Transport through quantum spin Hall insulator/metal junctions in graphene ribbons

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Quantum spin Hall insulator/metal interfaces are naturally formed in graphene ribbons with intrinsic spin-orbit coupling by selectively doping two regions creating a potential step. For a clean graphene ribbon, the transmission of the topological edge states through a n-n or p-p junction is perfect irrespective of the ribbon termination, width, and potential step parameters due to the orthogonality of incoming and outgoing edge channels. This is shown numerically for an arbitrary crystallographic orientation of the ribbon and proven analytically for zigzag and metallic armchair boundary conditions. In disordered ribbons, the orthogonality between left- and right-movers is in general destroyed and backscattering sets in. However, perfect transmission is restored by increasing the ribbon’s width, even in the presence of strong edge roughness.

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I. INTRODUCTION

Since the discovery of the quantum Hall effect, edge states have played an important role in condensed matter physics. With the prediction of the topological insulator phase and its observation in HgTe/CdTe quantum wells, the study of edge state physics has received renewed attention, both from the theoretical and experimental side. This new state of matter is identified by an energy gap in the bulk with gapless states propagating around the edges of the sample. In contrast to the normal quantum Hall effect, these edge states preserve time-reversal symmetry and must be spin-polarized as a consequence: at the system’s boundary a pair of counterpropagating spin-up and spin-down states exists as sketched in Fig. 1. As equal-spin states with opposite velocity are thus spatially separated at opposite edges of the sample, and since different-spin states at the same boundary form a Kramers’ double, edge states are protected against backscattering from time-reversal invariant impurities. This so-called quantum spin Hall (QSH) state has been first studied theoretically in graphene, where it results from the intrinsic spin-orbit coupling induced by the carbon atoms.

Graphene inherits interesting properties from its linear dispersion for low-energy quasi-particle excitations, making it a candidate for future spintronics applications. Part of its functionality comes from the ability to tune the carrier density and carrier type (electron or hole) with electric gates, which allows for the straightforward creation of n-p junctions in graphene. Such junctions allow the investigation of the dynamics of the effective massless Dirac-fermions in graphene, showing interesting properties such as Klein tunneling or beam collimation and lensing. Graphene’s functionality can be extended by forming junctions with different materials, such as ferromagnet or superconductor.

With the advent of topological insulators, the investigation of n-p junctions in the QSH phase (in graphene and in quantum wells) as well as interfaces between this phase and other materials has just been initiated.

In this paper we study the transmission properties of the QSH edge states in graphene ribbons through an electrostatic potential step, defined for example by se-
lectively doping left and right regions of the ribbon by means of two back gates. When the potential step height $U_0$ is such that the Fermi energy in both regions lies inside the spin-orbit induced band gap $\Delta_{SO}$, perfect transmission is trivially expected since transport in both regions occurs in the form of topological edge channels. Spin-preserving backscattering processes then amount to crossing the sample width and are forbidden as long as the ribbon’s width is larger than the width of the edge states\(^\text{[31]}\). However, when $U_0$ is bigger than $\Delta_{SO}$, a QSH insulator/metal junction is formed and topological edge channels in one region evolve into multiple bulk channels above the bandgap in the other (see Fig. 1). Backscattering of the QSH edge states could then in principle occur through the metallic region where a path opens up allowing the carriers to cross the sample’s width from one boundary to the other. This reflection process would lead to a spin-current parallel to the interface (a similar spin-current has been predicted at an interface between semi-infinite graphene planes in the presence of Rashba spin-orbit coupling\(^\text{[20]}\)). However, we show in this paper that the topological edge states in a clean ribbon of an arbitrary crystallographic orientation cannot be reflected at a QSH insulator/metal junction (either n-n or p-p) due to the orthogonality of left- and right-moving edge states at opposite boundaries. A similar mechanism was recently shown to be responsible for the perfect transmission of the zero Landau level edge state at a magnetic flux step in folded graphene nanoribbon\(^\text{[32]}\). Perfect transmission is also present in n-p junctions, but only when the ribbon is in the armchair or antizigzag configuration, because only then does the n-p junction not introduce intervalley scattering\(^\text{[33]}\). The orthogonality between edge states is proven by deriving analytic expressions for the QSH edge wavefunctions in zigzag and armchair terminated ribbons. For general ribbon terminations, the absence of backscattering is furthermore validated by numerical calculations. Interestingly, we also find that the topological edge state width depends on the ribbon’s termination. For an armchair ribbon, this width only depends on the magnitude of the spin-orbit induced gap, whereas it is practically independent of this parameter for zigzag ribbons where the edge state width becomes energy-dependent instead. This observation is further confirmed by numerical simulations of the charge density across the sample. These results for clean junctions are analyzed in Section II and in the Appendix.

The influence of disorder, produced for example by edge roughness, is analyzed in Section III. In general, the orthogonality between equal-spin left- and right-movers is then destroyed due to intervalley scattering and the conductance of the junction decreases as inter-boundary backscattering becomes possible through the metallic region. Backscattering is also present for intrinsic sources of intervalley scattering, like a (clean) n-p junction in a zigzag ribbon\(^\text{[33]}\). However, we find that in any case perfect transmission is restored upon increasing the ribbon’s width $W$, essentially because the probability of forward scattering increases with the ribbon’s width while the only available backscattering channel remains one. The conductance recovery with increasing $W$ depends on the ribbon termination due to the different edge state character for different ribbon boundaries. A summary of all our results and some concluding remarks are given in Section IV.

II. EDGE STATES IN A BALLISTIC JUNCTION

A. System description

We consider the system depicted schematically in Fig. 1. It consists of a graphene ribbon subject to the intrinsic spin-orbit coupling which opens a gap in the bulk graphene spectrum. The Fermi energy in the left part of the ribbon is considered to lay inside this gap, so that transport in this region can only take place through the topological edge channels (see Fig. 1). In the right part of the ribbon, the potential is shifted upwards or downwards by an electrostatic gate in order to reach doping levels above the spin-orbit induced bulk gap. Topological edge states then do not play a role anymore in this region and transport is mediated by normal propagating bulk modes. In this way we create a QSH insulator/metal junction in graphene (although the spin-orbit interaction is present throughout all the ribbon). The Hamiltonian of our system is given by

$$H = H_0 + H_{SO} + H_U.$$  \hfill (1)

The first term represents the standard hopping between nearest-neighbor carbon atoms,

$$H_0 = -t \sum_{\langle ij \rangle, s_z} c_{i,s_z}^\dagger c_{j,s_z},$$  \hfill (2)

where $c_{i,s_z}^\dagger$ is the creation operator for an electron with spin $s_z$ on site $i$. The second term in the Hamiltonian accounts for the intrinsic spin-orbit coupling introduced by Kane and Mele\(^\text{[21]}\):

$$H_{SO} = i \hbar SO \sum_{\langle \langle ij \rangle \rangle, s_z} \nu_{ij} s_z c_{i,s_z}^\dagger c_{j,s_z},$$  \hfill (3)

where the summation runs over next-nearest neighbors (note that in Eq. 2 hopping occurs between different sublattices $A$ and $B$, while in 3 hopping is within the same sublattice). The prefactor $\nu_{ij} = +1(-1)$ if the electron takes a left (right) turn to reach its next-nearest neighbor. Since this term commutes with the electron’s spin $s_z$, the Hamiltonian of the system decouples into two independent Hamiltonians for spin-up and spin-down that can be considered independently. In this case, we have edge states for each boundary with spin-up moving in one direction and spin-down moving in the opposite one (see Fig. 1). In the presence of spin-mixing terms


that do not break time-reversal symmetry (like for example the Rashba term), conserved currents do not have a well-defined spin projection. Nevertheless, it will still be possible to define two sets of counter-propagating currents at each boundary that are topologically protected against non-magnetic impurities. For simplicity, below we consider the case where $s_x$ is a good quantum number, but the physics we describe should be analogous if time-reversal symmetric spin-mixing terms were present.

The last term $H_U$ in the Hamiltonian describes the on-site graphene doping, given by

$$H_U = \sum_{i,s_x} U(x)c_{i,s_x}^\dagger c_{i,s_x}. \quad (4)$$

The sketch in Fig. 1 shows a n-n junction. In this case the doping profile along the boundary direction can be modeled by a smooth potential step of height $U_0$ of the form

$$U(x) = -\frac{U_0}{2} \left[ 1 + \text{erf} \left( \frac{2(x-L/2)}{\delta} \right) \right], \quad (5)$$

where $L$ is the length of the ribbon and $\delta$ controls the smoothness of the step. This gives $U(x) = 0$ when $x - L/2 < \delta$ (left part of the sample), while $U(x) = -U_0$ for $x - L/2 > \delta$ (right part of the sample). In order to have a QSH insulator/metal junction, we need $U_0 > \Delta_{SO}$ and consider the energy range $[0, \Delta_{SO}]$ depicted in grey in Fig. 1b). Here $\Delta_{SO}$ is the spin-orbit induced bulk gap (for an infinitely wide ribbon it is $\Delta_{SO} = 3\sqrt{3}\delta_{SO}$, and slightly larger for finite width ones). An equivalent p-p junction is obtained by changing $U_0$ by $-U_0$ in Eq. (5), and considering energies between $-\Delta_{SO}$ and 0. Furthermore, we could consider n-p (or p-n) junction if we choose $U_0 > 2\Delta_{SO}$. In the following we will focus on the n-n junction shown in Fig. 1 for simplicity.

### B. Perfect transmission

At a QSH insulator/metal junction in a graphene ribbon, an incoming edge state may in principle either be transmitted or reflected at the junction. Spin-preserving reflection is only possible when the electron is transferred from the incoming edge state into the counterpropagating edge state at the opposite boundary. Such an interboundary reflection is in principle possible because the electron’s wavefunction to the right of the junction is not constrained to the edges, but spans the whole bulk in multiple propagating metallic channels. However, one of the main points of our paper is that, at a valley-preserving junction, this reflection process is forbidden due to the orthogonality of forward and backward topological edge channels, much like in the Klein paradox. In Fig. 2, the conductance of the junction in units of $G_0 = 2e^2/h$ is plotted as a function of the Fermi energy of the incoming electrons (in units of $t$, the nearest-neighbor hopping amplitude). Different ribbon terminations are considered: armchair (parametrized by an angle $\theta = 0$, dashed blue curve), zigzag ($\theta = \pi/6$, solid red line), and an intermediate crystallographic orientation ($\theta = 0.4\pi/6$, thin green curve). The ribbon’s width is $W = 54a$ and the potential step has parameters $U = 0.25t$ and $\delta = 5a$. Perfect transmission is manifested by a flat first conductance plateau at energies where only edge states are present on the QSH insulator side. For higher energies, transport is carried by additional propagating modes above the spin-orbit gap that are not protected by orthogonality and thus the transmission is reduced (compared to the situation without a potential step, dotted curves). Perfect transmission below the gap holds irrespective of the ribbon’s crystallographic orientation and its width $W$ and is independent of $U_0 > 0$ and $\delta$ (as long as $\delta$ is larger than a few carbon-carbon lattice constants). Our numerical results for mesoscopic transport are obtained using the recursive Green’s function technique. A double-sweep generalization gives us access to the local charge density in real space. This allows for a direct visualization of the shape of the edge states and their propagation across the potential step, as depicted in Fig. 3 for different ribbon terminations and energies below the bulk spin-orbit gap. The charge density is shown in arbitrary units, with black representing the absence of charge, and white its maximum value. Since spin-up and spin-down are decoupled in our problem, they can be analyzed independently and their contribution summed up at the end. In Fig. 3 only the spin current incoming from the upper boundary is considered. A similar contribution (mirror symmetric with respect to the ribbon axes) coming in from the lower boundary with the opposite spin is not shown. In all ribbons, the incoming topological edge state in the left region propagates towards the junction and then spreads out into multiple channels.
FIG. 3: (Color online) Numerical results for the charge density across a potential step (U₀ = 0.25t and δ = 5a) for a clean ribbon of W = 54a with t₀ = 0.03t. A section L = 100a of the infinitely long ribbon is shown, and various ribbon terminations and Fermi energies below the spin-orbit gap are considered. At the left of the n-n junction (placed in the middle of each flake), transport is carried by a topological edge channel that evolves into multiple normal channels at the right. A similar contribution with opposite spin comes in from the lower boundary (not shown).

C. Edge states at an armchair boundary

First we consider an armchair ribbon extending along the vertical y-direction, so that the boundaries are at x = 0 and x = W (see Fig. 9 in the Appendix). For simplicity, we consider that the ribbon is wide enough so that the two opposite boundaries can be treated independently. In the armchair case, it is known that the topological edge states have wavefunction solutions around the K and K' points in the first Brillouin zone. Expanding the Hamiltonian for small momentum ķ = (qₓ, qᵧ) around these points and considering small energies below the spin-orbit induced gap, we make the following ansatz for the edge states of a wide ribbon at the left boundary (x = 0):

\[ \Psi_{ac}(x, y) = e^{i\eta_y} e^{-i\kappa x} \left[ \alpha_0 e^{i\vec{K} \cdot \vec{r}} |\psi\rangle + \beta_0 e^{i\vec{K}' \cdot \vec{r}} |\psi\prime\rangle \right]. \]  (6)

This is a superposition of modes around the two inequivalent K and K' points (K' = ±\( \frac{4\pi}{3\sqrt{3}a} \hat{x} \)) with amplitudes \( \alpha_0 \) and \( \beta_0 \). These are propagating in the y-direction and exponentially decaying in the x-direction. \(|\psi\rangle (|\psi\prime\rangle\) is a two-component spinor for the K (K') valley which contains the relative amplitude of the wavefunction on the A and B sublattices. In the Appendix we show that Eq. (6) satisfies the armchair boundary condition when

\[ \kappa = -\frac{\Delta_{SO}}{\hbar v_F} s_z sgn(q_y) sgn(E), \]  (7)

where \( s_z = +1(-1) \) for spin-up (spin-down) and \( sgn(q_y) \), \( sgn(E) \) are the signs of the particle’s wave vector and energy, respectively. The spin-orbit induced gap is \( \Delta_{SO} = 3\sqrt{t_{SO}} \) is the spin-orbit induced gap for a wide ribbon. The dispersion of these states is \( E = \pm \hbar v_F q_y \), where \( v_F = 3at/2 \) is the Fermi velocity. As \( \kappa \) needs to be positive for a bounded solution, positive energy states (electron-like) either propagate with positive wavevector \( sgn(q_y) = +1 \) and spin-down \( s_z = -1 \), or negative wavevector \( sgn(q_y) = -1 \) and spin-up \( s_z = +1 \) along the left boundary. For the right boundary we use the same ansatz (6) but now the ribbon extends to values \( x < W \) and the boundary condition is met at \( x = W \). Now \( \kappa \) needs to be negative and the positive energy edge state has positive (negative) wavevector with spin-up (down). If we rotate our lattice by 90 degrees, we get the electronic edge states propagating along the sample’s boundaries as sketched in Fig. 4.

The width of the edge states is given by the parameter \( \lambda = 1/|\kappa| \), and is thus determined solely by the spin-orbit coupling strength. In our numerical calculations we have chosen \( t_{SO} = 0.03t \) (the same value used by Kane and Mele in Ref. 2, although this value is thought to be overestimated), giving a decay length \( \lambda \approx 10a \). This is in good agreement with the edge state width observed in Fig. 8.

The orthogonality between forward- and backscattered edge states can be understood as follows. In the Appendix, we show that the Hamiltonian of the armchair ribbon with spin-orbit coupling can be transformed into a valley-isotropic form meaning that it has the same shape for both the K and K' valley. The valley degree of freedom (also called isospin) is thus conserved by the Hamiltonian. The potential step conserves the isospin as long as it is smooth on the scale of the lattice constant.
The isospin is described by a spinor $|\tau\rangle = (\alpha, \beta)$, where $\alpha$ and $\beta$ are the coefficients of the plane waves in the $K$ and $K'$ valley [see Eq. (A20)]. In the valley-isotropic basis, they are given by $|\tau\rangle = \frac{1}{2}(i\sigma_2, -1)$ for the left boundary, and $|\tau\rangle = \frac{1}{2}(i\sigma_2 e^{-2iK_W}, 1)$ for the right one.

Writing $W = \sqrt{2}(N + 1)\alpha$ in terms of the number $N$ of carbon atoms along the ribbon’s width, one can see that the isospins of counterpropagating equal-spin edge states (moving at opposite boundaries) are orthogonal when the armchair ribbon is metallic, i.e., for $N = 3n - 1$, with $n = 1, 2, \ldots$. Scattering between these states is thus forbidden which leads to the absence of reflection.

The case of semiconducting armchair ribbons is a bit more involved. Let us show this with an example. Imagine we had a ribbon without potential step but with a smooth intrinsic spin-orbit step instead. The left region is then exactly the same as in Fig. 3, but the right region now is plain graphene (i.e., without spin-orbit coupling). For metallic armchair ribbons (actually for zigzag and intermediate ones too), such a junction constitutes a QSH insulator/metal interface and we observe numerically a perfect transmission for energies below the induced spin-orbit bulk gap. However, the semiconducting armchair ribbon is insulating for small energies in the right region, and the transmission is zero for such energies. Therefore, knowledge of the wavefunction in the left region only is not sufficient in order to make a statement for the transmission in semiconducting armchair ribbons. In our case of a constant spin-orbit coupling and a potential step we can only state that numerically we also observe perfect transmission as long as the ribbon is metallic in the presence of spin-orbit coupling, i.e., $W \gtrsim 2\lambda$, even though the isospins of the incoming and outgoing edge states are not orthogonal.

D. Edge states at a zigzag boundary

Now we consider a wide zigzag ribbon that extends along the horizontal $x$-direction, so that the boundaries are at $y = 0$ and $y = W$ (see Fig. 4 in the Appendix). For zigzag ribbons, the dispersive topological edge states are centered around the $M$ point ($q_x a = \pi/\sqrt{3}$). Therefore, the standard low energy expansion of the Hamiltonian around the $K$ and $K'$ points (that leads to the Dirac equation in the absence of spin-orbit interaction) is not reasonable anymore, since the low-energy solutions in the presence of the intrinsic spin-orbit coupling occur for momenta far away from those points. In Ref. [22] Zarea and Sandler resorted to a tight-binding method to calculate the wavefunctions and dispersion of the topological edge states. In the Appendix, we follow a slightly different approach that allows us to study the edge state width in some more detail. We find that the wavefunction at the lower boundary $y = 0$ can be written as

$$\Psi_{zz} = e^{i\eta x}\left[|\alpha e^{-\kappa_1 y}|\psi^{(1)}\rangle + |\beta e^{-\kappa_2 y}|\psi^{(2)}\rangle\right]. \tag{8}$$

It is interesting to note that one needs a superposition of two plane waves in order to satisfy the boundary conditions, both for the armchair and the zigzag ribbon. In the absence of spin-orbit coupling, the wavefunction has to vanish at both $A$- and $B$-sites at the boundary of an armchair ribbon, but only at one sublattice for the zigzag ribbon [23]. However, as spin-orbit coupling induces next-nearest neighbor hoppings, the wavefunction now has to vanish on both sublattices for the zigzag termination too. For the armchair ribbon, the superposition in Eq. (6) consisted of plane waves around the $K$ and $K'$ points (as in the absence of spin-orbit coupling). In the zigzag case we need a superposition of two plane waves with different decay lengths in the transverse direction. These decay lengths, up to second order in $\epsilon \equiv E/\Delta$ and $\tau \equiv t_{SO}/t$, are given by $\lambda_i = 1/\kappa_i = -\frac{4\pi}{\tau} (\log(\phi_i))^{-1}$, where

$$\phi_1 = -\tau^2 \frac{Q_1^2}{Q_c^2}, \tag{9a}$$

$$\phi_2 = -Q_c + \frac{\epsilon^2}{Q_c^2} \frac{Q_c}{Q_c^2 - 1} + \tau^2 \frac{(Q_1 + Q_c(Q_2 + Q_1 Q_c))^2}{Q_c(Q_c^2 - 1)}. \tag{9b}$$

Here we have defined $Q_c \equiv 2\cos(\sqrt{3}q_x a/2)$, $Q_1 \equiv 2\sin(\sqrt{3}q_x a/2)$, and $Q_2 \equiv 2\sin(\sqrt{3}q_x a)$. The energy dispersion at the lower boundary is given by (see Appendix) $E = -6t_{SO} a \sin(\sqrt{3}q_x a)$. The spin-up and spin-down bands thus cross at the wave vector $q_x a = \pi/\sqrt{3}$ with zero energy. The spin-up (down) electrons therefore propagate to the right along the lower (upper) boundary.

At low energies and for small values of the spin-orbit coupling, the contribution $\phi_2$ in Eqs. (9) is clearly dominating. Furthermore, the spin-orbit coupling $\tau$ only contributes a second order correction to $\phi_2$. We thus
find that the edge state width for zigzag ribbons is only weakly dependent on the exact value of the spin-orbit coupling. On the other hand, it is rather strongly dependent on the wavevector $q_x$ (through $Q_z$), and thus on the energy. In Fig. 4 we have plotted the edge state widths $\lambda$ for armchair and zigzag orientations as a function of the Fermi energy $E$. Except for energy values close to the spin-orbit gap, the width of the zigzag edge states is considerably smaller than the armchair one. This is precisely what we found in Fig. 3. However, for energies close to $\Delta_{SO}$, the zigzag edge state width increases dramatically (as is also evident in Fig. 3). For these energies, $\lambda$ also becomes dependent on the spin-orbit coupling strength, as shown in Fig. 4 with the red solid, dashed and dotted lines.

To understand the perfect transmission found in zigzag ribbons, first consider a ribbon without spin-orbit coupling. In that case, one can perform the low energy approximation around the two inequivalent $K^{\uparrow}$ points in the same fashion as with armchair terminated ones. In the valley isotropic basis, the isospin is then simply given by $|\gamma\rangle^\uparrow = (1,0)$ for a left moving particle and $|\gamma\rangle^\downarrow = (0,1)$ for a right moving one at the lower and upper boundaries. Edge states along zigzag boundaries thus belong to opposite (orthogonal) valleys for opposite propagation directions. By turning on the spin-orbit coupling, the low energy dispersionless bands evolve into dispersive helical bands crossing at the $M$ point, as shown in Fig. 1 and their isospin is not well defined anymore. The latter bands are no longer separated by a large momentum, and one might therefore think that the potential step, even if it is smooth, could induce scattering between these bands. The key point now is that for a fixed spin, these two bands belong to opposite boundaries in the left region, so no large momentum can connect them. Scattering between these bands is only possible if the wavefunction is able to spread through the bulk of the ribbon. When this happens, to the right of the junction, the Fermi energy of the quasiparticles lies above the bulk gap where the high energy modes in this region have again a well defined valley polarization. Hence, all modes injected from a left moving helical edge state will belong to the $K$ valley and not to the $K'$ one. The backscattering channel, that is derived from the $K'$ valley, will therefore remain inaccessible.

### III. INFLUENCE OF EDGE ROUGHNESS

For a clean ribbon, perfect transmission was due to the orthogonality between equal-spin left- and right-moving edge channels, combined with valley-preserving scattering throughout all the ribbon. Disorder in general will break the orthogonality between topological edge channels and a decrease in the transmission through a QSH insulator/metal junction is thus to be expected. However, even if the disorder conserves the orthogonality of the topological channels, e.g., when disorder is only present in the right (metallic) region of the junction, it will in
general induce inter-valley scattering which will connect counterpropagating edge channels through the bulk of the metallic region. Note that there are no topological edge states running along the junction, since this would require that both sides of the junction be bulk insulators with different values of the $Z_2$ topological invariant.

To analyze the influence of disorder in more detail we have considered rough edge boundaries, which break the orthogonality between topological edge states. We model rough edges by randomly removing carbon atoms up to a depth $d$ (in units of $a$) from the ribbon’s boundaries. In particular, we model a rough edge with a function of the form

$$f(x) = y_b + \sum_{n=1}^{N/2} A_n \frac{d}{\sqrt{N}} \sin \left( \frac{2\pi n}{N} x - \varphi_n \right). \quad (10)$$

Here $y_b$ is $W-d/2$ for the upper boundary and $d/2$ for the lower one. The rough ribbon is obtained by removing all the carbon atoms in positions $(x, y)$ for which $y > f(x)$ ($y < f(x)$) at the upper (lower) boundary. The number of modes $N$ in the Fourier series is chosen to be of the order of the number of atoms along the length of the ribbon. The amplitudes $A_n$ and phases $\varphi_n$ are random numbers between 0 and 1 or $-\pi$ and $\pi$ respectively. Note that this function generates a boundary profile that varies strongly at the scale of the lattice spacing $a$ and therefore is a source of strong inter-valley scattering. Examples of ribbons with different roughness depths are sketched in the lower panels of Figs. 5 and 6, where sections of width $W = 5a$ (as used in the calculations) are shown.

The conductance of a QSH insulator/metal junction in the presence of edge roughness is depicted in Figs. 5 and 6 for armchair and zigzag ribbons respectively. Results for intermediate ribbons are similar to one or the other (depending on the crystallographic orientation) and are not shown. All conductance points in these plots are obtained by averaging over 256 disorder realizations. The non-perfect transmission of the topological edge states through the junction is manifested by a reduction of the first conductance plateau. This reduction is however much less pronounced than the conductance decrease in a disordered n-n (or p-p) junction in the absence of spin-orbit coupling (and thus without topological edge states in the left region), as shown in the insets of Figs. 5 and 6.

This increased protection against backscattering can be understood from plots of the charge density in the sample, as depicted in Fig. 7. In the presence of edge roughness, the spin-polarized edge state incoming from the upper boundary does not follow a straight line anymore (like in the flakes of Fig. 3) but its wavefunction accommodates to the roughened boundary. Therefore, unless $d$ is so large that upper and lower topological edge state wavefunctions can overlap, there are still no available intra-boundary backscattering channels. Only a single reflection channel is open, namely to cross to the topological edge state at the lower boundary. This is radically different in a ribbon without intrinsic spin-orbit coupling, where multiple transmission and reflection channels are available throughout the bulk and disorder will have a bigger impact. The previous argument explains the small sensitivity of the conductance on roughness depth $d$ for energies below the spin-orbit induced gap in Figs. 5 and 6. However, when the edge state width $\lambda$ becomes comparable to the ribbon’s effective width (given approximately by $W - 2d$), direct inter-boundary backscattering can take place in the left region due to the overlap of counter-propagating (non-orthogonal) edge channels, significantly reducing the transmission probability. This happens for zigzag ribbons with energies close to the band-gap edge, where the edge state width diverges (see Fig. 4), which manifests itself as a conductance dip in the left region due to the overlap of counter-propagating (non-orthogonal) edge channels, significantly reducing the transmission probability.

In Fig. 8 we plot the conductance through a QSH insulator/metal junction as a function of the ribbon’s width $W$ in the presence of edge roughness with a depth $d = 5a$. The disordered region has a length $L = 100a$, and the potential step parameters are $U_0 = 0.25t$ and $\delta = 5a$. Zigzag and armchair ribbons are considered, and energies either close to the Dirac point or close to the spin-orbit induced gap are compared. For all parameters, we clearly see that the conductance increases with $W$, so
that perfect transmission is recovered in the thermodynamic limit. This can be understood by realizing that, as the ribbon width is increased, the number of available forward scattering channels grows while the available backscattering channels remains one. Note that for the potential step parameters selected, all curves behave similarly except for the one of the zigzag terminated ribbon for energies close to the gap. The slower conductance increase in that case is a result of the large overlap of the opposite boundary topological edge states, as discussed previously. Although the junction used for the calculations in Fig. 8 is a n-n junction, we have found similar results for p-p and n-p (p-n) junctions and conclude that conductance recovery with increasing ribbon width is a general trend.

IV. CONCLUSIONS

Transport through QSH insulator/metal junctions has been analyzed in graphene ribbons in the presence of an electrostatic potential step. We have found that for clean ballistic ribbons (with arbitrary crystallographic orientation), the topological edge states are transmitted perfectly through such a junction, independent of the ribbon’s width, the parameters of the potential step and the value of the intrinsic spin-orbit coupling, as long as inter-valley scattering is not present. This has been explained by proving the isospin orthogonality between forward and backward edge channels analytically, a mechanism that is analogous to the Klein tunneling. We have also found that the edge state width only depends on the spin-orbit coupling strength for armchair ribbons but is in addition strongly energy dependent for zigzag ribbons. In the presence of edge roughness, the orthogonality, and thereby the perfect transmission, is destroyed and the upper (lower) edge channel can be reflected to the lower (upper) one through the metallic region where the particle’s wave function spans the whole ribbon’s width. However, even in the presence of strong disorder, reflection from a QSH insulator/metal junction is small as compared to a similar ribbon in the absence of intrinsic spin-orbit coupling. This protection can be understood as a spin-orbit proximity effect since to the left of the junction the edge states are still topologically protected (as long as time-reversal symmetry breaking disorder is absent). Finally, we found that perfect transmission is gradually restored in the presence of disorder as the ribbon’s width increases, since the number of available forward-scattering channels grows. This recovery is dependent on the ribbon’s crystallographic orientation, and was explained by analytical considerations as well as by numerical simulations of the charge density across the junction. In the present work, the QSH insulator/metal junction was realized by means of a constant spin-orbit coupling and an electrostatic potential step. An analogous junction could be achieved in the presence of a spin-orbit potential step if the intrinsic spin-orbit coupling could be externally tuned across the ribbon. We analyzed this scenario numerically and found similar results for metallic ribbons.

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Appendix A: Topological Edge States

In this Appendix we derive the edge state energies and wavefunctions for armchair and zigzag graphene ribbons in the presence of the intrinsic spin-orbit interaction. Moreover, we prove the orthogonality between same spin left and right moving edge states at the opposite boundaries of the ribbon and obtain the edge state width as a function of spin-orbit coupling and energy.

We consider the lattice and the reference system shown in Fig. 9. In terms of the lattice vectors $\vec{r}_i$ (linking nearest-neighbor carbon atoms) and $\vec{a}_i$ (linking next-nearest neighbors), the tight-binding Hamiltonian can be written as $H = H_0 + H_{SO}$, where

$$H_0 = -t \sum_{s_1, s_2} \sum_{n=1}^{3} a_{r_i, s_1}^\dagger b_{r_i+n, s_2} + h.c.,$$

and

$$H_{SO} = i\epsilon_{SO} \sum_{s_1, s_2} \sum_{n=1}^{6} (-1)^{n+1} s_2 \left[ a_{r_i, s_1}^\dagger a_{r_i+n, s_2} - b_{r_i, s_1}^\dagger b_{r_i+n, s_2} \right].$$
sured from the center of the first Brillouin zone and sites, the total Hamiltonian can thus be written as

\[ \vec{b} = a(\pm \sqrt{3}/2, 0), \quad b_3 = a(0, 3/2), \quad a_1, a_2 = a(\pm \sqrt{3}/2, 3/2), \quad a_6, a_3 = a(\pm \sqrt{3}, 0) \text{ and } a_5, a_4 = a(\pm \sqrt{3}/2, -3/2), \]

where \( a \) is the interatomic distance.

In the previous two equations, \( i \) runs over equal sublattice sites, \( a^\dagger \) and \( b \) are creation operators on sublattice \( A \) and \( B \) respectively, and \( s_z = \pm 1 \) is the \( z \)-component of the electron spin.

Fourier transforming these Hamiltonians into momentum space, one gets:

\[ H_0 = \sum_{\vec{q}, s_z} \xi(\vec{q}) a_{\vec{q}, s_z}^\dagger b_{\vec{q}, s_z} + \text{h.c.}, \quad \text{(A3)} \]

where \( \vec{q} \) is the wave vector in the graphene plane measured from the center of the first Brillouin zone and

\[ \xi(\vec{q}) = -\frac{t}{a} \sum_{n=1}^3 e^{-i\vec{q}\vec{r}_n} = -t \left[ 2 \cos \left( \frac{\sqrt{3}}{2} ax \right) + e^{-i\frac{\pi}{2} q_y} \right], \quad \text{(A4)} \]

with \( a \) the interatomic distance. On the other hand

\[ H_{SO} = \sum_{\vec{q}, s_z} \chi(s_z, \vec{q}) \left( a_{\vec{q}, s_z}^\dagger a_{\vec{q}, s_z} - b_{\vec{q}, s_z}^\dagger b_{\vec{q}, s_z} \right), \quad \text{(A5)} \]

with

\[ \chi(s_z, \vec{q}) = i s_z t_{SO} \sum_{n=1, \ldots, 6} (-1)^{n+1} e^{-i\vec{q}\vec{a}_n}. \quad \text{(A6)} \]

The total Hamiltonian can thus be written as

\[ H = \sum_{\vec{q}, s_z} \left( a_{\vec{q}, s_z}^\dagger b_{\vec{q}, s_z} \right) \left( \chi(s_z, \vec{q}) \xi(\vec{q}) - \chi(s_z, \vec{q})^* \right) \left( a_{\vec{q}, s_z} b_{\vec{q}, s_z}^\dagger \right), \quad \text{(A7)} \]

with eigenvalues

\[ E(\vec{q}) = \pm \sqrt{\left| \xi(\vec{q}) \right|^2 + \chi(s_z, \vec{q})^2} \quad \text{(A8)} \]

and eigenvectors

\[ \left( \psi_A(s_z, \vec{q}) \psi_B(s_z, \vec{q}) \right) \propto \left( \frac{\xi(\vec{q})}{\xi(\vec{q}) + \chi(s_z, \vec{q})} \right). \quad \text{(A9)} \]

The total wave function is then

\[ \Psi_{s_z, \vec{q}}(x, y) = e^{i q_x x} e^{i q_y y} \left( \psi_A(s_z, \vec{q}) \psi_B(s_z, \vec{q}) \right). \quad \text{(A10)} \]

1. Armchair ribbon

With the geometry depicted in Fig. 9, armchair edges extend along the \( y \)-direction. To obtain an edge state localized in the \( x \)-direction, we replace \( q_x \rightarrow i \kappa \) in Eq. (A10). The boundary condition amounts to setting the wavefunction to zero at \( x = 0 \), both on \( A \) and \( B \) sublattice sites. To obtain a nontrivial solution, we have to consider a superposition of two wavefunctions. In the armchair case, one can consider a combination of waves around the \( K \) and \( K' \) points of the Brillouin zone of graphene, because the low-energy limit corresponds to having wavevectors in the vicinity of these points. Our ansatz is thus

\[ \Psi^{ac}(x, y) = e^{-\kappa x} e^{i q_y y} \left[ \alpha_0 e^{i R_x \kappa} \left( \psi_A \psi_B \right) + \beta_0 e^{i R_x' \kappa} \left( \psi_A' \psi_B' \right) \right], \quad \text{(A11)} \]

where \( q_y \) is measured from the \( K' \) point (with \( K' = \pm 3\sqrt{3}a \)) and \( \alpha_0, \beta_0 \) are the relative amplitudes of the wavefunction in each valley.

After expanding the quantities \( \xi \) and \( \chi \) in Eqs. (A4) and (A6) around the \( K' \) point, one arrives at \( \xi' = \pm \sqrt{3} t_{SO} \) and \( \chi' = \pm s_z \Delta_{SO} \), where the upper (lower) sign corresponds to the \( K (K') \) point, and \( \Delta_{SO} = 3 \sqrt{3} t_{SO} \). The spinors in Eq. (A11) are then given by (c.f. Eq. (A9)):

\[ \left( \psi_A' \psi_B' \right) \propto \left( \frac{i hv_F (\pm \kappa + q_y)}{E \mp s_z \Delta_{SO}} \right). \quad \text{(A12)} \]

A nontrivial wavefunction (A11) fulfilling the boundary condition \( \Psi^{ac}(x = 0, y) = \left( \begin{array}{c} 0 \\ 0 \end{array} \right) \) can only be found when

\[ \left| \begin{array}{c} \psi_A \\ \psi_B' \end{array} \right| = 0. \quad \text{(A13)} \]

This leads to the following expression for \( \kappa \): \( \kappa = -s_z \frac{\Delta_{SO}}{E} \). Inserting this into the dispersion relation \( E = \pm \sqrt{\Delta^2_{SO} + (hv_F q_y)^2} \), one obtains \( E = \pm hv_F q_y \). The result for \( \kappa \) can then be written as:

\[ \kappa = \frac{-\Delta_{SO}}{hv_F} s_z \text{sgn}(q_y) \text{sgn}(E). \quad \text{(A14)} \]
At the left boundary, $\kappa$ should be positive to get a decaying solution, so, e.g., electrons ($E > 0$) propagate either with spin-up downwards ($q_y < 0$), or with spin-down upwards $q_y > 0$. The pseudospin associated with these electrons is

\[
\begin{pmatrix}
\psi_A^{\uparrow} \\
\psi_B^{\uparrow}
\end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix}
-s_i \\
1
\end{pmatrix}.
\]  

(A15)

At the right boundary one needs $\kappa < 0$ and the propagation directions are reversed. The pseudospin is then

\[
\begin{pmatrix}
\psi_A^{\downarrow} \\
\psi_B^{\downarrow}
\end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix}
s_i \\
1
\end{pmatrix}.
\]  

(A16)

In terms of the Pauli matrices for the pseudospin degree of freedom, $\sigma$, and for the isospin one, $\tau$, the Hamiltonian $[A7]$ around the K and K’ valleys can be expressed:

\[
H = \hbar v_F(q_x \sigma_x \otimes \tau_z - q_y \sigma_y \otimes \tau_0) + s_z \Delta_{SO} \sigma_z \otimes \tau_z, \quad (A17)
\]

acting on the Dirac 4-component spinor $\psi = (\psi_A, \psi_B, \psi_A^T, -\psi_B^T)$. In order to prove the orthogonality between equal-spin incoming and outgoing edge channels, it is convenient to express the previous Hamiltonian in the ”valley isotropic” basis [8], where $H$ is isotropic in the valley degree of freedom. The Hamiltonian in the valley isotropic basis is related to $H$ through the unitary transformation $H^{iso} = U^* H U$, where

\[
H^{iso} = [\hbar v_F(q_x \sigma_x - q_y \sigma_y) + s_z \Delta_{SO} \sigma_z] \otimes \tau_0 \quad (A18)
\]

and

\[
U = \frac{1}{2}(\tau_0 + \tau_z) \otimes \sigma_0 - \frac{1}{2}(\tau_0 - \tau_z) \otimes i \sigma_y. \quad (A19)
\]

In a similar way, the pseudospins are transformed like $\psi^{iso} = U \psi = (\psi_A, \psi_B, \psi_A^T, -\psi_B^T)$. The total wave function in this basis is

\[
\psi^{iso}_{\alpha c}(x, y) = e^{-\kappa x} e^{i q_y y} \left[ \alpha e^{i R^z \tau} \begin{pmatrix}
\psi_A \\
\psi_B
\end{pmatrix} + \beta e^{i R^z \tau} \begin{pmatrix}
\psi_B^T \\
-\psi_A^T
\end{pmatrix} \right] \quad (A20)
\]

where $\alpha$ and $\beta$ represent the valley polaritazion or isospin of the wave function.

2. Zigzag ribbon

Now we consider a semi-infinite zigzag-terminated graphene sheet to find expressions for the topological edge states. In the absence of spin-orbit coupling, it is known that the boundary condition amounts to a vanishing wavefunction on one of the sublattices. However, as spin-orbit coupling induces next-nearest neighbor hopping, the total wave function in our case has to vanish in both the A and the B sublattice sites at the edge.

This condition can never be met by a single wavefunction of the form $[A10]$, so we will look at a superposition of two of them. Furthermore, as we are looking for an edge state solution the wavefunction has to decay from the edge into the bulk. Considering the lower boundary (the semi-infinite graphene sheet extends towards $y > 0$, see Fig. [9]), we then substitute $q_y \to \kappa$ and make the following ansatz:

\[
\psi_{s_z, q_y}(x, y) = \alpha e^{-\kappa y} e^{i q_y x} \begin{pmatrix}
\psi_A(s_z, q_z, \kappa_1) \\
\psi_B(s_z, q_z, \kappa_1)
\end{pmatrix} + \beta e^{-\kappa y} e^{i q_y x} \begin{pmatrix}
\psi_A(s_z, q_z, \kappa_2) \\
\psi_B(s_z, q_z, \kappa_2)
\end{pmatrix}, \quad (A21)
\]

In the following, the notation

\[
Q_c = 2 \cos \left( \frac{\sqrt{3}}{2} q_x a \right), \quad (A22a)
\]

\[
Q_1 = 2 \sin \left( \frac{\sqrt{3}}{2} q_x a \right), \quad (A22b)
\]

\[
Q_2 = 2 \sin \left( \sqrt{3} q_x a \right), \quad (A22c)
\]

\[
\phi_i = e^{-\frac{\kappa x}{2 a_n}}, \quad (A22d)
\]

will prove to be convenient. The terms $\xi$ and $\chi$ in Eqs. [A4] and [A6] can then be written as

\[
\xi(q_x, \phi_i) = -t (Q_c + \phi_i^{-1}), \quad (A23a)
\]

\[
\chi(s_z, q_x, \phi_i) = -t_{SO} s_z (Q_2 - Q_1 (\phi_i + \phi_i^{-1})) \quad (A23b)
\]

and the energy dispersion (A8) becomes

\[
e^2 = (Q_c + \phi_i^{-1}) (Q_c + \phi_i) + \tau^2 (Q_2 - Q_1 (\phi_i + \phi_i^{-1}))^2. \quad (A24)
\]

Here we defined $\epsilon \equiv E/t$, and $\tau \equiv t_{SO}/t$. Multiplying this equation with $\phi_i^2$ gives a fourth order equation in $\phi_i$ from which one can in principle calculate the allowed values of $\phi_i$ as a function of energy. Solving this equation exactly proves to be too difficult. However, as we are interested in small values of the energy $\epsilon$ and spin-orbit coupling strength $\tau$, we can make an expansion to second order in these parameters. From the four solutions to Eq. (A24), only two fulfill the condition $|\phi_i| < 1$ for a decaying wavefunction around the M-point ($q_x a = \pi/\sqrt{3}$ corresponding to zero energy $\epsilon = 0$). They are

\[
\phi_1 = -\tau^2 \frac{Q_2^2}{Q_c}, \quad (A25a)
\]

\[
\phi_2 = -Q_c + \epsilon^2 \frac{Q_c}{Q_c^2 - 1} - \tau^2 \frac{(Q_2 + Q_c Q_1 + Q_1)^2}{Q_c (Q_c^2 - 1)}. \quad (A25b)
\]

The quantities $\phi_1$ still depend explicitly on both energy and wavevector $q_x$. In order to find the dispersion relation $\epsilon(q_x)$, we have to apply the boundary condition $\psi_{s_z, q_y}(x, y = 0) = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$ to the wavefunction defined in
Eq. (A21). A non-trivial solution for the coefficients $\alpha$ and $\beta$ is then obtained when

$$
\begin{vmatrix}
\psi_A(s_z, q_x, \phi_1) & \psi_A(s_z, q_x, \phi_2) \\
\psi_B(s_z, q_x, \phi_1) & \psi_B(s_z, q_x, \phi_2)
\end{vmatrix} = 0. \tag{A26}
$$

With Eq. (A9) for the spinors, this gives

$$
\xi(q_x, \phi_1)[E(s_z, q_x) - \chi(s_z, q_x, \phi_2)] = \xi(q_x, \phi_2)[E(s_z, q_x) - \chi(s_z, q_x, \phi_1)]. \tag{A27}
$$

Using Eqs. (A23) and inserting the allowed values for the $\phi_i$ from Eq. (A25), one obtains the dispersion relation (up to first order in $\tau$):

$$
\epsilon(s_z, q_x) = -3 s_z \tau Q_2 = -6 s_z \frac{t_{SO}}{t} \sin(\sqrt{3} q_x a). \tag{A28}
$$

The zero of energy lies at $q_x a = \pi/\sqrt{3}$ (at $q_x a = 0$ there is no edge state solution with $|\phi_i| < 1$). Quasiparticles with spin-up (spin-down) thus move with positive (negative) velocity $\pm \frac{\sqrt{3} t_{SO}}{2t}$ at the lower boundary. At the upper boundary, the role of spin-up and spin-down is interchanged (see below).

The $\phi_i$ in Eq. (A25) can assume negative values. With the definition $\phi_i \equiv e^{-\tau_{\alpha} \kappa}$, this means that the solutions for $\kappa_i$ can be complex and the wavefunction oscillates in the $y$-direction with a decaying envelope. In particular, we find that the wavefunction changes sign when propagating from one zigzag dimer line to the next. The edge state width has thus to be defined as $\lambda_i = 1/Re(\kappa_i)$. With Eq. (A22d), one obtains

$$
\lambda_i = -\frac{3a}{2\log(|\phi_i|)}. \tag{A29}
$$

Until now, we only considered the lower boundary. For the upper boundary, the semi-infinite graphene sheet extends now to negative $y$-values. A localized state is then found by substituting $q_y \to -q_y = -i\kappa$ in Eq. (A10). This will interchange the off-diagonal terms $\xi$ and $\xi^*$ in the Hamiltonian (A7). If we further substitute $s_z \to -s_z$, then the diagonal terms are interchanged too. The Hamiltonian in Eq. (A7) for the upper boundary then looks exactly as the one for the lower boundary, but with the $A$- and $B$-sites interchanged. Using Eq. (A9) and the condition (A27), it is possible to see that the pseudospin for the lower boundary is

$$
|\psi^l(s_z, q_x, \phi_i)\rangle = \left( \begin{array}{c}
1 \\
-s_z \tau Q_1
\end{array} \right). \tag{A30}
$$

to first order in $\tau$, both for $i = 1, 2$. With the substitution $A \leftrightarrow B$ and $s_z \to -s_z$ mentioned above, the pseudospin for the upper boundary is

$$
|\psi^u(s_z, q_x, \phi_i)\rangle = \left( \begin{array}{c}
-s_z \tau Q_1 \\
1
\end{array} \right). \tag{A31}
$$

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45 For semiconducting armchair ribbons, $W$ has to be much bigger than the edge state width $\lambda$ so that the ribbon in the presence of intrinsic spin-orbit coupling is metallic.
46 Note that the actual with of the ribbon is $W' = \frac{\sqrt{3}}{2}(N - 1)a$, but the wave function has to vanish one site away from the ribbon’s boundary at each side of the ribbon, so that $W = W' + \sqrt{3}a$. 