Magnetotransport signatures of 3D topological insulator nanowire structures

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Abstract

We study the magnetotransport properties of patterned nanowire structures such as kinks or Y-junctions by performing ballistic transport simulations for topological insulator materials. Similar to straight wires, a gapless helical subband can be obtained in the nanowire structures when they are pierced by a half-integer magnetic quantum flux but, unlike for straight wires, the direction and perpendicular component of the magnetic field play an important role for the conductance spectrum. Resonances with perfect transmission through the structure can be found near the Dirac point only when the input and output leads have gapless subbands with aligned spin polarization, for which we present a general criterion. These transport signatures depend crucially on spin-momentum locking and could be relevant for quantum transport experiments on topological insulator nanowires.
Introduction

A decade ago, three-dimensional topological insulators (3D TIs) entered the scene of condensed matter physics and since then they have remained in the center of attention. Rightfully so, as they offer an interesting theoretical and experimental playground for fundamental research as well as applications, combining relativistic and quantum physics in a single condensed matter system, based on aspects of topology.\textsuperscript{1,5}

Typical properties of 3D TIs are strong spin-orbit coupling, leading to a band inversion in the bulk spectrum, and the appearance of gapless surface states which are protected by time reversal symmetry. These surface states are well described by a single 2D spin-momentum locked Rashba-Dirac cone, which has been confirmed by angle-resolved photoemission spectroscopy (ARPES) measurements in a wide range of 3D TI materials.

As the 3D TI materials are typically heavily doped, identifying surface state transport in bulk samples has proven to be quite a challenge.\textsuperscript{6,7} By studying 3D TI nanostructures instead,\textsuperscript{8–10} the surface-to-volume ratio is increased which in turn increases the detectability of surface state transport. However, confinement generally induces a gap in the surface state spectrum which increases as the cross section is reduced. Interestingly, a gapless spectrum can be restored through the Aharonov-Bohm (AB) effect by piercing the nanostructure with a half-integer magnetic flux.\textsuperscript{11,12} This leads to unique magnetotransport signatures that one is able to measure systematically in various 3D TI nanowire samples,\textsuperscript{13–29} e.g. shifted Shubnikov-de Haas and quantum flux-periodic AB oscillations and weak antilocalization due to the absence of backscattering. Furthermore, these surface states have been probed directly, using e.g. nano-ARPES or Kelvin probe microscopy techniques.\textsuperscript{28,30,31}

There is a solid understanding of uniaxial 3D TI nanowire (or ribbon) surface states in the presence of a magnetic field and different approaches have been introduced to model this system, e.g. effective and continuous (Dirac-like) surface models,\textsuperscript{32–35} surface and bulk lattice models,\textsuperscript{36,37} and a Luttinger liquid description in the 1D limit.\textsuperscript{38} Here, we extend these efforts to other 3D TI nanowire structures, such as kinks or junctions, which have been
proposed as the basic building blocks of 3D TI nanowire circuits for Majorana-based quantum information processing.\cite{39,40} We will show that the unique magnetotransport signatures of 3D TI nanowire structure reveals valuable information about their surface states, and could thus be interesting for further experimental exploration.

**Model**

For straight cylindrical 3D TI nanowires, one can safely resort to an effective 2D surface Rashba-Dirac model. For 3D TI nanowire structures with arbitrary shapes and cross sections made of a certain TI material, we employ a tight-binding model based on the 3D $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian, introduced by Zhang et al.\cite{32} These two approaches will be discussed in the following subsections.

![Figure 1](image-url)  
*Figure 1: A sketch of a (a) cylindrical (b-c) rectangular 3D TI (a) nanowire (NW) (b) kink (c) $\Upsilon$-junction in the presence of a magnetic field. The bulk region and its surface, which hosts the topological surface states, are indicated in blue and orange, respectively.*

**2D Rashba-Dirac Hamiltonian**

The surface states of a 3D TI can be effectively described by the bound states of a massive 3D Dirac Hamiltonian for which the Dirac mass undergoes a sign flip at the TI surface. For a flat surface of a 3D TI slab for example, this leads to the well-known 2D Rashba-Dirac Hamiltonian, $H^{RD} = v_F(\hat{p}_y\sigma_x - \hat{p}_x\sigma_y)$, featuring a single orthogonally spin-momentum locked Dirac cone. For a general curved surface, the 2D Hamiltonian obtains a curvature term and
can be written as follows:  

\[ \hat{H}_{\text{surf.}} = -\left( v_F / 2 \right) [\hbar \nabla \cdot \mathbf{n} + \mathbf{n} \cdot (\hat{p} \times \hat{\sigma}) + (\hat{p} \times \hat{\sigma}) \cdot \mathbf{n}] , \]  

(1)

with \( \hat{p} \) the momentum operator on the surface and \( \mathbf{n} \) a unit vector normal to the surface. We can also add a magnetic field to the surface Hamiltonian through minimal coupling, \( \hat{p} \to \hat{p} - eA \), with electron charge \( e \) \( (< 0) \). We will now consider the surface of a cylindrical 3D TI nanowire oriented along the \( x \)-direction \( (\mathbf{n} = \mathbf{e}_r) \) with radius \( R \) (constant curvature \( 1/R \)) and a constant magnetic field parallel to the cylinder described by the vector potential \( A(r, \phi) = B\parallel r \mathbf{e}_\phi / 2 \). We will only consider divergenceless vector potentials throughout the text according to the Coulomb gauge. The eigenstates \( \Psi(x, \phi) \) of this system have the following form, based on the symmetries of the system:

\[ \Psi(x, \phi) \equiv e^{ikx+i\ell\phi} \begin{pmatrix} \Psi_1 \\ e^{i\phi} \Psi_2 \end{pmatrix} \quad (l = 0, \pm 1, \pm 2, \ldots), \]  

(2)

with wave vector \( k \) and quantized angular momentum \( l \). The Hamiltonian and energy dispersion relation become:

\[ \hat{H}_{\text{cyl.}}(j, k) = \hbar v_F \begin{pmatrix} -j/R & -ik \\ ik & -j/R \end{pmatrix} , \quad E_\nu(j, k) = \nu \hbar v_F \sqrt{k^2 + (j/R)^2} \quad (\nu = \pm 1), \]  

(3)

with \( j \equiv l+1/2+\Phi/\Phi_0 \) and \( \Phi = B\parallel \pi R^2 \) the magnetic flux piercing the cylinder, \( \Phi_0 = -\hbar/e > 0 \) being the magnetic flux quantum and \( j \) the generalized angular momentum, containing contributions from the curvature of the surface and the magnetic flux. The spectrum has a pair of gapless helical subbands \( (\nu = \pm 1, \ j = 0) \) when a half-integer magnetic flux, \( \Phi/\Phi_0 = (2m+1)/2 \ (m \in \mathbb{Z}) \), is piercing the wire.

From Eqs. (2-3) and box normalization of the wave function \( (x \in [-L/2, L/2], \ k = \)
2\pi n/L, n \in \mathbb{Z})

we get the following spinor solutions:

\[ (\Psi_1, \Psi_2) = \frac{1}{\sqrt{2\pi RL}} \begin{cases} 
\left( \sin \gamma_{\nu}(j,k), i \cos \gamma_{\nu}(j,k) \right) & (\nu j \geq 0) \\
\left( \cos \gamma_{\nu}(j,k), i \sin \gamma_{\nu}(j,k) \right) & (\nu j \leq 0)
\end{cases} \tag{4}\]

with:

\[ \gamma_{\nu}(j,k) \equiv \arctan \left( \frac{\nu k R}{|j| + \sqrt{k^2 R^2 + j^2}} \right) \tag{5}\]

always chosen to lie in the interval \([-\pi/4, \pi/4]\). This solution is a 2-component spinor \(\Psi\) that lives on the 2D surface of the cylinder. The corresponding 3D 4-component spinor \(\chi\) that extends into the bulk region, with constant Dirac mass \(M\) (and infinite Dirac mass with opposite sign considered outside of the cylinder), is given by:

\[ \chi(x, r, \phi) = \vartheta (R - r) e^{i|\nu v_F|(r-R)/\hbar} \begin{pmatrix} 
\Psi(x, \phi) \\
i\sigma, \Psi(x, \phi)
\end{pmatrix}, \tag{6}\]

allowing us to assign the penetration depth \(\lambda = \hbar/|\nu v_F|\) to the surface state. These 4-component spinors can be compared with the 4-orbital surface state wave functions that are obtained with the \(\mathbf{k} \cdot \mathbf{p}\) model.

A magnetic field perpendicular to the axial direction of the wire will in general break time reversal symmetry as well as the rotational symmetry around the \(x\)-axis. To assess its impact, we apply perturbation theory with perturbation Hamiltonian \(\hat{H}_\perp = -e v_F B_\perp R \sin \phi \hat{\sigma}_\phi\), arising from a vector potential \(\mathbf{A} = B_\perp r \sin \phi \mathbf{e}_y\) that corresponds to a magnetic field along the \(y\)-direction, \(B_\perp \mathbf{e}_y = B_\perp (\cos \phi \mathbf{e}_r - \sin \phi \mathbf{e}_\phi)\). The wave vector along the axial (transport) direction remains a valid quantum number, while states with different values for \(\nu\) and \(j\) get mixed. The gapless \(j = 0\) subband remains gapless up to second order in the perpendicular magnetic field \(B_\perp\), such that the topological protection is, at least up to a certain extent, maintained in the presence of a perpendicular magnetic field. The first-order correction cancels out completely for the \(j = 0\) subband while the second-order correction yields a
renormalization of the Fermi velocity,

\[ v_F \rightarrow v_F \left[ 1 - (eB_R^2)/(\pi \hbar^2) \right] = v_F \left[ 1 - (2B_R^2/\Phi_0)^2 \right], \quad (7) \]

which is symmetric around \( E = 0 \) and always reduces the magnitude. Unlike for the surface of a 3D TI slab, the energy spectrum remains gapless and the conductance near the Dirac point is unaffected. When the perpendicular magnetic field approaches the critical value of \( B_{\text{crit}} \equiv \Phi_0/(2R^2), \) the Fermi velocity is renormalized to zero and the perturbative result breaks down. The flat gapless subband spectrum that is obtained in this limit is in agreement with the formation of Landau levels when a strong perpendicular magnetic field is applied. Note that this calculation depends on the rotational symmetry of the nanowire and electron-hole symmetry. To what extent this result holds for general nanowire structures will be verified numerically.

### 3D \( k \cdot p \) Hamiltonian

For a more realistic (low energy) description of the surface states of various 3D TI materials, Zhang et al. introduced the following 3D effective \( k \cdot p \) Hamiltonian:

\[ H^{kp}(k) \equiv \epsilon(k) + \tau_z M(k) + \sigma_z \tau_x A_z k_z + \sigma_x \tau_x (k_x + i k_y) A_\perp, \]

\[ \epsilon(k) \equiv C_0 - C_\perp (k_x^2 + k_y^2) - C_z k_z^2, \quad M(k) \equiv M_0 - M_\perp (k_x^2 + k_y^2) - M_z k_z^2, \quad (8) \]

with \( z \) the direction of uniaxial anisotropy and \( k \equiv (k_x, k_y, k_z) \). The four orbitals refer to the electron and hole bands with spin up and spin down (|\( E, \uparrow \rangle \), |\( H, \uparrow \rangle \), |\( E, \downarrow \rangle \) and |\( H, \downarrow \rangle \) respectively), with \( \sigma \) (\( \tau \)) acting on the spin(electron-hole)-subspace. This Hamiltonian describes an insulator when \( C^2_{\perp,z} < M^2_{\perp,z} \) and a topologically nontrivial regime can be unambiguously assigned, namely when the band inversion parameters \( M_\perp, M_z \) and the mass (bulk gap) parameter \( M_0 \) have equal signs: \( M_0 M_{\perp,z} > 0 \). The band inversion of the E and H bands is governed by \( M_{\perp,z} \), while electron-hole asymmetry is captured by \( C_{\perp,z} \). The parameters
A_{⊥,z}$ determine the group velocity of the gapless surface states and finite values for $M_{⊥}$, $M_z$ prevent the fermion doubling theorem from applying.\cite{3} Hence, this Hamiltonian can be safely put on a lattice without acquiring unphysical Dirac points at $k_{x,y,z} = ±\pi/a$ for a cubic lattice with lattice constant $a$ for example. The corresponding terms in the Hamiltonian are also known as Wilson mass terms.\cite{3,44} Specific values for the parameters representing various 3D TI materials can be found in Table 1.

When considering a 3D TI slab with surface orthogonal to the $z$-direction with this Hamiltonian, an isotropic gapless surface state spectrum is obtained, described by the following 2D effective Hamiltonian:\cite{4}

$$\hat{H}^{k \cdot p}_{\text{surf.}} = -C_z M_0/M_z - M_{⊥}(\hat{p}_x^2 + \hat{p}_y^2) + \text{sgn}(M_z)\sqrt{1 - (D_z/M_z)^2} A_{⊥}(\hat{p}_x \sigma_y - \hat{p}_y \sigma_x).$$

(9)

The wave function profile perpendicular to the $x$-$y$ surface of the $k_x = k_y = 0$ surface state has the following form when the 3D TI is confined to the $z > 0$ region:\cite{3,44}

$$\chi(z) = \begin{pmatrix} c_1 & -c_1 & c_2 & c_2 \end{pmatrix}^T \left[ \exp(-q_z^+ z) - \exp(-q_z^- z) \right],$$

$$q_z^\pm \equiv \frac{1}{2} \sqrt{\frac{A_z^2}{M_z^2 - C_z^2}} \pm \sqrt{\frac{1}{4} \frac{A_z^2}{M_z^2 - C_z^2} - \frac{M_0}{M_z}},$$

(10)

with two independent parameters $c_1$ and $c_2$ (up to normalization). The wave function extends into the bulk with a characteristic penetration depth (or one could say surface state thickness) $\lambda_z$ that can be defined as $\lambda_z \equiv \max\{1/\Re(q_z^+), 1/\Re(q_z^-)\}$. This solution is for confinement along $z$ and analogous solution can be obtained for confinement along $x$ and $y$. The different depth values are presented for the different parameter sets and confinement directions in Table 1. As the band gap of a typical topologically trivial insulator is very large compared to that of the known 3D TIs, hard wall confinement at the 3D TI surfaces, which is understood throughout this text, is an appropriate approximation.

To model 3D TI nanowires with an arbitrary cross section, we consider a tight-binding
Table 1: The parameters of the $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian for Bi$_2$Se$_3$, Bi$_2$Te$_3$ and Sb$_2$Te$_3$ are listed$^{33,34}$ as well as a set of parameters for an isotropic and electron-hole symmetric toy model.

| Toy model | Bi$_2$Se$_3$ (A) | Bi$_2$Se$_3$ (B) | Bi$_2$Te$_3$ | Sb$_2$Te$_3$ |
|-----------|------------------|------------------|-------------|-------------|
| $M_0$ (eV) | 0.3              | 0.28             | 0.28        | 0.30        | 0.22        |
| $M_\perp$ (eV·Å$^2$) | 15              | 56.6             | 44.5        | 57.38       | 48.51       |
| $M_z$ (eV·Å$^2$) | 15              | 10.0             | 6.68        | 2.79        | 19.64       |
| $A_\perp$ (eV·Å) | 3               | 4.1              | 3.33        | 2.87        | 3.40        |
| $A_z$ (eV·Å) | 3               | 2.2              | 2.26        | 0.30        | 0.84        |
| $C_\perp$ (eV·Å$^2$) | 0               | -19.6            | -30.4       | -49.68      | 10.78       |
| $C_z$ (eV·Å$^2$) | 0               | -1.3             | -5.74       | -6.55       | 12.39       |
| $\lambda_\parallel$ (Å) | 10              | 9.01             | 14.09       | /           | 36.28       |
| $\lambda_\perp$ (Å) | 10              | 25.90            | 19.52       | 20.01       | 27.82       |

formulation of the $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian on a cubic lattice with artificial lattice constant $a$ with a uniform magnetic field inserted through a standard Peierls substitution. All (band structure and transport) simulations for this tight-binding model have been carried out with a parallelized implementation of Kwant$^{46}$.

The spectrum of a nanowire with and without magnetic field along the wire axis is presented in Fig. 2. On the one hand, the gap in (a) agrees well with the value of $\hbar v_F/R$ obtained from the 2D Rashba-Dirac model when considering $R = \sqrt{A/\pi}$ with $A$ the cross sectional area of the nanowire. This can be expected when the surface states cannot tunnel through the bulk region$^{35,38}$, something which is exponentially suppressed as long as the surface state thickness is significantly smaller than the minimal distance required to cross the bulk region$^{47}$. On the other hand, a minimal total flux of $\Phi/\Phi_0 \approx 0.6$ appears to be required in (b) to close the gap, seemingly incompatible with the condition that can be obtained from the Rashbda-Dirac spectrum in Eq. (3). The cause of this offset is found to be the finite thickness of the surface states and will be discussed below.

An example of a surface state wave function resulting from the tight-binding $\mathbf{k} \cdot \mathbf{p}$ model for a 3D TI nanowire with square cross section can be found in Fig. 3 next to the Rashbda-Dirac-based counterpart for a cylindrical nanowire. The local density and phase dependence of the different orbitals are gauge-dependent, but the surface state solutions for orbitals $E_{\uparrow}$...
cross section is too small to neglect the surface state thickness, a rescaling of the flux needs to be considered for a precise tuning of the amplitude and orientation of the magnetic field. A rescaling ratio $\alpha$ can be estimated by $\alpha \approx 1 - \langle \lambda \rangle C / (2A)$, with $\langle \lambda \rangle$ the average surface state thickness along the circumference $C$. Note that there is an exact agreement between the Rashba-Dirac and $k \cdot p$ model surface state thickness, but this is generally not the case as their thicknesses are governed by the unrelated parameters in Eqs. (6) and (10) respectively. From Table 1 it is clear that the rescaling ratio $\alpha$ can vary significantly between different 3D TI materials and nanowire orientations. In principle, one should be able to verify this
with precise magnetotransport measurements.

![Image](image-url)

Figure 3: A cross section of the wave function of a gapless subband state (see Fig. 2 (b)) of a (a-b) cylindrical (c-d) rectangular 3D TI nanowire is presented. (a,c) The phase of the different orbitals (spinor components) is shown in color, with the brightness proportional to the local orbital density. (b,d) The local density of the total wave function is indicated. The surface of the nanowire is marked with a (a,c) black (b,d) gray dashed line. (a-b) The Rashba-Dirac surface state spinor with $M = 0.3$ eV/$v_F^2$ and $v_F = 3$ eV·Å and the (c-d) $k \cdot p$ Hamiltonian with toy model parameter set of Table 1 and $a = 1$ Å are considered, both for a nanowire with cross section equal to 100 nm$^2$.

**Magnetotransport**

We will focus on the magnetotransport properties of three different nanowire structures: a straight nanowire, a kink with angle $\gamma_K$ and a Y-junction (see Fig. 1). The simulations are limited to nanowires with a uniform square cross section of 10 × 10 nm$^2$ without disorder, considering the toy model and the Bi$_2$Se$_3$ (A) parameter set of Table 1. The main trade-off when considering a larger (smaller) cross sectional area will be a smaller (larger) required magnitude of the magnetic field ($\propto \mathcal{A}$) versus a smaller (larger) doping level energy window.
\( \propto \sqrt{A} \) in which the magnetotransport signatures of the gapless subband will appear. The dependency on cross section size and shape (e.g. the aspect ratio of a rectangular cross section) and disorder has already been investigated and reported in detail elsewhere and will not be discussed further. For the Bi\(_2\)Se\(_3\) transport simulations, the direction of uniaxial anisotropy is considered to be perpendicular to the plane \((x-z)\) spanned by the legs of the kink or the Y-junction, in line with the experimental feasibility of these structures. The external magnetic field on the other hand is always considered with in-plane orientation, minimizing its perpendicular component.

**Straight nanowire**

The conductance of a straight 3D TI nanowire with toy model and Bi\(_2\)Se\(_3\) parameter sets is presented in Fig. 4. The Dirac point is centered at 0 meV for the electron-hole symmetric toy model and near 71 meV for Bi\(_2\)Se\(_3\). The value of the latter is well estimated by 

\[-M_0(C_\perp/M_\perp + C_z/M_z)/2 \approx 67 \text{ meV},\]

the average of the Dirac point energy for TI slab surface states parallel to the \(x-z\) and \(y-z\) planes, respectively. The typical diamond tile pattern for the magnetoconductance is clearly visible in both cases and the electron-hole asymmetry of Bi\(_2\)Se\(_3\) is barely visible. The flux rescaling ratio \(\alpha\) which can be extracted from the conductance profile is significantly smaller for the Bi\(_2\)Se\(_3\) parameter set, as expected from the estimate \(\alpha \approx 1 - \langle \lambda \rangle C/(2A)\) because \(\langle \lambda \rangle\) is larger for Bi\(_2\)Se\(_3\). The agreement between this estimate for \(\alpha\) and its fitted value from the conductance profile is not perfect, however, because the lattice constant in our simulations, \(a = 10\ \text{Å}\), is too large for an accurate retrieval of the surface state depth profile.

**Kink**

Compared to straight wires, a much richer magnetotransport behavior can be expected for kinks. The lack of translational invariance and time reversal symmetry allows for backscattering processes, even in ideal nanowire kinks without disorder. It is already known for 3D
Figure 4: The conductance of a $10 \times 10$ nm$^2$ 3D TI nanowire is shown as a function of the energy (near the Dirac point) and magnetic flux $\Phi$ from a fully aligned uniform magnetic field. The results were obtained with a tight-binding version of the $k \cdot p$ Hamiltonian presented in Eq. (8) with the (a) toy model (b) Bi$_2$Se$_3$ (A) parameter set of Table 1 and $a = 10$ Å. The Dirac point energy equal to (a) 0 meV (b) 71 meV and the effective half-integer magnetic fluxes with rescaling ratio (a) $\alpha = 1$ (b) $\alpha = 0.77$ are indicated with pink dashed lines and white dotted lines, respectively.

TI slabs which are tilted with respect to each other that angle-dependent reflections will occur at their interface, but here we focus on the nanowire regime with well separated sub-bands where confinement plays an important role. As is the case for straight TI nanowires, the confinement gap can be closed in both legs of the kink simultaneously by applying an external magnetic field with the appropriate magnitude under the correct angle $\gamma_B$. This can be translated to the following condition:

$$\cos \gamma_B/(2n_I + 1) = \cos(\gamma_K - \gamma_B)/(2n_O + 1),$$

(11)

with $n_{I,O}$ integers such that $\Phi_{I,O} = (2n_{I,O} + 1)\Phi_0/2$, where $\Phi_I = |B\cos \gamma_B|A$ and $\Phi_O = |B\cos(\gamma_K - \gamma_B)|A$ are the piercing magnetic fluxes of the input and output leg, respectively (see Fig. 1). Evidently, unlike for straight TI nanowires, the appearance of a perpendicular component of the magnetic field cannot be prevented throughout the whole structure, but the gapless Dirac spectrum is expected to survive as long as the amplitude of the perpendicular component stays below $B_{\text{crit}} \equiv \pi \Phi_0/(2A)$, in analogy to the perturbative result based on
Figure 5: The conductance of a 3D TI nanowire kink, with $\gamma_K = \pi/2$ and both legs effectively pierced by a half-integer quantum magnetic flux, is shown as a function of the angle $\gamma_B$ of the applied magnetic field ($|\mathbf{B}| = \sqrt{2}\Phi_0/(\alpha A)$) and the (equal) energy level of the leads. The nanowire parameters for (a) and (b) are the same as in Fig. 4 and the same Dirac point energy is indicated with a pink dashed line.

We proceed by considering a kink with fixed angle $\gamma_K$ while letting the magnetic field rotate, the setup which is most easily set up experimentally. When $\gamma_K = \pi/2$ and the magnitude of the magnetic field is tuned to $\sqrt{2}\Phi_0/(\alpha A)$, the perpendicular component is within limits (when $\alpha$ is reasonably large) and a gapless subband channel should appear in both legs of the kink when $\gamma_B = \pi/4 + m\pi/2$ with $m \in \mathbb{Z}$. Hence, for these angles one could expect transmission across the kink at energies arbitrarily close to the Dirac point. Results of conductance simulations for this system are presented in Fig. 5 and the expected transmission behavior can indeed be identified. However, the signal generally appears to be very weak for $m$ even as compared to $m$ odd. This implies a dependence on the relative direction of the projection of the magnetic field on both legs and its resulting spin polarization. We can define two types of projections of the magnetic field for the $\gamma_K = \pi/2$ kink: a symmetric projection when $\pi/2 < \gamma_B < \pi$ or $3\pi/2 < \gamma_B < 2\pi$ and an anti-symmetric projection when $0 < \gamma_B < \pi/2$ or $\pi < \gamma_B < 3\pi/2$. A symmetric ($m$ odd) projection instigates a spin polarization in both legs with maximal overlap for the states moving in the same direction, and the opposite holds for an anti-symmetric projection. This behavior transfers from the
toy model kink to Bi$_2$Se$_3$ as well as to the Y-junction and is and depends crucially on the spin-momentum locking characteristics of the topological surface states. Spin-momentum locking implies that a 90 degree rotation of the momentum should be accompanied by a 90 degree spin rotation in the same direction. For spin degenerate surface states, this constraint would not be present and a $\pi/2$-periodic conductance profile would be obtained as a function of $\gamma_B$.

For the Bi$_2$Se$_3$ kink, the electron-hole asymmetry becomes noticeable in the conductance near the Dirac point, unlike for a straight nanowire. The gap closes asymmetrically and the closing point is shifted about 15 meV in energy as compared to the Dirac point of the straight wire with an aligned magnetic field. A gap persists at the gap closing angles, implying that the symmetric Dirac velocity renormalization, as derived perturbatively above for perpendicular magnetic fields, is not entirely valid for an electron-hole asymmetric and/or anisotropic 3D TI $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian. However, this gap is very small compared to the confinement and reflection gap and does not conceal the unique $\pi/2$-periodic surface state conductance signature.

**Y-junction**

In this section, a 3D TI Y-junction configuration (see Fig. 1 (c)) is considered, with three nanowire legs having identical cross sections. Lead by the interpretation of the conductance results for kinks in the previous section, we can expect that a properly tuned and oriented external magnetic field can close the confinement gap in any selection of the three legs. A T-junction for example would not offer the same flexibility, as two of the three legs always align identically with the applied magnetic field.

The results for conductance simulations of a Y-junction, with an external magnetic field having an amplitude of $2\Phi_0/(\alpha A)$, are shown in Fig. 6. This amplitude closes the confinement gap of the two output legs simultaneously when $\gamma_B = m\pi$ ($m \in \mathbb{Z}$), and the input (I) and left (OL) or right (OR) output legs simultaneously when $\gamma_B = \pi/3 + m\pi$ or $\gamma_B = 2\pi/3 + m\pi$, respectively.
Figure 6: (a,c) The conductance between the different legs of a 3D TI nanowire Y-junction is shown as a function of the angle $\gamma_B$ of the magnetic field ($|B| = 2\Phi_0 / (\alpha A)$) and the energy level of the input leg, (b,d) as well as a measure for the relative conductance of the left and right output legs. The (a-b) toy model (c-d) Bi$_2$Se$_3$ (A) parameter set was considered, with the remaining parameters identical to those considered in Fig. 4. The Dirac point energy of the corresponding straight TI nanowire is indicated with a pink dashed line. The angle of $\pi/3$ between the $z$ axis and the two output channels was approximated by $\arctan(3/5)$ in the tight-binding simulations for sufficient lattice commensurability.

respectively. Furthermore, the amplitude is within limits for the perpendicular component, such that the phenomenology of the gapless helical subband should survive. From the simulation results, the different expected conductance regimes can be clearly identified near the Dirac point for both the toy model and the Bi$_2$Se$_3$ Y-junction: a fully gapped regime ($\gamma_B \approx m\pi$), a reflection dominated regime ($\gamma_B \approx \pi/2 + m\pi$), a left-transmitting regime ($\gamma_B \approx \pi/3 + m\pi$) and a right-transmitting regime ($\gamma_B \approx 2\pi/3 + m\pi$). As for the results of the 90 degree kink, the main difference between the toy model and the Bi$_2$Se$_3$ simulations is the particle-hole asymmetry in the conductance signature and an upward shift in energy of about 15 meV for the gap closing with respect to the straight nanowire Dirac point energy.

Note that one can also consider an amplitude of $2\Phi_0 / (\sqrt{3}\alpha A)$ to obtain similar gap closing
conditions. This would lead to gap closings in two of the three legs when zero magnetic flux pierces the remaining third leg. This results in an anti-symmetric projection of the magnetic field with respect to the gapless legs however. Based on the results presented above, one can expect a much weaker conductance signature for this setup as compared to the setup being considered here, which has a symmetric projection. Unlike for the 90 degree kink, gapless transmission with symmetric and anti-symmetric projections cannot be realized in a single Y-junction setup where only the angle $\gamma_B$ of the magnetic field is varied.

Conclusions and outlook

Based on an analysis of the 2D surface Rashba-Dirac model and a tight-binding simulations of a 3D $\mathbf{k} \cdot \mathbf{p}$ model, we have studied the magnetotransport properties of patterned 3D TI nanowire structures, in particular a 90 degree kink and a Y-junction. A perturbative treatment for the 2D Rashba-Dirac model shows that the magnetic flux-driven gap closings and their resulting conductance signatures survive as long as the perpendicular component of the magnetic field, which is unavoidable for this type of structures, stays below a critical value. This result is confirmed with a 3D $\mathbf{k} \cdot \mathbf{p}$ model, which also accounts for the impact of the surface state thickness, the cross sectional shape of the nanowire and anisotropy and/or electron-hole asymmetry of the band structure. Compared to effective surface models, the surface state thickness induces a rescaling of the effective piercing magnetic flux, which in turn governs the magnetic field that is required to induce gapless helical subbands and gapless transmission across a structure.

For a Y-junction, we demonstrated that, in addition to reflection, gapless transmission can be obtained and steered to either of the two output legs, applying an external magnetic field with appropriately tuned magnitude and orientation. Apart from piercing the input and output channels with a half-integer quantum magnetic flux, a compatible spin polarization of both channels is required to obtain maximal overlap and transmission. This can only be
realized by a magnetic field with a symmetric (rather than an anti-symmetric) projection with respect to both channels. This additional constraint depends crucially on surface state spin-momentum locking, and can be exploited to realize a unique $\pi$-periodic conductance profile as a function of the magnetic field angle for a 90 degree kink.

The magnetotransport properties of these types of kinks and junctions provide a new way to explore 3D topological insulator surface states experimentally with quantum transport measurements and could lead to new possibilities for applications. A notable example is the Y-junction, which has also been proposed by Cook et al. as a trijunction device for non-Abelian Majorana state braiding when combined with proximity-induced $s$-wave superconductivity.\textsuperscript{[89]} It would be interesting to investigate whether these magnetotransport signatures could be exploited for electrical detection of a Majorana bound state at the end of a Y-junction leg. An analysis of the impact of diffusive transport behavior of the surface states over longer length scales remains for future work.

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