Topological superconducting domain walls in magnetic Weyl semimetals

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Recent experimental breakthrough in magnetic Weyl semimetals have inspired exploration on the novel effects of various magnetic structures in these materials. Here we focus on a domain wall structure which connects two uniform domains with different magnetization directions. We study the topological superconducting state in presence of an s-wave superconducting pairing potential. By tuning the chemical potential, we can reach a topological state, where a chiral Majorana mode or zero-energy Majorana bound state is localized at the edges of the domain walls. This property allows a convenient braiding operation of Majorana modes by controlling the dynamics of domain walls.

Introduction – The last decade has witnessed spectacular advancements in the understanding, prediction, and synthesis of new topological materials with diverse exotic emergent phenomena originating from the nontrivial band topology. One of the most interesting classes is the Weyl semimetal where the low-energy electronic dispersion closely follows the three dimensional Weyl Hamiltonian. The salient properties originate from the nontrivial Berry curvature exhibited around the nodal points in the three-dimensional band structure. Moreover, by integrating the Berry curvature over a closed manifold around a given node yields its topological charge and chirality. Recently, magnetic Weyl semimetals have gained great interest since the broken time-reversal symmetry prevents the Weyl nodes with opposite chirality from overlapping and annihilating one another. Thus, this new class of materials provide a new platform to study the interplay between nontrivial band topology, magnetism, and correlations, thereby opening up new routes to novel quantum phenomena.

Magnetic Weyl semimetals are expected to host topological superconductivity when put in proximity to a trivial superconductor. This delicate state is predicted to support chiral Majorana modes or localized Majorana bound states at edges, endings or defects. These zero-energy Majorana modes mimic the Majorana fermion and can follow nontrivial trajectories originating from the nontrivial Berry curvature exhibited around the nodal points in the three-dimensional band structure. The last decade has witnessed spectacular advancements in the understanding, prediction, and synthesis of new topological materials with diverse exotic emergent phenomena originating from the nontrivial band topology. One of the most interesting classes is the Weyl semimetal where the low-energy electronic dispersion closely follows the three dimensional Weyl Hamiltonian. The salient properties originate from the nontrivial Berry curvature exhibited around the nodal points in the three-dimensional band structure. Moreover, by integrating the Berry curvature over a closed manifold around a given node yields its topological charge and chirality. Recently, magnetic Weyl semimetals have gained great interest since the broken time-reversal symmetry prevents the Weyl nodes with opposite chirality from overlapping and annihilating one another. Thus, this new class of materials provide a new platform to study the interplay between nontrivial band topology, magnetism, and correlations, thereby opening up new routes to novel quantum phenomena.

Controlled magnetic switching and domain wall motion have formed a basis for magnetic random access memory and magnetic nanowire device concepts, which lie in the core of spintronics. Large metastable magnetic domains have also been observed in a noncentrosymmetric ferromagnetic Weyl semimetal candidate CeAlS. Therefore, the existence and control of these magnetic domain walls in magnetic Weyl semimetals provides a hope to realize new electronic states.

In this Letter, we propose that a magnetic Weyl semimetal with magnetic domain walls in proximity to a superconducting pairing potential can host chiral Majorana edge modes, or zero-energy Majorana bound states, at the edge of the domain walls. The appearance of these modes follows from the highly anisotropic dependence of the nontrivial band topology on the direction of the magnetization. Specifically, we show that the magnetization orientation induced area difference of nontrivial topology in the phase diagram can be utilized to enable topologically trivial superconductivity away from the domain wall, whereas a topologically nontrivial superconductivity on the domain wall, thus realizing localized topological edge states on the domain walls. Lastly, we demonstrate that the braiding of Majorana modes can be straightforwardly achieved by tuning the magnetization of the domains.

Method – The effective Hamiltonian of a magnetic Weyl semimetal may be written for a cubic lattice as

$$H_0 = \sum_j \left( -\mu c_j^\dagger c_j + \left[ -t_\sigma c_j^\dagger \mathbf{\sigma} c_{j+\hat{x}} - i (c_j^\dagger \mathbf{\sigma} c_{j+\hat{y}} + c_j^\dagger c_{j+\hat{z}}) - i\Delta c_j^\dagger \mathbf{\sigma} c_{j+\hat{x}} + c_j^\dagger c_{j+\hat{z}} + H.c. \right] + m_c c_j^\dagger \mathbf{\sigma} c_j + m_s c_j^\dagger \mathbf{\sigma} c_j \right) \right)$$

where $\mu$ is the chemical potential, $t_\sigma$, $t$, and $t'$ are the coefficients of spin-orbit coupling, $m_c$ and $m_s$ are the projected Zeeman field strengths on the $x$ and $z$ axes, respectively. By inspection, time-reversal and inversion symmetry are both broken in this Hamiltonian. Upon Fourier transforming, the energy eigenvalues are $E = -\mu \pm \sqrt{h_x^2 + h_y^2 + (h_z + m_c)^2}$ with $h_x = m_c - 2t_\sigma \cos k_x - 2t \cos k_y - 2t \cos k_z$, $h_y = 2t' \sin k_x$, and $h_z = 2t' \sin k_z$, where the position of the Weyl nodes satisfies $h_x = h_y = h_z + m_c = 0$.

To include the presence of superconductivity, we add the pairing potential in the mean-field,

$$H_{sc} = \sum_j \left[ \Delta c_j^\dagger c_{j+\hat{x}} + \Delta' c_j^\dagger c_{j+\hat{y}} \right] ,$$

where $\Delta$ is a momentum independent uniform s-wave gap function. Here we do not restrict the source of superconductivity. It can be either intrinsic or induced by proximity. To model a domain wall in this system, we allow $m_c$ and $m_s$ to be spatially dependent over the whole $x-z$ plane. Without loss of generality, we take $m_c = m_c \cos Q(x-x_0)$ and $m_s = m_s \sin Q(x-x_0)$, where the magnetization rotates through an...
angle of $Q(x - x_0)$ between points $x_0$ and $x$, as shown in Fig. 1(a). Since translational invariance is broken along the $x$-axis, the domain wall system is governed by the two-dimensional topological classification rules. Consequently, the topological charge is obtained from the Chern number of the $k_y$ - $k_z$ plane in the momentum space. Furthermore, the eigen-energy and wavefunction of the edge states are obtained within a thin-film geometry, which leads to a quasi-one-dimensional domain wall.

**Results** – Figure 1(b) and 1(c) show the band structure at $k_y = 0$ for the magnetization along the $z$ and $x$ axes, respectively, with no superconductivity. The hopping parameters $t_x = 0.4t$, $t_y = 0.4t$ were used. For the Zeeman field along the $z$-axis $[m_z = 0.5\mu]$, four Weyl nodes are present at $k_y = (\pm 0.68\pi, 0, -0.79\pi)$ and $(\pm 0.32\pi, \pi, -0.21\pi)$ in the Brillouin zone. For the magnetization along the $x$-axis $[m_x = 0.5\mu]$, the four Weyl nodes are located at $(\pm 0.29\pi, 0, \pi)$ and $(\pm 0.29\pi, \pi, 0)$. These two cases are called “Weyl phase I” and “Weyl phase II” for convenience.

To characterize the effect of the superconducting pairing potential on the electronic band structure, we perform a Wilson loop analysis on a $16 \times 1 \times 1$ supercell with periodic boundary conditions to obtain the Chern number. By tuning the chemical potential $\mu$ and gap function $\Delta$, we map out the phase diagram, as shown in Fig. 2, for the various Weyl phases. The purple and yellow regimes denote topological trivial and nontrivial phases, respectively. Since time-reversal symmetry is broken, this system belongs to the class D topological superconductors.

Figure 2(a) and 2(b) present the phase diagram of Weyl phase I as a function of superconducting pairing strength versus the chemical potential and filling factor, respectively. Interestingly, in comparing these results to the phase diagram for Weyl phase II [Fig. 2 (c) and (d)] we find the regime of nontrivial topological phase is larger in Weyl phase II than Weyl phase I. This key difference is what allows us to restrict a topologically nontrivial superconducting phase to a magnetic domain wall. That is, by choosing a $(\mu, \Delta)$ to be nontrivial for Weyl phase II, but trivial for Weyl phase I, we can design a domain wall structure where away from the domain the magnetization is aligned along the $z$-axis while at the domain wall the magnetization is pointing along the $x$ direction, thus inducing a local topologically nontrivial phase.

The phase boundary may also be obtained analytically from the Hamiltonian in momentum space

$$H = \begin{bmatrix}
-\mu + m_z + h_z & h_z - ih_y & 0 & \Delta \\
 h_z + ih_y & -\mu - m_z - h_z & -\Delta & 0 \\
 0 & -\Delta^* & \mu - m_z + h_z & -h_z + ih_y \\
\Delta^* & 0 & -h_z - ih_y & \mu + m_z - h_z
\end{bmatrix},$$

by recognizing that the determinant is the product of the eigenvalues. Therefore, if the bands are gapless $\det(H) = 0$ otherwise the system is gapped. Using this fact, the phase boundary can easily be determined as a function of $\mu$ and $\Delta$.

The determinant of the Hamiltonian in Eq. (3) is $D(h_x, h_y, h_z) = (h_x^2 + h_y^2 + h_z^2 - \Delta^2 - \mu^2)^2 + 4h_x^2\Delta^2 + 4h_z^2(\Delta^2 - m_z^2)$. To analyze the local minima of $D$ as a function of $h_x$, $h_y$, and $h_z$ we first start by tuning $h_x$. The minimum of $D$ is found at $h_z^2 = \Delta^2 + \mu^2 - m_z^2 - (h_x^2 + h_y^2)$ with minimum $D_{\text{min}} = 4h_x^2\Delta^2 + 4h_z^2(\Delta^2 - m_z^2)$. For Weyl phase II $[m_z = 0]$, the minimum value is 0 for $h_x = h_y = 0$, which implies the bands are always gapless as long as the minimum condition
cases: \[\Delta h\] above the minima condition obeys 4
corner [(−tum phase I and II we find (the phase boundary given by
near the Fermi level. The location of the domain wall is marked by
for a rectangular slab of superconducting magnetic Weyl semimetal.
arrow indicate the propagation direction of the chiral Majorana edge
the magnetization (red arrows) varying along the x-axis. The green
(∆2 + µ2 = (2t_x + 4t + m_z)m_z) 2. Comparing the phase boundary for Weyl
phase I and II we find \((2t_x + 4t + m)^2 \geq (2t_x + 4t + m)^2 + m_z^2\). For
produces a topologically nontrivial domain wall, parameters must be chosen to respect
the inequality \((2t_x + 4t + m)^2 \geq \Delta^2 + \mu^2 > (2t_x + 4t + m)^2 + m_z^2\).
Figure 3(a) shows a schematic of the domain wall geometry
where the magnetization rotates clockwise by \(\pi\) across the first
domain wall (DW-I) and then rotates by \(\pi\) again across the
second domain wall (DW-II) allowing for periodic boundary
condition along x and avoiding spurious defect states intro-
duced by an edge. Since the magnetization is uniform along
y and translational invariance is only broken along the x-axis,
the domain walls are two-dimensional, covering the y-z plane.
To study the edge states in the y-z plane, we need to take an
open boundary condition in the y or z dimension. For the
remaining discussion, let \(t_x = 0.4t, m = 0.5t, \mu = 5t, \) and
\(\Delta = 0.3t\) all of which satisfy the condition for localized Majorana modes.

Figure 3(b) shows the electronic band structure along the \(k_z\)
direction for the slab geometry with \(N_x = 16\) and \(N_y = 130\). DW-I and II are constrained at \(x \in (4, 8)\) and \((12, 16)\). Two
pairs of linearly dispersing bands are clearly seen crossing the
Fermi level at 0 and ±\(\pi\) along \(k_z\), indicating the existence of
topological edge modes. For the first pair, the corresponding
Bogoliubov wavefunction amplitude [Fig. 3(c) and 3(d)] is
highly localized at the edges of the DW-I, decaying rapidly
into the bulk. The propagation direction of each Majorana mode is further elucidated from the sign of the Fermi velocity and indicated by the green arrows in Fig. 3(a). Similarly, the amplitude of the wavefunction for the second pair [Fig. 3(e) and 3(f)] is located at the edges of DW-II, with propagation
directions opposite to those pinned to DW-I. Fundamentally,
this is driven by the fact that DW-I and DW-II have opposite
magnetizations due to the opposing magnetizations on the do-
 mains. As a result the winding numbers in the Wilson loop
analysis mutually cancel, as discussed further in the supple-
mental material[40]. Furthermore, if a single domain wall with open boundary conditions is equivalently examined, a finite
winding number is found[40].

We now shift our discussion to the case of an atomically-
thin film breaking z-axis translational invariance, as depicted
in Figure 4(a), to elucidate our Majorana mode braiding proto-
ocol. In this case, there is a single one-dimensional domain wall and running along the y-axis. Specifically, we utilize a
9 × 60 × 4 super cell with \(\mu = 3.5t\) and \(\Delta = 0.9t\) and study its
nontrivial topology directly by diagonalizing the Hamiltonian
in the real space. Here, the magnetization is positive (neg-
ative) in the upper (lower) half plane centering the domain wall
at \(x = 0\). Figure 4(b) shows the eigen-energy spectrum close
of these levels onto the second layer in the
existence of two localized Majorana bound states. Projecting
the wavefunction of these levels onto the second layer in the z
direction [Fig. 4(c)] we confirm the presence of the localized
edge modes. For the projected wavefunction on the various
layers in the system, see the appendix[40].

From the two examples above, we clearly see that nontrivial
topology comes about at the interface between two differing
magnetization domains in the Weyl semimetal. Therefore, by
patterning various magnetic domain topologies with external
magnetic fields we can control and manipulate the presence
and position of the localized Majorana states. Thereby, pro-
viding a mechanism by which to facilitate braiding.

Figure 4(d) presents our proposed Majorana braiding proto-
ocol using a magnetic Weyl semimetal thin-film. The surface
of the film is divided into four quadrants with independently
tunable magnetic fields. To initialize a state, the upper and
lower half-planes are oppositely polarized creating a domain
wall with Majorana bound states at either end, labeled as \(\gamma_1\)

FIG. 3. (Color) (a) schematic of the two domain wall geometry with
the magnetization (red arrows) varying along the x-axis. The green
arrows indicate the propagation direction of the chiral Majorana edge
modes. (b) Electronic band dispersions along \(k_z\) in the Brillouin zone
for a rectangular slab of superconducting magnetic Weyl semimetal.
(c), (d), (e), and (f) show the amplitude of wavefunction at \(k_z\) momentum −0.926\(\pi\) and 0.074\(\pi\) for the pairs of linearly dispersing bands
near the Fermi level. The location of the domain wall is marked by
the white dash lines.

can be reached. Therefore, the phase boundary corresponds
to a critical point where \(h_z^2 + h_y^2 + h_x^2 = \Delta^2 + \mu^2\). The max-
imum value of \(h_z^2 + h_y^2 + h_x^2\) is \((2t_x + 4t + m_z)^2\) located at a
corner [(\(\pi, \pi, \pi\)] of the Brillouin zone when \(t' < t\), with a corresponding phase boundary \(\Delta^2 + \mu^2 = (2t_x + 4t + m_z)^2\).
The analysis of Weyl phase I [\(m_z = 0\)] were split into two
cases: \(\Delta > m_z\) and \(\Delta < m_z\). For \(\Delta > m_z\), following our steps
above the minima condition obeys \(4h_z^2(\Delta^2 - m_z^2) \geq 0\), with
the phase boundary given by \(\Delta^2 + \mu^2 = (2t_x + 4t + m_z)^2 + m_z^2\). For
\(\Delta < m_z\), the phase boundary is slightly perturbed away from
\((2t_x + 4t)^2 + m_z^2\). Comparing the phase boundary for Weyl
phase I and II we find \((2t_x + 4t + m)^2 \geq (2t_x + 4t + m)^2 + m_z^2\) when
taking \(m_x = m_y = m\). Therefore, to produce a topologically
nontrivial domain wall, parameters must be chosen to respect
the inequality \((2t_x + 4t + m)^2 > \Delta^2 + \mu^2 \geq (2t_x + 4t)^2 + m_z^2\).
FIG. 4. (Color) (a) An atomically-thin film slab of a magnetic Weyl semimetal with a one dimensional magnetic domain wall. (b) The eigen-energy spectrum close to the Fermi level with two zero-energy states corresponding to localized Majorana bound states. (c) Projected wavefunction amplitude of the Majorana bound states in real space. (d) Proposed four step Majorana braiding protocol. Direction of the external magnetic field along the $z$-axis in the various quadrants of the magnetic Weyl semimetal slab is indicated in red.

Due to the numerous experimental demonstrations inducing and controlling magnetic domain walls in real quantum materials, we are optimistic that the same level of robustness and precision can be achieved in the magnetic Weyl semimetals. Furthermore, a recent work by Xu et al. on CeAlSi has exemplified this claim. The key ingredients required by our proposal, such as strong anisotropy and fine tuning of the chemical potential, have been recently experimentally suggested in a several magnetic Weyl semimetals including Co$_3$Sn$_2$S$_2$, Mn$_3$Sn, Co$_2$MnGe and CeAlSi or is readily realized by chemical doping or electrostatic gating thin film samples.

Lastly, the presence of superconductivity is essential for the realization of Majorana modes on the domain walls. The superconductivity and magnetic Weyl phase can coexist intrinsically in materials, termed Weyl superconductors. Presently, there is mounting evidence suggesting UTe$_2$ and MoTe$_2$ to be Weyl superconductors. For generic magnetic Weyl semimetals, superconductivity can be induced by proximity effect, through heterostructuring with other bulk superconductors, such as Nb.

The four ingredients of this topological superconducting domain wall are anisotropic band structure, band topology, magnetism and superconductivity. In principle, the materials option does not restrict to the magnetic Weyl semimetal. However, these ingredients except for superconductivity is generically available in this material which makes it a natural platform to search for such domain walls.

**Conclusion** – We have demonstrated the existence of the chiral Majorana edge modes or zero-energy Majorana bound states on the domain walls of an anisotropic magnetic Weyl semimetal with intrinsic superconductivity or using a superconducting proximity effect. Because the magnetic domain wall emerges at the interface between two differing magnetic domains, they are easily controlled and manipulated by external magnetic fields. Finally, we have proposed a straightforward braiding protocol of zero-energy Majorana bound states.

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I. SINGLE DOMAIN WALL

The effective Hamiltonian of a magnetic Weyl semimetal including the mean-field pair potential for a three-dimensional lattice is given by

\[ H_0 = \sum_j -\mu c_j^\dagger c_j + \left[-t_x c_j^\dagger \sigma_x c_{j+\hat{x}} - t_y c_j^\dagger \sigma_y c_{j+\hat{y}} + \Delta c_{j+\hat{z}}^\dagger c_j + H.c.\right] \]

\[ + m_x c_j^\dagger \sigma_x c_j + m_z c_j^\dagger \sigma_z c_j + \Delta c_j^\dagger c_j + \Delta' c_{j+\hat{z}}^\dagger c_{j+\hat{z}}, \]  

(4)

where \( \mu \) is the chemical potential, \( t_x, t_y \) and \( t' \) are the spin-orbit coupling coefficients, \( m_x \) and \( m_z \) are the projected Zeeman field strengths along the \( x \) and \( z \) axes.

II. WANNIER CENTER CURVES

Figure 6 compares the evolution of the Wannier function center with \( k_y \) momentum for the cases of a single domain wall [Fig. 5(a)] and two domain walls [Fig. 3 of the main text]. For the single domain wall case, the Chern number is \( C = 1 \) since the Wannier center traverses from \( -\pi \) to \( \pi \) once, indicating the existence of a single chiral edge mode\(^2\). For the two domain case, the Chern number is zero, since one winding goes through \( 2\pi \) and the other goes to \( -2\pi \), thus mutually canceling. These two opposing winding numbers correspond to the opposite chirality of the chiral Majorana edge mode of the domain walls shown in Fig. 3 of the main text.
FIG. 6. (color online) The evolution of the Wannier center curves along the $k_y$ axis for a (a) single domain wall and (b) two domain walls.

III. ATOMICALLY-THIN FILM OF MAGNETIC WESYLM SEMIMETAL

To elucidate Majorana mode generation we consider to cases: In. the first case, the magnetization is equal and opposite in the upper and lower half-planes of a $9 \times 60 \times 4$ thin-film super cell of a typical magnetic Weyl semimetal. In the second case, the magnetization is uniform across the whole plane. For both cases we study its electronic structure and possible nontrivial topology directly by diagonalizing the Hamiltonian in the real space using open boundary conditions and the following parameters $t_x = 0.4t, t' = 0.4t, m = 0.5t, \mu = 3.5t$, and $\Delta = 0.9t$. In the first case, a single one-dimensional domain wall is formed running along the $y$-axis centered at $x = 0$ [Fig. 7(a)] with the magnetization rotating by $\pi$ across the domain wall. As a consequence, the corresponding electronic structure exhibits two zero-energy levels [Fig. 7(b)]. In contrast, for a uniform magnetization, no such modes are present [Fig. 7(c)].

FIG. 7. (color online) (a) An atomically-thin film slab of a magnetic Weyl semimetal with a one-dimensional magnetic domain wall. The eigen-energy spectrum close to the Fermi level with (b) and without (c) the domain walls. The panel (b) shows clearly the existence of two zero-energy modes corresponding to Majorana bound states.

Figure 8 presents the corresponding real space wavefunction amplitudes of the zero-energy modes. To capture an individual localized Majorana mode at the edge of the sample, we apply a unitary transformation to resolve the weak coupling between the edge states from the finite size effects, that is, $\psi_1 = (\psi_{+e} + \psi_{-e})/\sqrt{2}$ and $\psi_2 = (\psi_{+e} - \psi_{-e})/\sqrt{2}$, where $\psi_{\pm e}$ is the spatially
dependent Bogoliubov quasiparticle wavefunction \((u_\uparrow, u_\downarrow, v_\uparrow, v_\downarrow)\) for the level \(\pm \varepsilon\). Figure 8(a)-(d) and Fig. 8(e)-(h) show the projection of \(|\psi_1|^2\) and \(|\psi_2|^2\) on the four layers along the z-axis. Clearly, the Majorana modes are localized at either end of the domain wall.
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