$ is the effective mass and $D = -i\nabla h(\Delta, I(k) \cdot \sigma)$. We can introduce a vortex line along $z$ axis localized at the origin by adding a phase on gap functions for both singlet and triplet pairings. In the contin-
uum model, we need to linearize $I(k) = (a_1 k_x, a_1 k_y, a_3 k_z)$. In addition, we consider the asymptotic limit $\hbar/k \to 0$ that we can neglect all $\frac{1}{k}$ and $\frac{1}{\hbar}$ terms in the continuum BdG equation, where $r$ is the radius direction in the cylindrical coordinate. As the result, there is a localized zero energy solution that decays as a function of $r$ [49].
[51] For the $C_{4v}$ point group, $I(k)$ is independent of $k_z$ and $h(k)$ is an even function of $k_z$. Hence for a fixed $k_z$ surface, an effective two-dimensional layer satisfies time-reversal and particle-
hole symmetries, $U_T^{-1} \mathcal{H}(k_x, k_y) U_T = \mathcal{H}^*(-k_x, -k_y)$ and $U_p^{-1} \mathcal{H}(k_x, k_y) U_p = -\mathcal{H}^*(-k_x, -k_y)$. It turns out that each fixed $k_z$ surface belongs to class DIII and the two-dimensional $\mathbb{Z}_2$ topological invariant can be computed.
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Supplemental Material

A. q matrix

For a Hamiltonian $H = \sum_{k} \Psi_{k}^\dagger \mathcal{H}(k) \Psi_{k}$ in the presence of chiral symmetry, $\mathcal{H}(k)$ can be block off-diagonalized

$$\mathcal{H}(k) = V \mathcal{H}(k) V^\dagger = \begin{pmatrix} 0 & D(k) \\ D^\dagger(k) & 0 \end{pmatrix},$$

(4)

where $V$ is an unitary transformation that brings $\mathcal{H}(k)$ into off-diagonal form. Generically, one can deform a Hamiltonian into a flat-band Hamiltonian without altering the topological features of $H(k)$. The flat-band Hamiltonian $Q(k)$ can be defined in terms of the spectral projector $P(k)$

$$Q(k) = \mathbb{1}_{4N} - 2P(k)$$

$$= \mathbb{1}_{4N} - 2 \sum_{a=1}^{2N} \begin{pmatrix} \lambda_a^-(k) \\ \mu_a^+(k) \end{pmatrix} \begin{pmatrix} [\lambda_a^-(k)]^\dagger & [\mu_a^-(k)]^\dagger \end{pmatrix},$$

(5)

where $(\lambda_a^-(k), \mu_a^-(k))^T$ are the negative-energy eigenfunctions of $\tilde{H}(k)$, which are obtained from the eigenequation

$$\begin{pmatrix} 0 & D(k) \\ D^\dagger(k) & 0 \end{pmatrix} \begin{pmatrix} \lambda_a^+(k) \\ \mu_a^+(k) \end{pmatrix} = \pm E_a(k) \begin{pmatrix} \lambda_a^-(k) \\ \mu_a^-(k) \end{pmatrix}.$$  

(6)

Here, $a = 1, \ldots, 2N$ denotes the combined band and spin index (we consider $N$ bands and two spin degrees of freedom). Similar as $\tilde{H}(k)$, the flat band Hamiltonian holds the off-diagonal form,

$$Q(k) = \begin{pmatrix} 0 & q(k) \\ q^\dagger(k) & 0 \end{pmatrix}. $$

(7)

B. Continuum model

The continuum BdG equation can be expressed as

$$\mathcal{H}\psi = \begin{pmatrix} h & \Delta \\ \Delta^\dagger & -h^\ast \end{pmatrix} \psi = E\psi,$$

(8)

where $h = (-\nabla^2 + \mu)\mathbb{1}_{2x2} + \alpha l(k) \cdot \sigma$, with $m$ is the effective mass, $\mu$ is the chemical potential, and $\alpha l(k) \cdot \sigma$ is Rashba-type SOC with strength $\alpha$. The pairing term has the form $\Delta = (\Delta_s + \frac{1}{2} \mathbf{\nabla} \cdot \mathbf{D} + \mathbf{D} \cdot \mathbf{\nabla})/(i\sigma_2)$, with $\Delta_s$ is the singlet pairing amplitude and $\mathbf{D} = -i \nabla_k (\Delta_p I(k) \cdot \sigma)$ presents the triplet pairing, where $\sigma = (\sigma_1, \sigma_2, \sigma_3)$ are the Pauli matrices. Without loss of generality, we consider the spin-orbit coupling vector $l(k) = (a_1 k_x + a_4 k_y, a_1 k_y + a_4 k_x, a_3 k_z)$. A vortex line along z direction can be introduced by adding a phase on both singlet and triplet pairing amplitudes, $\Delta_s \to e^{i\theta} \Delta_s$ and $\Delta_p \to e^{i\theta} \Delta_p$. In the cylindrical coordinate, the normal-state Hamiltonian and the pairing term are

$$h = (-\frac{1}{2m} (\partial_r^2 + \frac{1}{r} \partial_r + \frac{1}{r^2} \partial_{\theta}^2 + \partial_z^2) - \mu)\mathbb{1}_{2x2} + \alpha \left( \begin{array}{c} a_3(-i\partial_z) \\ -ia_1 e^{i\theta}(\partial_r + \frac{i}{\tau} \partial_{\theta}) - ia_4 e^{-i\theta}(i\partial_r + \frac{1}{\tau} \partial_{\theta}) \end{array} \right),$$

$$\Delta = \Delta_s e^{i\theta} (i\sigma_2) - i\Delta_p \left( \begin{array}{c} a_1(-\partial_r + i\frac{1}{\tau} \partial_{\theta}) + ie^{2i\theta} a_4(\partial_r + i\frac{1}{r} \partial_{\theta}) - e^{2i\theta} a_4(\partial_r + i\frac{1}{\tau} \partial_{\theta}) - \frac{a_3 \partial_z}{r} \\ a_3 \partial_z \end{array} \right).$$

(9)

A general solution of this continuum BdG equation is $\psi(r, \theta, z) = e^{ik_z z}[\tilde{u}_\uparrow(r) e^{im_1 \theta}, \tilde{u}_\downarrow(r) e^{im_2 \theta}, \tilde{v}_\uparrow(r) e^{im_1 \theta}, \tilde{v}_\downarrow(r) e^{im_2 \theta}]^T$. The radial part of a localized solution must be a decay form $f(r) \sim e^{-\kappa r}$ with $\text{Re}[\kappa] > 0$. In the asymptotic limit $(1/r \to 0)$,
we can neglect all \( \frac{1}{r^2} \) and \( \frac{1}{r} \) terms. We find for \((m_1, m_2, n_1, n_2) = (0, 1, 0, -1)\) and \(a_4 = 0\), the continuum BdG equation has a localized zero energy solution for (i) \(k_z = 0\) or (ii) \(a_3 = 0\), that satisfies

\[
\begin{pmatrix}
-\frac{1}{2m} \kappa^2 - \mu & i\alpha a_1 \kappa e^{-i\theta} & -i\Delta_p a_1 \kappa & \Delta_s e^{i\theta} \\
i\Delta_p a_1 \kappa & -\frac{1}{2m} \kappa^2 - \mu & -\Delta_s e^{i\theta} & i\Delta_p a_1 \kappa e^{2i\theta} \\
i\Delta_p a_1 \kappa & -\Delta_s e^{-i\theta} & \frac{1}{2m} \kappa^2 + \mu & i\alpha a_1 \kappa e^{i\theta} \\
\Delta_s e^{-i\theta} & -i\Delta_p a_1 \kappa e^{-2i\theta} & i\alpha a_1 \kappa e^{-i\theta} & \frac{1}{2m} \kappa^2 + \mu
\end{pmatrix}
\begin{pmatrix}
\tilde{u}_1(r) \\
\tilde{u}_4(r) \\
\tilde{v}_1(r) \\
\tilde{v}_4(r)
\end{pmatrix}
= 0.
\]

Notice that this situation corresponds to a zero-energy localized solution at \(k_z = 0\) under \(D_4\) point group symmetry. In addition, the decay length \(\kappa\) is determined by solving the roots of the following determinant

\[
\text{Det}
\begin{pmatrix}
-\frac{1}{2m} \kappa^2 - \mu & i\alpha a_1 \kappa & -i\Delta_p a_1 \kappa & \Delta_s \\
i\alpha a_1 \kappa & -\frac{1}{2m} \kappa^2 - \mu & -\Delta_s & i\Delta_p a_1 \kappa \\
i\Delta_p a_1 \kappa & -\Delta_s & \frac{1}{2m} \kappa^2 + \mu & i\alpha a_1 \kappa \\
\Delta_s & -i\Delta_p a_1 \kappa & i\alpha a_1 \kappa & \frac{1}{2m} \kappa^2 + \mu
\end{pmatrix}
= 0.
\]