

Superconductor Vortex Spectrum Including Fermi Arc States in Time-Reversal Symmetric Weyl Semimetals

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Using semiclassics to surmount the hurdle of bulk-surface inseparability, we derive the superconductor vortex spectrum in nonmagnetic Weyl semimetals and show that it stems from the Berry phase of orbits made of Fermi arcs on opposite surfaces and bulk chiral modes. Tilting the vortex transmutes it between bosonic, fermionic, and supersymmetric, produces periodic peaks in the density of states that signify novel nonlocal Majorana modes, and yields a thickness-independent spectrum at magic “magic angles.” We propose (Nb,Ta)P as candidate materials and tunneling spectroscopy as the ideal experiment.

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Superconductor vortices are fundamentally quantum mechanical entities with discrete energy levels whose structure encodes properties of the parent superconductor and the normal metal. For instance, an ordinary Fermi gas and conventional superconductivity lead to a gapped vortex spectrum [1] while vortices in two dimensional (2D) spinless $p + ip$ superconductors [2] and s -wave superconductors that descend from a 2D Dirac fermion [3] host zero energy states known as Majorana modes (MMs). MMs are exotic states that equate a particle with its antiparticle. They harbor diverse potential applications ranging from topological quantum computing [4–10] and topological order [11] to supersymmetry (SUSY) [12–16], quantum chaos, and holographic blackholes [17,18]. In condensed matter, they invariably appear as topologically protected zero energy bound states in topological defects such as superconductor vortices and domain walls [2,3,5–7,10,19–31]. In recent years, the discovery of MMs in Fe-based superconductors with tunable band topology [22,32–44] and the observation of superconductivity in several topological semimetals [45–69] have motivated an urgent quest to theoretically determine the vortex spectrum given an arbitrary normal metal.

This pursuit hits a roadblock with gapless topological matter such as Weyl semimetals (WSMs) [70–88]. In the bulk, WSMs host accidental band crossings or Weyl nodes (WNs) that enjoy topological protection and spawn various topological responses [89–108]. WNs carry an intrinsic chirality or handedness, and are constrained to appear in pairs of opposite chirality [100]. Moreover, in time-reversal (\mathcal{T}) symmetric WSMs (TWSMs), each WN has a Kramer’s partner of the same chirality which leads to quadruplets of WN. The surface of a WSM hosts Fermi arcs (FAs) that connect the surface projections of pairs of WN of opposite chirality [77–86,109–127], resembling a broken segment of a 2D Fermi surface but forming a closed loop with a FA on

the opposite surface of a finite slab. The penetration depth of a FA into the bulk depends strongly on the surface momentum and diverges at the WN projections, thus making the surface inseparable from the bulk. Consequently, the Fermi “surface” of WSMs consists of FAs on the surface of the material and bulk Fermi points at the WNs (or Fermi pockets around WNs not at the Fermi level). Such a Fermiology is beyond a purely surface or purely bulk theory; yet, a basic physical question remains, What is the spectrum of a superconductor vortex in a WSM?

General vortex spectrum.—We answer this question using a powerful semiclassical approach that surmounts that above limitation. We restrict to TWSMs, since they generically host a weak pairing instability towards a gapped superconductor; WSMs that lack \mathcal{T} either lack a pairing instability or yield unconventional nodal or finite-momentum pairing [128–131]. For arbitrary pairing symmetry that yields a full gap when uniform, we propose the spectrum

$$E_n^\pm = \pm \varepsilon \left(n + \frac{1}{2} + \frac{\Phi_B + \Phi_S - \Phi_Q}{2\pi} \right); \quad \varepsilon = \frac{\Delta_0}{\xi l_{\text{FA}}} \quad (1)$$

where l_{FA} is of order the total length of FAs on opposite surfaces that form a closed loop, Δ_0 is the pairing amplitude far from the vortex, ξ is the superconductor coherence length, and $n \in \mathbb{Z}$. Additionally, Φ_B is the net phase acquired by a wave packet traversing the bulk. In the simplest case where FAs on opposite surfaces connect the same pairs of WN as depicted in Fig. 1, $\Phi_B = \Delta \mathbf{K} \cdot \mathbf{R}_v$ with $\Delta \mathbf{K}$ connecting these nodes in momentum space and \mathbf{R}_v connecting opposite ends of the vortex in real space. Henceforth, we parameterize $\mathbf{R}_v = (a_x \hat{x} + a_y \hat{y} + \hat{z}) L_z \equiv (\mathbf{a}_\perp + \hat{z}) L_z$, where L_z is the slab thickness and \hat{z} is the surface normal. Next, Φ_S is the total Berry phase of a “classical” path defined by the FAs on both surfaces that

ignores their bulk penetration. Finally, the penetration effectively reduces the thickness to $L_z - 2d$, where d is the average penetration depth of the FAs in a region of size $O(\xi^{-1})$ around the surface projections of the Weyl nodes. This induces a quantum correction

$$\Phi_Q = 2d\Delta\mathbf{K}_\perp \cdot \mathbf{a}_\perp \quad (2)$$

where $\Delta\mathbf{K}_\perp = \Delta K_x \hat{x} + \Delta K_y \hat{y}$. Thus, Eq. (1) predicts a generically nondegenerate, discrete spectrum with equally spaced energy levels, while the zero-point energy is determined by the Berry phase of the FAs, WN locations, sample thickness, and vortex orientation. The spectrum is generically gapped, contrary to a naive bulk approach that predicts a generically gapless spectrum [132].

Equation (1) is inspired by results in Refs. [19,133], and [132]. Reference [133] showed that quasiparticle dynamics in inhomogeneous superconductors can be faithfully captured by quantizing the semiclassical action for wave packets traveling in closed orbits in real space. The action, which appears as a phase in the relevant path integral, was shown to consist of three terms: (i) a Bohr-Sommerfeld phase $\oint \mathbf{k}_{cl} \cdot d\mathbf{r}_{cl}$ for the classical orbit, (ii) a Berry phase due to rotation of the Nambu spinor, and (iii) a π phase if a unit vortex is encircled. Within a complementary momentum-space picture, Ref. [19] proved that a smooth 2D Fermi surface in the normal state and arbitrary pairing symmetry that produces a full gap when superconductivity is uniform yield a superconductor vortex spectrum $\epsilon_n^\pm = \pm(\Delta_0/\xi l_{FS})[n + \frac{1}{2} + (\Phi_{FS}/2\pi)]$ for $l_{FS}\xi \gg 1$, where l_{FS} and Φ_{FS} are the Fermi surface perimeter and Berry phase, respectively. The normal state is assumed to be \mathcal{T} symmetric, which leads to a pair of Fermi surfaces with opposite Berry phases in the normal state that produce particle-hole conjugate eigenstates inside the vortex.

To propose Eq. (1) for a TWSM, we first note that the Bohr-Sommerfeld phase, π phase from the vortex, and the Nambu-Berry phase contribute shifts proportional to n , $1/2$, and $\Phi_{FS}/2\pi$, respectively in ϵ_n . Then, we recall that a WN with chirality $\chi = \pm 1$ produces a chiral MM in the vortex core with chirality χw , where $w = \pm 1$ is the winding number of the vortex [132]. Thus, for $w = 1$, a right- (left-) handed WN produces a chiral MM inside the vortex with upward (downward) group velocity. For a smooth vortex, defined by $|\Delta\mathbf{K}\xi| \gg 1$, these chiral modes allow wave packets to travel between FAs on opposite surfaces without scattering. The smoothness also ensures that a wave packet on the surface travels along a single FA without scattering into other FAs. Thus, the semiclassical orbit naturally involves travel along a FA on the top surface, tunneling through the bulk via a downward chiral MM, FA traversal on the bottom surface followed by tunneling up the bulk via an upward chiral MM. Since a TWSM contains quadruplets of WNs and an even number of FAs on each surface related by \mathcal{T} , such orbits appear in \mathcal{T} -related pairs but with opposite energies in the vortex to preserve overall particle-hole symmetry. This picture inspires the generalization of Φ_{FS} to $\Phi_{tot} = \Phi_B + \Phi_S - \Phi_Q$, the total phase acquired by a wave packet traversing a closed orbit in mixed real and momentum space, as depicted in Fig. 1.

A peculiar situation occurs when $\Phi_{tot}/2\pi$ equals a half-integer. Then, Eq. (1) predicts a gapless vortex with a pair of zero modes that can always be decomposed into a pair of MMs in a suitable basis [134]. These MMs are highly nonlocal as they are composed of mixed real- and momentum-space orbits. They are not protected by symmetry; rather, they appear at a series of critical points as Φ_{tot} is varied. These critical points separate trivial and topological phases of the vortex, which behaves as a 0D superconductor with a \mathbb{Z}_2 topological classification [135]. The MMs decouple at criticality by definition and, when probed via

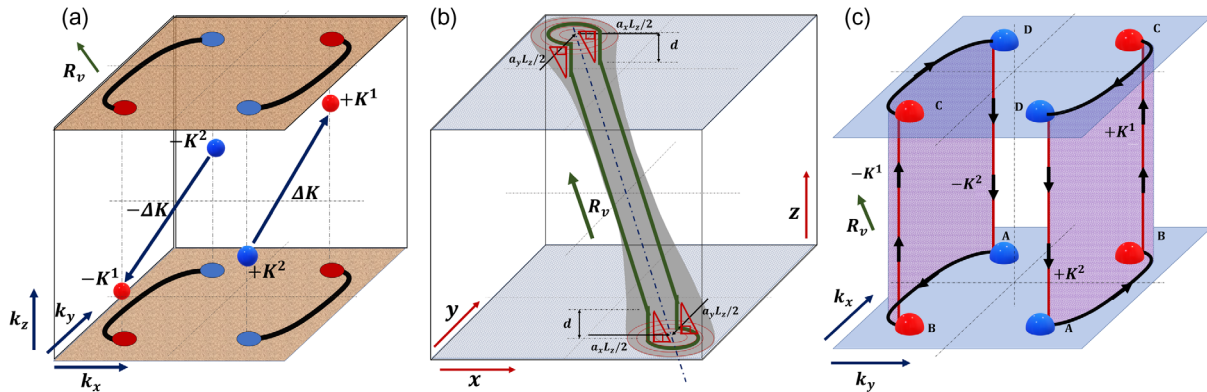


FIG. 1. Schematic picture. (a) k -space illustration of a minimal TWSM. Red (blue) spheres at $\pm K^1$ ($\pm K^2$) denote right- (left-)handed WNs, red (blue) discs denote their projections onto the surface Brillouin zone, and black curves are FAs. (b) Real space illustration of the vortex (grey tube) and the semiclassical orbit (green curve). The classical bulk path parallels the tube axis, but quantum tunneling causes deviations near the surface. (c) Semiclassical orbits in mixed real (z) and momentum (k_x, k_y) space. Each orbit is a closed loop consisting of bulk chiral modes tied to a pair of WNs interspersed by FAs that connect their surface projections.

an STM whose tip metal has doubly degenerate bands, contribute separately to the tunneling conductance. Thus, the peak height in the dI/dV spectrum must be twice that of topological MMs [136,137], $2 \times 2e^2/h = 4e^2/h$, while the regions between critical tilts must contain quantized plateaus separated by $4e^2/h$ in the I - V characteristics.

Now, pairs of MMs separate gapped superconductors differing in fermion parity [138]. Thus, the vortex is fermionic with odd fermion parity on the topological side of criticality, and bosonic on the trivial. Naturally, the critical vortex is impartial to bosonic or fermionic statistics and therefore exhibits SUSY—a mysterious and elusive symmetry between bosons and fermions first proposed in the standard model and more recently, in certain condensed matter systems [12–16,139,140] (see Ref. [134] for details). Remarkably, vortices here can be tuned between bosonic, fermionic, and supersymmetric by varying Φ_{tot} which, we show below, can be accomplished by simply tilting the magnetic field that threads the vortex. While disorder, the Zeeman effect and other perturbations can modify the critical tilt angles, SUSY will persist at criticality as it is purely a property of the critical vortex and oblivious to how criticality was achieved.

In general, the vortex also contains purely bulk states that do not involve the FAs. First, WNs at the Fermi level will produce modes $E_{\text{bulk}}^{\pm}(n_1, n_2, q_3) = \pm \sqrt{2\hbar(v_1 n_1 + v_2 n_2)\Delta_0/\xi + (v_3 \hbar q_3)^2}$, where $n_{1,2} \in \mathbb{Z} \geq 0$, $n_1 + n_2 \geq 1$, q_3 is the momentum along the vortex axis measured relative to the WN and (v_1, v_2, v_3) are the canonical Weyl speeds. These modes are nonchiral and lie above the bulk gap $E_g = \sqrt{2\hbar v \Delta_0/\xi}$, where $v = \min(v_{1,2})$. Clearly, $E_g \gg \varepsilon$ if $l_{\text{FA}} \xi \gg \sqrt{\Delta_0 \xi/\hbar v} \sim 1$, assuming the standard Ginzburg-Landau relation $\Delta_0 \sim \hbar v/\xi$. Since $l_{\text{FA}} \sim |\Delta \mathbf{K}_{\perp}| \leq |\Delta \mathbf{K}|$, the smooth vortex limit of $|\Delta \mathbf{K} \xi| \gg 1$ is consistent with nonchiral bulk modes from undoped WNs being at parametrically higher energies.

Second, the bulk can also contain Fermi pockets. In the weak-pairing, smooth vortex limit, these pockets give rise to the spectrum $E_{\text{bulk}}^{\pm}(n, q_3) = \pm[\Delta_0/\xi l_{\text{FS}}(q_3)]\{n + \frac{1}{2} + [\Phi_{\text{FS}}(q_3)/\Phi_{\text{FS}}(q_3)]\}$ with $n \in \mathbb{Z} \geq 0$. Trivial Fermi pockets that do not enclose band crossings have $\Phi_{\text{FS}}(q_3) \neq \pm\pi \forall q_3$ and contribute only nonchiral modes. In contrast, Fermi surfaces enclosing WNs have $\Phi_{\text{FS}} = -\pi$ at $q_3 = 0$ (relative to the WN) and contribute a single $n = 0$ chiral MM that combines with the FAs to form the states described in Eq. (1), while the $n \neq 0$ modes are nonchiral. For both types of Fermi pockets, the energy scale of the nonchiral modes $[\Delta_0/\xi l_{\text{FS}}(q_z)] \lesssim \varepsilon$ if $l_{\text{FS}} \gtrsim l_{\text{FA}}$. However, these modes can be easily distinguished from those defined in Eq. (1) by tilting the vortex, as we discuss shortly.

Finally, the normal state bulk can contain other point or line band crossings too which can invalidate various aspects of our results. For instance, vortices in Dirac semimetals contain a pair of counterpropagating modes for each Dirac

node [141–143], which can hybridize and ruin the semiclassical picture. We ignore crossings beyond unit WNs because they rely on crystalline symmetries while our focus is on generic band structures with only \mathcal{T} symmetry [144–146].

Numerical vortex spectrum.—We now support our general claims of Eq. (1) with numerics on an orthorhombic lattice model of a TWSM detailed in [134]. Given the Bloch Hamiltonian $H_0(\mathbf{k}, k_z)$ in the normal state, the corresponding Bogoliubov-deGennes Hamiltonian for a unit vortex along $(a_x, a_y, 1)$ can be written as

$$H_v = \begin{pmatrix} H_0(\mathbf{k}, k_z) & \Delta(\delta \mathbf{r}_{\perp})e^{-i\Theta(\delta \mathbf{r}_{\perp})} \\ \Delta(\delta \mathbf{r}_{\perp})e^{i\Theta(\delta \mathbf{r}_{\perp})} & -H_0(\mathbf{k}, k_z) \end{pmatrix} \quad (3)$$

where $\delta \mathbf{r}_{\perp} = (x - a_x z, y - a_y z)$, $\Theta(\delta \mathbf{r}_{\perp})$ is the polar angle of $\delta \mathbf{r}_{\perp}$ and $\Delta(\delta \mathbf{r}_{\perp}) = \Delta_0 \tanh(|\delta \mathbf{r}_{\perp}|/\xi)$. Direct numerical verification of Eq. (1) involves diagonalizing H_v in real space. However, the lack of translation invariance in every direction limits us to relatively small ξ , which causes departure from semiclassics for modest values of n . We bypass this limitation by tilting the vortex and comparing the locations of the zero modes with the predictions of Eq. (1). This way, we always probe the lowest few energy levels, which conform better to the semiclassical analysis. While this method allows a careful examination of the Berry phase terms and reveals various striking phenomena, ε is verifiable only up to its order of magnitude.

Figure 2(a) shows the FAs and WNs in a minimal TWSM with four WNs located at $\pm \mathbf{K}^1$ and $\pm \mathbf{K}^2$. We chose parameters such that all nodes are at different k_z and $|\Delta K_x| \ll |\Delta K_y|$ where $\Delta \mathbf{K} = \mathbf{K}^1 - \mathbf{K}^2$. Figure 2(b) shows the vortex spectrum for a finite slab when a vortex, initially along \hat{z} , is tilted separately towards the x and the y axis. Tilting towards the positive y axis ($a_x = 0$, $a_y > 0$) produces numerous level crossings, which is consistent with $\Phi_B = (\Delta K_y a_y + \Delta K_z)L_z$ changing by many multiples of 2π as a_y varies. In contrast, the spectrum varies weakly when the vortex is tilted towards the x axis, which is consistent with $\Phi_B = \Delta K_x a_x L_z$ varying negligibly with a_x since ΔK_x itself is small. In Fig. 2(c), we plot the wave functions of a pair of levels with equal and opposite energies in (k_x, k_y, z) space. The levels, which are related by particle-hole symmetry of the superconductor, are clearly localized around semiclassical orbits related by \mathcal{T} . This confirms the picture that motivated Eq. (1), namely, that the vortex spectrum follows from quantizing semiclassical orbits in mixed real and momentum space, and that semiclassical orbits related by \mathcal{T} turn into pairs of particle-hole conjugate quantum eigenstates. In [134], we use the zero mode locations to extract $\Delta K_{y,z}$ and Φ_S and find remarkable agreement with expectations.

Tilting the vortex.—Besides simplifying the numerics, tilting the vortex leads to striking qualitative phenomena.

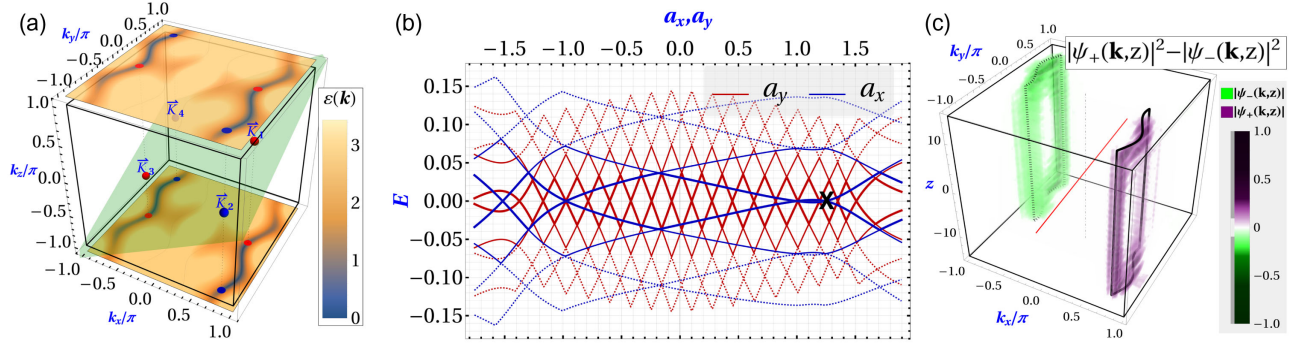


FIG. 2. Vortex spectrum for a tight-binding lattice model with unit interatomic spacing and $O(1)$ hoppings (see Ref. [134] for details). (a) Normal state band structure showing four bulk WNs (red and blue spheres), all at different k_z , and surface FAs connecting them. The four nodes lie on the green plane, which is clearly not parallel to the surface. (b) Vortex spectrum of a $L_x \times L_y \times L_z = 23 \times 23 \times 34$ system as the vortex is tilted separately towards the x axis and the y axis by $\tan^{-1} a_i$ ($i = x, y$). (c) Net probability density of the two lowest energy wave functions in (k_x, k_y, z) space at $a_y = 1.25$, marked “X” in (b), obtained by Fourier transforming the 3D real space wave functions with respect to x, y . We choose the band parameter $u = 1.2$ which yields $\Delta \mathbf{K}^{\text{calc}} = \{0.029, 0.428, 0.181\} \times 2\pi$, and superconducting parameters $\Delta_0 = 0.50$, $\xi = 2.0$, which yield $\varepsilon = \Delta_0/\xi l_{\text{FA}} \approx 0.04$ comparable to the scale of level spacings in (b).

First, since L_z enters Eq. (1) only through Φ_B , the spectrum becomes L_z independent when the vortex is tilted to a “magic angle” such that $\Delta \mathbf{K} \perp \mathbf{R}_v$ even though the semiclassical orbit still involves travel across the bulk. Moreover, we expect peaks in the density of states, $D(E) = \sum_{n,\lambda} \delta(E - E_n^\lambda)$, whenever $E_n^\pm = 0$. Noting that Φ_S does not depend on the vortex orientation, $D(0)$ peaks whenever $\Delta \mathbf{K}_\perp \cdot \mathbf{a}_\perp (L_z - 2d)$ equals a half-integer. Thus, the tilt parameters for two successive peaks obey

$$\Delta \mathbf{K}_\perp \cdot [\mathbf{a}_\perp^{(j)} - \mathbf{a}_\perp^{(j+1)}] = \frac{2\pi}{L_z - 2d}. \quad (4)$$

Thus, the peaks are periodic in \mathbf{a}_\perp with a period Δa governed by the WN locations through $\Delta \mathbf{K}_\perp$ and the effective thickness, $L_z - 2d$. Specifically, $\Delta a = [2\pi/(L_z - 2d)\Delta K_t]$, where ΔK_t is the component of $\Delta \mathbf{K}_\perp$ in the tilt direction.

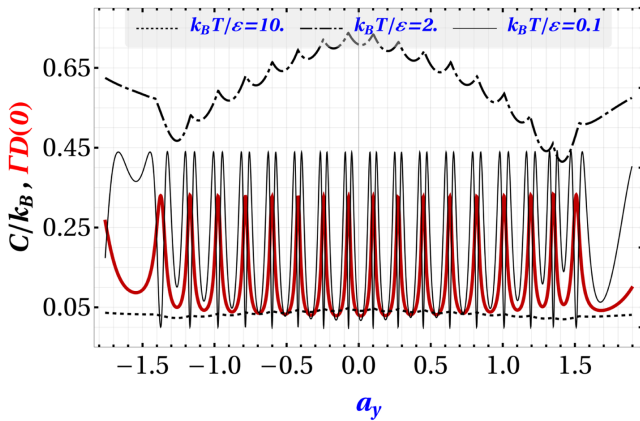


FIG. 3. Suitably normalized density of states $D(0)$ and specific heat C at different temperatures versus a_y . Zero modes in the spectrum lead to sharp peaks in $D(0)$ at periodic intervals of a_y , $\Delta a_y = [2\pi/(L_z - 2d)\Delta K_y]$, and induce oscillations in C at low T that get smeared out at high T . We approximate $D(E) = \pi^{-1} \text{Im} \sum_n [E - E_n - i\Gamma]^{-1}$ with $\Gamma = 0.0075$.

These peaks will induce characteristic oscillations with period Δa in transport and thermodynamic quantities at temperatures below the minigap, $T \lesssim \varepsilon/k_B$. For instance, the specific heat $C = k_B \sum_n [(E_n^+/k_B T) \text{sech}(E_n^+/k_B T)]^2$ will have oscillations with a “split-peak” structure (Fig. 3). Similarly, a scanning tunneling microscope (STM) should find zero bias peaks in the differential conductance, dI/dV , at periodic tilts with a peak height of $4e^2/h$. These oscillations can be used to distinguish the semiclassical modes depicted in Fig. 1 from nonchiral vortex modes generated by bulk Fermi pockets. The latter are expected to produce only quantitative variations due to the anisotropy of the Fermi pockets, but no oscillations or L_z dependence besides finite-size effects.

The magic angle and oscillations are reminiscent of quantum oscillations due to FAs in WSMs [126,127,147]. There, a magnetic field B induces cyclotron orbits involving surface FAs and bulk chiral modes, $D(0)$ has periodic peaks in $1/B$, and L_z enters the oscillation phase as an optical path length. Thus, at the quantum level, the discretization predicted by Eq. (1) is analogous to Landau levels rather than finite size quantization. Indeed, if the latter was at play, Eq. (1) in the thermodynamic limit should have yielded the gapless bulk spectrum described in Ref. [132] where FAs are irrelevant. It clearly does not, which can be attributed to the infinite penetration of the FAs into the bulk that forbids ignoring them even in this limit.

Application to (Nb,Ta)P.—NbP and TaP are TWSMs in which superconductivity induced at high pressure survives upon quenching to ambient pressure [51,62]. Superconductivity has also been reported in TaP directly at ambient pressure [69]. Both materials have 24 Weyl nodes interrelated by C_4 symmetry of a face-centered tetragonal lattice with conventional unit cell lattice constants $a_{\text{NbP}} = 0.3334 \text{ nm}$, $c_{\text{NbP}} = 1.1376 \text{ nm}$ and $a_{\text{TaP}} = 0.3318 \text{ nm}$, $c_{\text{TaP}} = 1.1363 \text{ nm}$ [148], and connected by 12 pairs of surface FAs. Although nonuniversal surface details

strongly modify the FAs and lead to nontopological gapless surface states from trivial Fermi surfaces [83,149], a smooth superconductor vortex tilted in a general direction is expected to produce 12 pairs of \mathcal{T} -related semiclassical orbits and hence, a superposition of 12 different oscillations frequencies in dI/dV . On the other hand, tilting in the yz plane ensures that only orbits with nonzero ΔK_y cause oscillations. If FAs connect surface projections of the nearest nodes of the same family, then $\Delta K_y = 0$ for all six orbits that involve WNs separated by the yz plane, while C_4^2 and \mathcal{T} symmetries ensure that the six orbits that cross the xz plane will result in precisely two frequencies: one from WNs with $\Delta \mathbf{K}_{\perp, \text{NbP}}^1 = 1.0198 \times (2\pi/a_{\text{NbP}})\hat{y}$ for NbP and $\Delta \mathbf{K}_{\perp, \text{TaP}}^1 = 0.9618 \times (2\pi/a_{\text{TaP}})\hat{y}$ for TaP, and another from WNs with $\Delta \mathbf{K}_{\perp, \text{NbP}}^2 = 0.5406 \times (2\pi/c_{\text{NbP}})\hat{y}$ and $\Delta \mathbf{K}_{\perp, \text{TaP}}^2 = 0.5486 \times (2\pi/c_{\text{TaP}})\hat{y}$. Discernible oscillations require $T \lesssim \varepsilon/k_B = \Delta_0/\xi l_{\text{FA}} k_B \sim T_c/\xi l_{\text{FA}}$. Using $T_c \sim 4$ K [51,62], $\xi \sim 4$ nm [58] and $l_{\text{FA}} \sim 10$ nm⁻¹ gives $T \lesssim 0.1$ K, which may be within reach of current STM experiments. Note that ε is of the same order as the vortex minigap in typical type-II superconductors, and STM can comfortably probe vortex modes in the latter including zero bias conductance peaks from MMs [22,33–38,150].

In summary, we have calculated the superconductor vortex spectrum in TWSMs including contributions from the surface FAs. While a naive bulk calculation for a general vortex orientation suggests a gapless spectrum consisting of a chiral mode corresponding to each WN, we found that the low-energy spectrum is gapped in general, and determined by the Berry phase of semiclassical orbits composed of the chiral modes and surface FAs. Such a spectrum is expected to produce a myriad of striking phenomena upon tilting the vortex. For instance, the vortex will alternate between bosonic and fermionic as it is tilted, while the critical points separating the two types of vortices exhibit SUSY and harbor unusual nonlocal MMs. Experimentally, we predict characteristic oscillations in the specific heat and periodic, $4e^2/h$ -quantized peaks in the differential tunneling conductance as a function of vortex tilt. At a certain tilt, dubbed the “magic angle,” the spectrum becomes independent of the slab thickness. We propose NbP and TaP as candidate materials and tunneling spectroscopy as the best experimental approach for studying this physics.

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