Conductance of gated junctions as a probe of topological interface states

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Energy dispersion and spin orientation of the protected states at interfaces between topological insulators (TIs) and non-topological materials depend on the charge redistribution, strain, and atomic displacement at the interface. Knowledge of these properties is essential for applications of topological compounds, but direct access to them in the interface geometry is difficult. We show that conductance of a gated double junction at the surface of a topological insulator exhibits oscillations and a quasi-linear decay as a function of gate voltage in different regimes. These give the values for the quasiparticle velocities along and normal to the junction in the interface region, and determine the symmetry of the topological interface states. The results are insensitive to the boundary conditions at the junction.

Introduction Using topological materials [1–3] as the basic component of future devices [4–6] requires making heterostructures of these systems together with a topologically trivial compounds that impact the desired properties on the interface states at the boundary between the two. Proposed partner compounds range from conventional semiconductors [7–9] to ferromagnets [10, 11] and superconductors [12–14]. For topological insulators it is commonly assumed that (apart from the imposed exchange field or proximity-induced superconductivity) the interface states have the same linear Dirac-like dispersion and helical spin-momentum locking that has been predicted and observed in the surface states by angle-resolved photoemission (ARPES) measurements [3]. It is well established, however, that symmetry breaking at interfaces, whether intrinsic [15] or due to the interface potentials [16] (arising from the polarity and broken bonds at the surface, strain and reconstruction due to lattice mismatch, etc.) may distort the Dirac cone, break the helicity of the topological states, and, in turn, affect the heterostructure properties [17]. Consequently, determining (and, ideally, controlling) the dispersion and spin texture of the topological interface states (TIS) is a critical step towards creating a platform for topological devices.

Direct access (ARPES or scanning tunneling spectroscopy) to the TIS is impossible due to the capping material, and indirect optical measurements (e.g. Kerr rotation [18, 19]) are often hard to interpret. Here we demonstrate that the dc conductance in a gated double junction setup for a topological heterostructure, shown in Fig. 1(a), exhibits a quasi-linear variation in one range, and Fabry-Perot-like oscillations in another range of gate voltages. The kink voltage at the edge of the linear regime and the period of the oscillations give the quasiparticle velocities parallel and normal to the junction, and hence the dispersion anisotropy, of the hidden topological interface state. Our proposal therefore establishes criteria for use of topological heterostructures in prototype devices.

Fabry-Perot-induced transmission resonances in gated graphene junctions are well-known [20, 21], but, in contrast to that case, the physics discussed here relies on the spinor structure of the TIS. Conductance oscillations were predicted in the TI surface states subject to the exchange field in the gated region [22, 23], but those studies assume no distinction between the interface and the surface states, and ignore the scattering at lateral junctions, see below, so the underlying physics is different. Our proposal provides quantitative measure of the symmetry-breaking effects intrinsic to the interface. We also show that the results are robust with respect to the details of the junction scattering [24, 25].

Vertical and lateral heterojunctions. Bulk-boundary correspondence guarantees the existence of a localized state at the interface between a TI and a non-topological material [1, 2]. In the absence of time-reversal breaking perturbations this state is generically gapless and, at low energy, linearly dispersing with the momentum in the plane of the interface, k. Since the band inversion that gives rise to the topological properties of the TI usually arises from the spin-orbit interaction (SOI), the resulting states also exhibit spin-momentum locking [1–3].

For prototypical TI Bi2Se3 the states at the surface terminations along the high symmetry directions ((111) in the rhombohedral/[001] in the hexagonal representation) are described by the effective Dirac Hamiltonian $H_D = v_1(\sigma \times k)z$ [26], where $\sigma$ is the vector of the Pauli matrices, $\hat{z}$ is the normal to the interface, $v_1$ is the effective velocity, and we set $\hbar = 1$. The eigenstates have isotropic dispersion, $E_{\pm} = \pm v_1 k_z$ and are helical (spin in the plane normal to the momentum direction), with the spinor structure $\Psi_D^\pm = (i, \pm e^{i\theta})^T$ for the positive and negative energy branches respectively, with $\theta$ the angle between $k$ and the x-axis.

Once the rotation symmetry is broken either by a choice of the lattice termination [15] or by the interface potentials [16], the topological state is described by a generalized form of $H_D$, namely

$$H_I = \sum_{i,j} c_{ij} \sigma_i k_j,$$

where the sum is over all the spin components, $i = x, y, z,$...
FIG. 1. The double junction setup for measuring the conductance oscillations. Top: experimental setup. Inset: top surface of the structure with the Dirac cones of the topological states, subject to the gate voltage \( V_g \). \( E \) is the chemical potential relative to the Dirac point. Bottom: matched states conserving the momentum along the junction for different \( V_g \) for the velocity discontinuity case discussed in text, showing the reduction in the available phase space for transmission for \( 0 < V_g < E \) and dominance of the near-normal incidence states in the interface region for \( V_g < 0 \).

but \( j = x, y \). For general \( c_{ij} \) the eigenstates of \( H_I \) have anisotropic dispersion, with non-helical spin texture and spins that point out of the plane if \( c_{zi} \neq 0 \). Since control of the interface potentials and, via them, the coefficients \( c_{ij} \) is difficult, the challenge is to determine the properties of these states for a given heterostructure.

For a single lateral junction between the surface and the interface states, the mismatch between the spinor structure of the eigenstates reduces the transmission probability. However, Klein tunneling ensures reflectionless transmission for quasiparticle at normal incidence irrespective of the exact form of \( H_I \). Since it is these quasiparticles that dominate the conductance, signatures of non-trivial TIS are weak in transport measurements on a single junction, but are clear and robust in the gated double-junction structure shown in Fig. 1(a).

Methodology and boundary conditions. We choose the \( x \)-axis normal to the junction. Then the Hamiltonian is piecewise defined as \( H = H_D \) for \( x < 0 \) and \( x > d \), and \( H = H_I + V_g \), where \( V_g \) is the gate voltage, for \( 0 < x < d \). The eigenstates in each region are given by \( \Psi_D(x, y) = \Psi_D \exp(ik_x \cos \theta + iky \sin \theta) \), and \( \Psi_I(x, y) = \Psi_I \exp(ik'x \cos \phi + ik'y \sin \phi) \), where \( \Psi_D \) are the spinor eigenvectors of the matrices \( H_D \) for momenta \((k, \theta)\) and \((k', \phi)\) in polar coordinates, respectively. To solve the scattering problem for an incoming particle with \( k = E/v_1 \) at angle \( \theta \), we write transmitted and reflected waves in each region, and match the wave functions at \( x_0 = 0, d \), using the conservation of energy and the momentum along the interface to determine \( k' \) and \( \phi \), see Fig. 1(b).

However, since the eigenvalue equation \( H \Psi = E \Psi \) is a first order differential equation, the wave functions are not continuous [27–29], but, instead, satisfy

\[
\Psi(x_0 - 0, y) = M \Psi(x_0 + 0, y),
\]

where the choice of the matrix \( M \) is constrained by conservation of the particle current normal to the interface, \( j_x = \delta H / \delta k_x \), and preservation of the time-reversal invariance. As is well known [30–32], this condition determines a single parameter family of matrices \( M(\alpha) \), where the value of \( \alpha \) depends on the details of junction potential. For the sandwich structure in Fig. 1(b) we therefore have two such parameters, \( \alpha \), and \( \beta \).

For each choice of \( H_I \) below we determine the matrix \( M \), compute the transmission probability, \( T(E, \theta, V_g, \alpha, \beta) \equiv T \), and evaluate the conductance using Landauer formalism,

\[
G(V_g) = \frac{G_0}{2} \int_{-\pi/2}^{\pi/2} T \cos \theta d\theta.
\]

Here \( G_0 = \frac{e^2}{3\pi^2} W k_F \), with \( W \) the width of the junction, and we assumed low temperature, \( E = v_1 k_F \). In all plots we use the value \( v_1 = 3.3 \text{ eV } \text{Å} \) for BiSe\(_3\) [33, 34].

Velocity discontinuity. Essential physics is already clear when considering the interface Hamiltonian which
differs from that for the surface only by the value of the velocity, \( H_I = v_2(\sigma \times \mathbf{k}) \). In that case \( M_k = \sqrt{v_2/v_1} \exp[i\sigma g] \) (\( M_k = \sqrt{v_1/v_2} \exp[i\beta g] \)) at the left (right) junction. The ratio of the velocities ensures conservation of the probability current, while the free parameter appears because \( j_k \propto \sigma \) remains invariant under rotations around the y axis in the spin space.

The energy and momentum conservation give \( v_2k' + V_g = v_1k = E \), and \( k' \sin \phi = k \sin \theta \). Since the mismatch between the Fermi surfaces is controlled by the gate voltage, see Fig. 1(b), for \( V_k < V_g < V_k^{(+)} \) with the “kink” voltages \( V_k^{(+)} = E(1 \pm v_2/v_1) \), the conductance of the junction is suppressed since the conservation laws cannot be satisfied for all the incoming momenta at the Fermi surface. Moreover \( G(V_g = E) = 0 \) since the Dirac point of the gated region coincides with the chemical potential, leaving no states to scatter into, and hence the measurement (or extrapolation to) this value gives the chemical potential of the surface state.

The quasi-linear decrease is clearly seen in Fig. 2 (we only plot \( G(V_g) \) for \( V_g < E \) since it is symmetric relative to \( V_g = E \) in our model). The value of \( V_k^{(+)} \), see Fig. 2 yields the ratio \( v_2/v_1 \), and allows determination of the interface velocity \( v_2 \) once \( v_1 \) is known from the ARPES surface measurements. Upon rescaling the computed conductance by \( v_2/v_1 \), the linear parts of the \( G(V_g) \) curves for different velocities \( v_2 \) match exactly, see Fig. 2.

Away from \( V_g = E \), the conductance \( G(V_g) \) shows oscillations. These arise because the net transmission probability across both junctions depends on the phase accumulated while traversing the gated region, \( \zeta = k'd \cos \phi \). Denoting \( \eta_\pm = \alpha \pm \beta \) and \( s = \text{sgn}(E - V_g) \), we find the transmission coefficient

\[
T = \frac{\cos^2 \theta \cos^2 \phi}{| \cos \phi \cos \zeta (\cos \theta \cos \eta_+ - i \sin \eta_+) + \sin \zeta (i \sin \theta \phi \cos \eta_+ - s(\cos \theta \sin \eta_+ + i \cos \eta_+))|^2 .
\]

For \( \alpha = \beta = 0 \) the result is particularly clear from the reflection coefficient \( R = 1 - T \),

\[
R = \frac{[(s \sin \phi \sin \theta - 1)^2 - \cos^2 \theta \cos^2 \phi] \sin^2 \zeta}{(s \sin \theta \sin \phi - 1)^2 \sin^2 \zeta + \cos^2 \theta \cos^2 \phi \cos^2 \zeta},
\]

which vanishes, ensuring perfect transmission, (a) for normal incidence, \( \theta = \phi = 0 \) (Klein tunneling); (b) when \( \zeta = k'd \cos \phi = n\pi \), corresponding to the incidence angles

\[
\sin^2 \theta_n(E) = \left[ \left( \frac{E - V_g}{v_2k_F} \right)^2 - \left( \frac{n\pi}{k_Fd} \right)^2 \right] \in [0, 1] .
\]

Fig. 3(a)-(b) shows the right hand side of Eq. (6), and gives the graphical solution for the allowed orders of maxima as a function of \( |V_g - E| \). Since shift of the parabolas depends on the length of the gated region, Fig. 1, for small \( d \) the gate voltage regions corresponding to different \( n \) do not overlap, yielding clear oscillations. For large \( d \) these regions strongly overlap at small to moderate values of \( n \), becoming more widely spaced as \( n \) increases, since the shift varies as \( n^2 \), see Fig. 3(c).

Assuming that the interface potentials don’t drastically change the Dirac velocity, \( v_2/v_1 \sim O(1) \), and taking \( E \sim 0.1 - 0.2eV \), a reasonable value for \( \text{Bi}_2\text{Se}_3 \) [33, 35], we find \( k_F^{-1} \sim 30 - 60A \), so that \( k_Fd \gg 1 \) for realistic structures. The oscillations start aperiodic and non-sinusoidal, as implied by Fig. 3(b). They become more pronounced at \( n \gg 1 \), with the period \( \Delta V_g \approx \pi v_2/d \), which directly gives the quasiparticle velocity \( v_2 \) in the interface region.

For these values we find pronounced oscillations for \( d \sim 10 - 100nm \), while for greater \( d \) their amplitude is reduced. These values for \( d \) also allow coherent quasiparticle propagation across the gated region according to the values of the mean free path reported for \( \text{Bi}_2\text{Se}_3 \) [36, 37], the mean free path may be longer for systems with the Fermi level tuned to the Dirac point \([38]\). We plot the results for \( d = 40 \) nm \((k_Fd = 24) \), and the inset of Fig. 2 shows that the leading frequency of the oscillations is in excellent agreement with our estimate of \( \Delta V_g \), which gives \( f_1 = 38.6eV^{-1} \) and \( 116eV^{-1} \) for \( v_2 = v_1 \) and \( v_2 = v_1/3 \) respectively.

The oscillation amplitude in Fig. 2 grows with \(|V_g - E|\): For a large Fermi surface in the gated region, Fig. 1(b) all the transmitted quasiparticles in the interface region travel close to the normal direction, \( \phi \to 0 \) for all \( \theta \), increasing their contribution to \( G(V_g) \). In reality for large \( V_g \) there appears a contribution to the current from the bulk bands, making the oscillations harder to detect, especially if \( v_2 \gg v_1 \). Therefore samples tuned to detect, especially values of \( E \) [38] offer wider dynamical range for the observation of oscillations.

In all cases we consider we confirmed that the kink voltage and the period of oscillation are independent of the specific values of \( \alpha, \beta \), and \( E \) [25]. For finite interface scattering the peak transmission value is reduced, and the slope of \( G(V_g) \) changes slightly, but the extracted velocity values remain the same.

**Conductance oscillations for non-helical interface states.** The above analysis was for a system with helical states, and the key question is whether broken symmetry with violated helicity can be detected. Ref. 16 provided the symmetry analysis of the possible linear in
FIG. 3. Location of the transmission maxima. Panels (a) and (b) show parabolas in the right-hand side of Eq. (6) for large and small gate length, \( d \). The function must be in the [0,1] interval (shaded) to have a solution for \( \theta_n \). The corresponding ranges \( (w_n, \text{ shown by thick horizontal lines}) \) of gate voltage \( V_g \) for different orders, \( n \), do not (do) overlap for small (large) and large (bottom) values of \( d \). \( \Delta V_a \) is the interval between the appearance of two successive (generally aperiodic and non-sinusoidal, see text for details) oscillations. Panel (c) shows the evolution of maxima from overlapping at small \( V_g \) to non-overlapping. Dashed vertical lines show that the number of maxima depends on the gate voltage.

\( k \) interface Hamiltonians, Eq. (1). When the rotational symmetry of \( H_I \) is broken, the Dirac dispersion becomes anisotropic, with elliptical constant energy contours. At the same time, the spins of the interface states may point out of the plane of the interface. Both effects reduce the symmetry to the \( B_2 \) representation of the \( C_{2v} \), symmetry group [16]. To capture these effects, we consider

\[
H_I = v_2 (\sigma_x k_y - a \sigma_y k_x) + v_2 b \sigma_z k_x .
\]  

(7)

The energy dispersion is anisotropic \( E(k_x, k_y) = v_2 \sqrt{(a^2 + b^2) k_x^2 + k_y^2} \), with elliptical constant energy contours. We made the natural assumption that the symmetry breaking (e.g. due to strain) yields the principal axes for the ellipse which are parallel and perpendicular to the interface For \( a = 1, b = 0 \) we recover the previous case.

The spins acquire a non-zero out of plane component for \( b \neq 0 \). We find the boundary condition matrix for this case to be

\[
M_L(\alpha) = \sqrt{\frac{v_2 \chi}{2v_1}} e^{i \alpha \sigma_y} - i \frac{v_2 b}{\sqrt{2v_1 v_2 \chi}} \sigma_x e^{-i \alpha \sigma_y} \quad (8)
\]

where \( \chi = a + \sqrt{a^2 + b^2} \) and \( M_L(\beta) = [M_L(-\beta)]^{-1} \).

We then compute the transmission coefficient and the conductance as described above.

Since the conserved component of the momentum parallel to the interface, \( k_y \), in Eq. (7), does not depend on \( a, b \), the kink voltage, \( V_k^{(\pm)} \), is still determined by the condition in Fig. 1(b), and depends only on the velocity along the junction, \( v_2 \). Note that the slope of \( G(V_g) \) in the linear regime weakly depends on \( a, \beta \), but \( V_k^{(\pm)} \) determined from the intercept of that slope and the extrapolation of the averaged, over the oscillation period, conductance, does not, see Fig. 4. On the other hand, in the oscillatory regime, when the Fermi surface in the gated interface region is large, most of the transmitted quasiparticles travel and at near-normal direction \( k_y' \approx 0 \), see Fig. 1(b). Then the relevant velocity is \( v_{F,x}^{\text{max}} = v_2 \sqrt{a^2 + b^2} \), and the period of oscillations is \( \Delta V_{F,x} = \frac{\pi v_{F,x}^{\text{max}}}{d} \). This is exactly the behavior shown in Fig. 4. Consequently, the velocities obtained from the two measurements characterize two orthogonal directions of the quasiparticle dispersion and provide a quantitative test of the symmetry breaking in the interface region.

Discussion. We showed that the conductance of a gated mesoscopic scale double junction at a surface of topological insulator exhibits two regimes that can be
used to determine the quasiparticle dispersion normal to and along the junction in the (otherwise hidden) interface region. These features are robust with respect to the doping level and scattering at the junctions, providing a quantitatively accurate measurement of the parameters of TIS from straightforward transport measurements.

Importantly, even though the overlap of the spinors between surface and interface states depends on the out-of-plane spin component controlled by parameter $b$ in eq. (7), the oscillation frequency only depends on the quasiparticle velocity. Hence this method detects and measures the symmetry breaking in dispersion, but not the out-of-plane spin tilt of TIS [16]. Measurements in a magnetic field may test for the latter effect, but we leave this for future work.

Hexagonal lattice structure of many TIs modulates the dispersion of topological states away from the Dirac point [39]. This modulation is negligible in Bi$_2$Se$_3$ [33, 35], but relevant in Bi$_2$Te$_3$ [40], so a comparison between the two materials would be useful. Gating renormalizes the velocity of the interface state [41], but this effect is too small to be relevant here.

In conclusion, we proposed a conductance measurement that quantitatively determines the properties of the topological interface states, and the consequences of the symmetry breaking interface potentials. These interface states are different from the TI surface states, and are difficult to access by other methods, but are critical for future applications, and our proposal is the first step towards tailoring their properties to specific devices.

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Supplementary material for Conductance of gated junctions as a probe of
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In the main text, we proposed a conductance measurement to study the dispersion anisotropy of the interface state formed at the boundary between a topological and a conventional insulator or semiconductor. The measurement involves quasiparticle transport across a lateral double junction, and we showed that the disorder potentials at each such junction can be encoded into boundary conditions with a single free parameter, see Eq. (2) and Eq. (8) in the main text. The goal of this supplementary material to show that the measurements we propose are robust against the choice of these boundary parameters, $\alpha$ and $\beta$.

![Polar plot of transmission probability as a function of the angle of incidence for different values of junction parameters $\alpha$ and $\beta$.](image)

Figure 1: Polar plot of transmission probability as a function of the angle of incidence for different values of junction parameters $\alpha$ and $\beta$. Values of other parameters used: $E = 0.2$ eV, $v_1 = 3.3$ eV Å, $v_2 = 2.2$ eV Å and $V_g = 0.05$ eV.

In the main text we argued that the main source of oscillations of the junction conductance is due to the Fabri-Perot-like transmission maxima. Figure 1 shows the transmission probability for two different choices of $\alpha, \beta$, and illustrates two main effects of the boundary scattering: (i) Even at the maxima the transmission is not perfect, $T \neq 1$ except for Klein Tunneling at $\theta = 0$. Consequently, the maximal conductance $G/G_0 < 1$, in agreement with Fig. 4 of the main text. (ii) For a fixed gate voltage, $V_g$, the transmission maxima shift and sharpen or broaden, depending on the specific values of $\alpha, \beta$, but the number of maxima is independent of that choice.
The same behavior is manifested in the color plot of the transmission probability as a function of the voltage and the incidence angle, Fig. 2. Once the Dirac cone is sufficiently shifted by the gate voltage, \( V_g < 0 \), the period of the oscillations, corresponding to the spacing, \( \Delta V_g \), between dark red fringes, is the same for both cases.

![Figure 2: Transmission Probability as a function of the angle of incidence and the gate voltage \( V_g \) for \( E = 0.2 \) eV, \( v_1 = 3.3 \) eV Å, and \( v_2 = 2.2 \) eV Å. Left panel: \( \alpha = \beta = 0 \), right panel: \( \alpha = -\pi/3 \) and \( \beta = -\pi/4 \).](image)

The main features of the conductance, evaluated from Eq. (3) of the main text, and shown as a function of the gate voltage in Fig. 3 confirm these observations. The maximal conductance, \( G = G_0 \), is reached only for \( \alpha = \beta = 0 \), when there are no scattering potentials at the interface. The oscillations are non-sinusoidal, and are phase-shifted between different curves. The period, however, remains the same, as is visually clear from Fig. 3 for the case of equal Dirac velocities, and confirmed in Fig. 4 for \( v_1 \neq v_2 \). Note also that the frequency is also independent of the choice of the chemical potential, \( E \), indicating that the result is robust against the doping level and temperature.

Note that the slope of \( G(V_g) \) in the linear region, \( V_g \approx E \) does depend on the interface potentials, but the “kink” voltage, \( V_k^{(\pm)} \), defined in the main text, has a much weaker dependence on these parameters, making this a preferred method for evaluating the velocity \( v_2 \). We show the “worst” case for our analysis, \( v_1 = v_2 \), in Fig. 3, where the variation in the slope for different \( \alpha, \beta \) is about 20\%, but the change in \( V_k^{(\pm)} \) is only about 5\%.

For the non-helical interface state, \( H_I = v_2(\sigma_y k_y - a\sigma_z k_x) + v_2b\sigma_z k_x \), the same conclusions hold. The frequency of the oscillations does not depend on the values of \( \alpha \) and \( \beta \). Variation in both the change of the initial slope and the determination of the kink voltage are smaller than for the case described above, and the dependence of \( V_k^{(\pm)} \) on \( \alpha, \beta \) is very weak. The slope of the conductance

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Figure 3: Conductance oscillations for different values of $\alpha$ and $\beta$. Values of other parameters used: $E = 0.2 \text{ eV}$, $v_1 = v_2 = 3.3 \text{ eV Å}$

Figure 4: Lead frequency of conductance oscillations for different values of $\alpha$, $\beta$ and $E$. Values of other parameters used: $v_1 = 3.3 \text{ eV Å}$ and $v_2 = 1.1 \text{ eV Å}$

is independent of the values of $a$ and $b$, see Fig. 6, confirming that it does depend solely on the velocity $v_2$. The lead frequency of oscillations is also independent of $E$ (i.e. chemical potential) (See Fig. 7).

In conclusion, our proposal to study the features of the interface state using the conductance measurement gives reliable results irrespective of the particular values of the a priori unknown
junction potentials.

Figure 5: Conductance oscillations for different values of $\alpha$ and $\beta$ for the non-helical interface state characterized by $H_I = v_2(\sigma_x k_y - a\sigma_y k_x) + v_2 b\sigma_z k_x$. Values of other parameters used:

$v_1 = 3.3$ eV Å, $v_2 = 1.1$ eV Å and $E = 0.2$ eV.

Figure 6: Independence of the initial slope and the kink voltage of the conductance on the ellipticity and non-helicity parameters $a, b$. 
Figure 7: Lead frequency of conductance oscillations for different values of $E$ for the non-helical interface state characterized by $H_I = v_2(\sigma_y k_x - a\sigma_y k_x) + v_2 b \sigma_z k_x$. Values of other parameters used: $v_1 = 3.3$ eV Å, $v_2 = 1.1$ eV Å $\alpha = \pi/3$ and $\beta = -\pi/4$