The appearance of gapless modes at the interface between insulating phases with distinct topologies is one of their quintessential traits, and holds many promises for novel device designs. This feature is usually attributed to the so-called bulk-edge correspondence. Roughly speaking, in order to “unwind” one band structure into another one must close the gap at some point, rendering protected localized states, that usually display chiral properties. The prime example of this is the Quantum spin Hall (QSH) effect. There, counter-propagating modes belonging to opposite spins will emerge within the bulk band gap at the boundary between two time-reversal symmetric insulators with different $Z_2$ topological invariants.

While the manifestation of chirality in transport has been thoroughly researched, in this paper we will examine in detail what happens when the chiral states are forced into a loop, a subject unexplored until now. We will show that, depending on the particular topology and the type of material on either side of the loop, the chirality manifests as a spin and/or valley coupling between the states bound to the orbit and their angular momentum, making these loops potential building blocks for artificial magnets with tunable and highly diverse properties.

We start by introducing our general model, which is valid for arbitrarily shaped loops, is shown by solving Eq. (1) for the geometry depicted in the upper row of Fig. I. Note that in the domains $I$ and $II$ only a single mass term of the form $\Delta_{I/II}\sigma_z$ is used in Eq. (1). For instance, in case (c) $\Delta_I = s\tau\Delta_{KM}$ and $\Delta_{II} = \Delta_{SP}$. Then the evanescent modes, decaying exponentially away from the interface read

$$\Psi_{I/II} = e^{ik_zz} e^{i\kappa_{g/II}/\hbar v_F} \left[ \frac{1}{\Delta_{I/II}^2 + \varepsilon^2} \right],$$

and we are interested in solutions $E = \pm \hbar v_F k_z$, with $\kappa_{g/II} = |\Delta_{I/II}|/\hbar v_F$. Matching the wavefunctions at the absence of magnetic field, inducing the quantum anomalous Hall (QAH) phase. Finally, $\Delta_{SP}$ is the staggered potential breaking the inversion symmetry, and opening a trivial band gap unlike the previous two.

An interface between any of the aforementioned insulating phases will support boundary modes. This can be shown by solving Eq. (1) for the geometry depicted in the upper row of Fig. I. Note that in the domains $I$ and $II$ only a single mass term of the form $\Delta_{I/II}\sigma_z$ is used in Eq. (1). For instance, in case (c) $\Delta_I = s\tau\Delta_{KM}$ and $\Delta_{II} = \Delta_{SP}$. Then the evanescent modes, decaying exponentially away from the interface read

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FIG. 1. (a) - (d) The set of interfaces between insulating phases considered. The upper row shows the parameters related to each region, while the middle row depicts the corresponding dispersion of the emerging modes. The bottom row illustrates the hypothesis for the persistent currents in the closed loops inferred from the linear dispersion relations. Red (blue) lines depict the states belonging to the $K$ ($K'$) valley, while the spin is denoted by arrows.
TABLE I. Summary of the numerical solutions. The symbol “×” means that there are no allowed solutions, while the allowed modes are characterized by the corresponding angular momentum numbers $j$.

|   | $\uparrow K$ | $\uparrow K'$ | $\downarrow K$ | $\downarrow K'$ |
|---|-------------|-------------|-------------|-------------|
| (a) | $j > 0$ | $j < 0$ | $j > 0$ | $j < 0$ |
| (b) | $\times$ | $j < 0$ | $\times$ | $j < 0$ |
| (c) | $\times$ | $j < 0$ | $j > 0$ | $\times$ |
| (d) | $\times$ | $\times$ | $j < 0$ | $j < 0$ |

The boundary leads to the dispersion relations shown in the middle row of Fig. 4. These demonstrate chirality of the topological modes bound to the interface [2, 3]. Unlike the cases in Figs. 1(c) and 1(d), the first two cases are spin degenerate.

We now present the main premise of our paper. Instead of straight interfaces, we consider circular ones, depicted in the bottom row of Fig. 4. The chirality of the boundary modes suggests that the angular momentum of the states in these loops must obey certain selection criteria depending on the particular phases in regions I and II. For instance, in the cases (b) and (d) one would expect to see that only negative angular momentum valley and spin filtered states are allowed, respectively.

To explore this explicitly, we solve the problem in polar coordinates, in which the Hamiltonian (11) reads

$$H = \left[ \frac{\Delta_{I/II}}{\pi^+} \frac{\pi^-}{-\Delta_{I/II}} \right].$$

where $\pi^\pm = \tau \hbar v_F e^{\pm i \theta} (i \partial_r \pm \tau \partial_\phi)$. Because of the radial symmetry the total angular momentum $J_z = I_z + J_{\tau/2}$ is a good quantum number denoted by $j$ [19, 20], and therefore the solution can be sought in the form

$$\Psi = e^{i(j-\tau/2)\phi} \left[ \chi_A(r) \right. e^{i\tau \phi} \chi_B(r) \right].$$

The coupled system of equations reduces to the differential equation

$$\left[ r^2 \frac{d^2}{dr^2} + r \frac{d}{dr} - \frac{\Delta_{I/II}^2 - E^2}{\hbar^2 v_F^2} r^2 - (j - \tau/2)^2 \right] \chi_A = 0.$$  

Having in mind that we are interested in states lying within the bulk band gap $\Delta_{I/II}^2 - E^2 > 0$, so that the solutions are the modified Bessel functions $I_{j-\tau/2}(r)$ and $K_{j-\tau/2}(r)$, which are exponentially divergent at $r \to \infty$ and $r = 0$, respectively. The radially bound modes read

$$\Psi_I = e^{i(j-\tau/2)\phi} \left[ I_{j-\tau/2}(z_I(r)) \right.$$

$$-i\tau e^{i\tau \phi} \frac{\Delta_{I/II}^2 - E^2}{\Delta_{I/II} + E} I_{j+\tau/2}(z_I(r)) \left. \right],$$

and

$$\Psi_{II} = e^{i(j-\tau/2)\phi} \left[ K_{j-\tau/2}(z_{II}(r)) \frac{\Delta_{I/II}^2 - E^2}{\Delta_{I/II} + E} K_{j+\tau/2}(z_{II}(r)) \right],$$

where $z_{II} = \sqrt{\Delta_{I/II}^2 - E^2} r$. Matching $\Psi_I$ and $\Psi_{II}$ at the interface $r = R$ results in the eigenvalue equation

$$\sqrt{\Delta_{I/II}^2 - E^2} I_{j+\tau/2}(z_I(R)) I_{j-\tau/2}(z_{II}(R)) = 0,$$

which we solve numerically.

Our numerical results are summarized in Table I for four cases shown in Fig. 1. For those spin and valley flavors for which there exists a solution for a given interface we give the allowed angular momentum values, while the cases for which no solution is found are indicated by “×”. Only results for positive energies are given, since the negative energy solutions are the same, albeit with opposite values of $j$. By inspecting Table I and comparing it with Fig. 4 one can see that the numerical results agree with the expectations deduced from the chirality of the topological modes. Namely, the angular momentum of the states bound to the loops does not only display the expected orientation but are also: (a) valley-coupled, (b) valley-filtered, (c) spin-valley-filtered, and (d) spin-filtered.

In Fig. 2 the solid black lines are the numerically computed energies of the bound states for the radial interface corresponding to Fig. 4(a) for spin up in the $K$ valley. Note that for all the modes that are allowed, the set of energies is the same (only the angular momentum number $j$ varies), such that it suffices to show the spectrum for only one particular case. One can see that the larger loops can support states with higher $j$. Note also that, as a rule, there exists only one state for a given $j$. This is due to the exponential localization at the loop, which prevents oscillatory behavior in the radial direction and the emergence of a corresponding degree of freedom.

Interestingly, the energy curves follow a $1/R$ form with amazing precision, and it is relatively easy to obtain a good analytical fit of the energy levels using the following reasoning. Given the exponential localization of the modes near $r = R$, the loops effectively become 1D closed lines carrying states with pseudospin degree of freedom, described by $\psi$. Then, by requiring single-valuedness of $\psi$ upon one full revolution we must have $\psi(\phi + 2\pi) = -e^{i\phi} \psi(\phi)$, where the contour is oriented counterclockwise. The minus sign comes from the spinorial nature of the state, and it forces the phase factor accumulated along the trajectory $\theta = \text{sgn}(j) p L/h$ ($L = 2\pi R$ is the loop length) to be quantized in half integer multiples of $2\pi$. Denoting this half integer number by $j$, and recalling the dispersion of the topological
modes $E = v_F p$, yields the following expression

$$E = |j| \frac{h v_F}{R},$$

for the energy levels. They are shown in Fig. 2 in dashed red lines, and show an excellent agreement with the numerical results. Only a small deviation between the two sets of curves is found for the loops with the smaller radius. This is to be expected, given that for smaller loops overlap of the wavefunction must occur, permitting tunneling of the modes between sections of the loop.

Having analytically elucidated the chiral nature of the angular momenta, we now employ the TB method to study the behavior of the loops in a magnetic field. On the one hand, this is important because it can offer insights into intervalley scattering. Indeed, the most critical case is the setup (a), since valley flipping can cause back-reflection and mixing of the states, something not captured within the continuum approach. All the other cases are more robust, since either there are no counter-propagating states ((b) and (d)), or backscattering requires the simultaneous flipping of the valley and spin indices (setup (c)). On the other hand, the TB method will help us to resolve important details of the magnetic moments originating from the loops. The TB Hamiltonian that we used reads

$$H = -t \sum_{\langle i,j \rangle} \epsilon^{\nu_{ij}} c_i^\dagger c_j + i \frac{s \Delta_K M}{3 \sqrt{3}} \sum_{\langle (ij) \rangle} \nu_{ij} \epsilon^{\nu_{ij}} c_i^\dagger c_j. \quad (10)$$

We use $t = 2.7$ eV for the hopping between nearest neighbor $p_z$ orbitals, while the second term is the SOC. Note that $\nu_{ij} + 1$ ($\nu_{ij} - 1$) if an electron makes a right (left) turn at the intermediate atom when hopping from site $j$ to site $i$. The Peierls term $\varphi_{ij} = -\frac{e}{\hbar} \int_{r_j}^{r_i} A \cdot dl$ accounts for the phase the electron acquires while traveling in the presence of the magnetic field. The staggered potential is simply added along the main diagonal of the Hamiltonian, like in the continuum model.

Our calculations were performed for a loop of radius $R = 10$ nm contained within a larger circular quantum dot, with a 15 nm radius, so that a proper decay of the topological modes is ensured. The results are shown by solid lines in Figs. 3(a) and (b) for the loop setups depicted in Figs. 1(a) and (c), respectively, as a function of the magnetic flux through the loop $\Phi = BR^2 \pi$ in units of the flux quantum $\Phi_0 = \hbar / e$. For setup (a) the results are shown in black, since the TB model cannot resolve the two valleys, while for setup (c) (Fig. 3(b)) the valleys can be distinguished due to the additional spin polarization. In Fig. 3(a), for $B = 0$ the majority of the levels are degenerate indicating the preservation of the valley index. Only a handful of levels (for instance those around 0.1 eV) are offset by an equally small amount in the opposite directions with respect to the continuum solutions. This behavior indicates that such states are susceptible to intervalley scattering, causing bonding and anti-bonding states. As the magnetic field is turned on, the remaining valley degeneracy is lifted due to the opposite magnetic moments (see below). Moreover, an anticrossing behavior occurs at energies where intervalley scattering is prominent, resulting in an Aharonov-Bohm-like pattern of the curves. On the other hand, for the setup (c), such scattering is impossible in the TB picture due to the absence of spin-flipping terms in the Hamiltonian, as demonstrated by Fig. 3(b). Consequently, the spin up in the $K$ valley (solid blue curve), with a magnetic moment oriented along the magnetic field, and the spin down in the $K$ valley (solid red curve) with the opposite orientation of the magnetic moment are independent of each other, and experience a rigid, linear, decrease and an increase in energy, respectively.

In order to capture the behavior of the topological modes in the presence of a magnetic field, we again resort to the consideration of the phase change upon a single rotation around the loop. Now, due to magnetic field the additional phase factor of the form (assuming $B$ is constant inside the loop) $-\frac{e}{\hbar} \oint A \cdot dl = -\frac{e}{\hbar} BS$ appears, where $S$ is the loop area. As before, $\theta$ must be a half integral multiple of $2\pi$, yielding

$$E = |j| \frac{h v_F}{L} + \text{sgn}(j) \frac{e v_F}{L} SB. \quad (11)$$

These levels are depicted by dashed curves in Fig. 3 and show excellent agreement with the TB results, with small deviations at very large magnetic fields [21]. Note that the change in energy due to magnetic field can be captured entirely by the classical formula for the energy of a closed current contour given by $-\mu B$. Besides the area of the loop, the magnetic moment of a classical contour $\mu = IS$ depends on the current due to one topo-
Finally, the loops in setup (d) not only reduce the loop length and area due to tunneling, and the effect to a certain degree. Nevertheless, no amount of scattering can change the orientation of the persistent current, which is related to the topology of the surrounding band structures, and the emptied states should quickly become repopulated. Note that, while the interplay of the orbital magnetism emerging in insulating Dirac systems [35–37], and the magnetism of topological-state loops remains to be explored, the main obstacle for realizing this effect is most likely related to the size of the bulk band gaps. This can not only restrict the amount of persistent current supported by the loops, but more importantly limit the temperature range of applicability.

In conclusion, we investigated the behavior of electronic states bound to the circular interfaces between insulating phases of distinct topologies. These loops can be a source of magnetic moments due to persistent currents flowing along the interfaces. The chirality of the states bound to these loops manifests as a chirality in the angular momentum and the corresponding magnetic moments. We have shown that a simple 1D model, whose validity extends to noncircular loops, captures both the qualitative and the quantitative behavior of the electrons. Because of the intimate link between the magnetic moments and spin and valley degrees of freedom, novel magnetic structures and devices can be envisioned.

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In this supplemental material we show that the 1D model derived in the main paper is valid for arbitrarily shaped loops. Towards this end, we display the numerical TB spectrums, and the levels predicted by

\[ E = |j| \frac{\hbar v_F}{L} + \text{sgn}(j) \frac{e v_F}{L} S B, \]  

(1)

for an elliptic, and hexagonal zigzag and armchair loops in Fig. 1, Fig. 2 and Fig. 3, respectively. Note that \( j \) does not denote the total angular momentum now, due to the lack of rotational symmetry. However, it is still required to be a half-integer, while its sign reflects the orientation of the chiral current. For the elliptic loop we have used \( R_1 = 5 \text{ nm}, \ R_2 = 15 \text{ nm}, \ \mathcal{S} = R_1 R_2 \pi, \) and for the loop length we have used the approximation of the form

\[ L = \pi (R_1 + R_2) \left( 1 + \frac{3h}{10 + \sqrt{4 - 3h}} \right), \]  

(2)

where \( h = (R_1 - R_2)^2 / (R_1 + R_2)^2. \)

The hexagonal loops are distinguished by the number of zigzag (\( N_{ZG} \)) or armchair (\( N_{AC} \)) segments along one edge. The loop length (\( L = 6l \)) and area (\( S = 6l^2 \sqrt{3}/4 \)), depend on the length of one side of the hexagon \( l_{ZG} = N_{ZG} \sqrt{3}a \) (\( l_{AC} = (3N_{AC} - 2)a \)), where \( a \) is the nearest neighbor distance. The results depicted here are for \( N_{ZG} = 42 \) and \( N_{AC} = 25. \) For the nearest neighbor hopping in the TB model we have adopted the value found in graphene (\( t = 2.7 \text{ eV} \)), while the connection with the continuum model is made by employing the Fermi velocity value corresponding to this parameter \( v_F = \frac{3a}{2\pi}. \)

All the loops are surrounded by a region large enough to ensure the decay of the topological modes.

On the one hand, for setup (c) from the main paper (where counterpropagating states belong to opposite spins), it can be seen that regardless of the shape, the persistent current is robust, and that Eq. (1) predicts the energy levels with great accuracy. On the other hand, the spectrum of setup (a) shows some deviation depending on the particular case, although Eq. (1) still provides a very good fit for the results in general. While elliptic loops display stronger intervalley scattering and subsequent hybridization than the circular loops, intervalley scattering in zigzag hexagonal loops is practically nonexistent. In armchair hexagonal loops a gap is opened for
low-energy chiral states. Remarkably, away from this energy region a behavior indicating chirality preservation is observed.

FIG. 3. Same as in Fig. but for a armchair hexagonal loop.