A Green’s function approach to topological insulator junctions with magnetic and superconducting regions

Oscar E Casas\textsuperscript{1,3}*, Shirley Gómez Páez\textsuperscript{1,2} and William J Herrera\textsuperscript{1}

\textsuperscript{1} Departamento de Física, Universidad Nacional de Colombia, Bogotá, Colombia
\textsuperscript{2} Departamento de Física, Universidad el Bosque, Bogotá, Colombia

E-mail: oecasasb@unal.edu.co

Received 16 April 2020, revised 10 August 2020
Accepted for publication 17 August 2020
Published 7 September 2020

Abstract

This work presents a Green’s function approach, originally implemented in graphene with well-defined edges, to the surface of a strong 3D topological insulator with a sequence of proximitized superconducting (S) and ferromagnetic (F) surfaces. This consists of the derivation of the Green’s functions for each region by the asymptotic solutions method and their coupling by a tight-binding Hamiltonian with the Dyson equation to obtain the full Green’s functions of the system. These functions allow the direct calculation of the momentum-resolved spectral density of states, the identification of subgap interface states and the derivation of the differential conductance for a wide variety of configurations of the junctions. We illustrate the application of this method for some simple systems with two and three regions, finding the characteristic chiral state of the quantum anomalous Hall effect at the NF interfaces, and chiral Majorana modes at the NS interfaces. Finally, we discuss some geometrical effects present in three-region junctions such as weak Fabry–Pérot resonances and Andreev bound states.

Keywords: Green functions, topological insulators, magnetic-superconducting junctions, Majorana states, Andreev reflections

(Some figures may appear in colour only in the online journal)

1. Introduction

The unusual electronic properties of topological insulators (TI) and their underlying physics have been subject of intense research in the last decade [1–4]. The relativistic and helical nature of the surface states, combined with topological protection against time-reversal symmetry perturbations, make these materials suitable candidates for the construction of nanodevices free of dissipation and decoherence [1, 2, 5]. Among these materials stand out the family of strong TI’s Bi\textsubscript{2}Se\textsubscript{3}, Bi\textsubscript{2}Te\textsubscript{3}, and Sb\textsubscript{2}Te\textsubscript{3} whose surface states present a conical dispersion relation and left-handed helical spin texture, that can be described by a simple relativistic model at the $\Gamma$ point in momentum space [1, 6–8]. These particular features have already been observed by spin-resolved angle-resolved photoemission spectroscopy (ARPES) [9, 10], and in some transport experiments at very low temperatures, either by the weak anti-localization [11–16] or Shubnikov–de Haas oscillations analysis [17–20].

The introduction of the ferromagnetic and superconducting order on these materials surface by proximity effect, also give rise to a rich and novel phenomenology. Magnetization induced by a ferromagnetic insulator results in the quantum anomalous Hall effect (QAHE) which exhibits a chiral bound state at the system’s boundaries [21–27]. On the other hand, the proximity effect with conventional superconductor results in an effective topological spinless p-wave order parameter. Its zero energy Andreev bound states at vortices and FS interfaces constitute Majorana modes, that could be implemented in topological quantum computations technologies [28–31]. The robust topo-
logical character of these interface states lies in the bulk-boundary correspondence, which relates the change of some topological invariant between two phases with the emergence of interface bound states (IBS) [1–4]. Additionally, in these systems the NS interfaces would present specular Andreev reflections for low doping of the N region analogous to those predicted for graphene, provided that transport is restricted to the surface [32–34].

The study of the electrical transport properties of junctions on the TI’s surface with magnetic, superconducting or mixed regions requires the explicit calculation of the differential conductance and the identification of the transport channels involved. In a first approximation, this problem has been addressed through the scattering matrix or Blonder-Tinkham-Klapwijk (BTK) formalism, where the problem has been addressed through the scattering matrix and the associated reflection and transmission coefficients determine the conductance of the system. Besides, this approach considers the different dispersion processes at the NS interface, making it physically intuitive and computationally undemanding for simple junctions [33, 35–52]. Other works use sophisticated and exhaustive Green’s function techniques that allow the direct calculation of all transport observables and can be implemented even for systems with time-dependent perturbations, particle interactions and disorder [53–61]. The study of the transport properties of heterostructures using the Green’s function formalism usually requires a significant amount of numerical calculation, except in some simple non-interacting systems in the stationary regime.

For translationally-invariant 2D systems, the McMillan’s Green’s functions method has the advantage of combining the rigor and generality of Green’s functions approaches with the simplicity and physical intuition of the BTK formalism, since Green’s functions are calculated analytically from the full wave function of the system, that is, from the linear combination of the scattering states present in all the subregions of the junction [54, 56, 61, 62]. However, the Green’s functions obtained by this method are exclusive of each system and cannot be implemented to describe other configurations. Thus, this method becomes inconvenient for the study of junctions with many subregions, as in the case of the scattering matrix formalism.

In this paper we study the transport properties of junctions on the surface of Bi2Se3 in contact with ferromagnetic and conventional superconducting materials. For this, we adapted a Green’s functions approach that had previously been applied in graphene with well-defined edges [63–66]. In this approach, the Green’s functions of N, F, or S regions in a junction are calculated from the asymptotic solutions method. Then, they are coupled by a tight-binding Hamiltonian with the Dyson equation to obtain the Green’s functions and the transport observable of a system with multiple regions. In section 3, it is discussed the concordance between our results for the NF and FS junctions and the known in the literature, principally on the induced topological phases and the associated IBS. In section 4, the transport properties of systems with three regions are explored and discussed. Finally, in section 5 our conclusions and perspectives are presented.

### 2. Model and transport observables

This section is focused on the analysis of the energy spectrum and transport observables of systems that can be modeled as 2D junctions with different parallel interfaces and translational invariance. The surface states of a strong TI of the Bi2Se3 family are described by an effective zero-mass Dirac Hamiltonian at the Γ point [6, 7]. For the plus z surface it is given by $H_z(r) = \frac{1}{2} \mu v_T (\sigma \times \hat{p})_z$, where $v_T$ is the speed of the charge carriers at the Fermi level, $\mu = -i\hbar \nabla$, is the momentum operator and $\sigma_\tau$ is the Pauli vector in the spin subspace. First, was considered the case of a superconducting region (S) on the surface of a TI. There, the direct contact of the TI with a conventional superconductor favors the tunneling of Cooper pairs, inducing a superconducting state by the surface proximity effect. For this region, the elementary excitations of the system are described by the BdG–Dirac Hamiltonian with a spin-singlet s-wave order parameter

$$H(r) = \begin{pmatrix} H_\sigma(r) - E_F & \Delta_{\sigma_\tau} \\ -\Delta_{\sigma_\tau} & -H_\sigma(r) - E_F \end{pmatrix},$$

where $E_F$ is the surface Fermi energy. This Hamiltonian can also describe normal regions (N) by doing $\Delta_\sigma = 0$. If the surface of an N region contacts a ferromagnetic material with perpendicular magnetization vector $M = Mz$, a ferromagnetic region (F) is obtained. Hence, the surface Hamiltonian $H_{\sigma}(r)$ in equation (1) acquires an additional Zeeman-type term of the form $H_Z = M \cdot \sigma = Mz \sigma_z$ (in this work we consider $E_F = 0$).
for ferromagnetic regions to avoid possible transport channels through the ferromagnetic insulator bulk [33]).

By assuming translational invariance of the regions in y direction, the eigenspinors of the Hamiltonian (1) have the form \( \psi^{\mu}(x)e^{iqy} \) where the superscript \( \mu = qe, qh \) indicates electron- or hole-like quasiparticle solutions, and \( q \) the conserved wave vector in y direction. Then, the advanced and retarded Green’s functions can be written as
\[
g^{a,a}(E, x, x', y - y') = \int dq e^{iq(y-y')} g^{a,a}(E, q, x, x') / 2\pi,
\]
where Fourier transform satisfies the inhomogeneous equation
\[
[(E \pm 0^+ - \mathcal{H}(x, q)) g^{a,a}(E, q, x, x') = \delta(x - x'), \tag{2}
\]
with \( E \) the excitation energy of the system and \( 0^+ \) represents an infinitesimal scalar.

The asymptotic solutions method was implemented to obtain solutions of equation (2) that satisfy specific boundary conditions for each region. This method has been used to find the Green’s functions for the Schrödinger equation [70], the Bogoliubov–de Gennes equation in NS junctions (McMillan’s formalism) [62], and in some graphene-based superconducting systems with finite-sized regions [63–66]. In this method, the equilibrium Green’s functions for each region are calculated from the scattering solutions of (1) at the boundaries as follows
\[
\tilde{g}(x, x') = \begin{cases} 
\sum_{\mu,e,h} \tilde{C}_{\mu} \Psi_{\mu}^{e}(x) \tilde{\Psi}_{\mu}^{e}(x') & x < x' \\
\sum_{\mu,e,h} \tilde{C}_{\mu} \Psi_{\mu}^{h}(x) \tilde{\Psi}_{\mu}^{h}(x') & x > x',
\end{cases}
\tag{3}
\]
where \( \Psi_{\mu}^{e,h}(x) \) are the asymptotic solutions of the region that obeys the boundary conditions at the left (L) or right (R) edge. \( \tilde{\Psi}_{\mu}^{e,h}(x) \) are the asymptotic solutions associated with \( \mathcal{H}(x, q) (\tilde{\Psi}_{\mu}^{e,h}(x) = \mathcal{P} \Psi_{\mu}^{e,h}(x) \) with \( \mathcal{P} = I \) the inversion operator for this case), and \( \tilde{C}_{\mu} \) are coefficient matrices determined by the equation (2), as shown in appendix A, where we present the specific analytical expressions of the Green’s functions implemented in the following sections.

For normal and ferromagnetic surfaces we have normal excitations \( [\mu = e, h \text{ in equation (3)}] \) and asymptotic solutions consist of conventional reflection processes at the boundaries, where the reflected particle is the same type as the incident particle [processes \( a \) and \( b \) in figure 1(a)]
\[
\Psi_{\mu}^{e}(L/R)(x) = \psi_{\mu}^{a}(x) + r_{L/R}^{a} \psi_{\mu}^{a}(x),
\Psi_{\mu}^{h}(L/R)(x) = \psi_{\mu}^{b}(x) + r_{L/R}^{a} \psi_{\mu}^{a}(x),
\tag{4}
\]
where \( \psi_{\mu}^{a}(x) \) are the eigenspinors of (1) with \( \Delta_0 = 0 \) propagating in \( x \) direction, and the \( r_{L/R}^{a} \) with \( i = a, b \) are the reflection coefficients at left (L) or right (R) edge defined by the boundary conditions (see appendix A.1 for details).

For a superconducting region, asymptotic solutions include besides quasiparticle reflection processes, branch crossing processes (due to the fast variation of the pair potential near the boundary), where the incident and reflected quasiparticles are of different type [processes \( c \) and \( d \) in figure 1(b)]. Then these can be written as
\[
\Psi_{\mu}^{e}(L/R)(x) = \psi_{\mu}^{a}(x) + r_{L/R}^{a} \psi_{\mu}^{a}(x),
\Psi_{\mu}^{h}(L/R)(x) = \psi_{\mu}^{b}(x) + r_{L/R}^{a} \psi_{\mu}^{a}(x),
\tag{5}
\]
where \( \psi_{\mu}^{a}(x) \) (with \( \mu = qe, qh \)) are the eigenspinors of (1) and \( r_{L/R}^{i} \) with \( i = a, b, c, d \) are the quasiparticle reflection coefficients at L/R edge (see appendix A.2 for details). On the other hand, for semi-infinite regions, the open boundary condition at a given side implies no reflected contributions, as summarized in table 1.

| Extension               | Normal/magnetic | Superconducting |
|-------------------------|-----------------|-----------------|
| Semi-infinite (left)    |                  |                 |
| Finite                  |                  |                 |
| Semi-infinite (right)   |                  |                 |

Since TI’s surface lacks of borders, it is necessary to introduce artificial boundary conditions for each region provided that perfect transparency is recovered when coupling different regions. To simplify the calculations, we adopted artificial boundary conditions for the spin simulating opposite infinite magnetic barriers in \( x = x_L \) and \( x = x_R \) (analogous to those of a graphene ribbon with zigzag edges along the y axis [63]). Here, we adopted the following choice for the boundary conditions
\[
\Psi_{\mu}^{e}(L/R)\big|_i = \Psi_{\mu}^{e}(L/R)\big|_{i+} = 0. \tag{6}
\]
According to the selected boundary conditions, the coupling of different regions placed in series is modeled by the Hamiltonian approach [67]. There, the microscopic hopping of charge carriers between available channels at the edges of adjacent regions (figure 2) is described by a tight-binding Hamiltonian of the form [63–67]

\[ H_T = t \int dq \hat{c}_{qL}^\dagger \hat{c}_{qR} + \text{h.c.}, \]

where \( t = \hbar v_F \) is the hopping amplitude associated with the perfect (or transparent) coupling between regions on the TI’s surface, and \( \hat{c}_{q\sigma} \) are the annihilation operators for charge carriers at the edge of the \( i = L, R \) region with wave number \( q \) and spin projection \( \sigma = \uparrow, \downarrow \). Consequently, given the equilibrium Green’s functions of the two adjacent regions \( \hat{g}_i = \hat{g}(x_i, x'_i) \), as those defined above, it is possible to calculate the equilibrium Green’s function \( \hat{G}_{ij} = \hat{G}(x_i, x'_j) \) of the entire system by using a Dyson equation of the form [63–67]

\[ \hat{G}_{ij} = \hat{g}_{ij} + \hat{g}_{ik} \hat{\Sigma}_{ki} \hat{g}_{kj}, \]

where \( \hat{g}_{ij} = \hat{g}(\delta_{ij}) \) and \( \hat{\Sigma}_{ij} \) are the coupling ‘self-energies’ between the adjacent edges of the two regions and are given by the matrix form of the hopping Hamiltonian

\[ \hat{\Sigma}_{LR} = \hat{\Sigma}_{RL} = t \tau_c (\sigma_\tau - i \sigma_y)/2. \]

The formal details in the implementation of the Dyson equation for junctions with two or more coupled regions are illustrated in appendix B.

Once the equilibrium Green’s functions of the system have been calculated with the Dyson equations, the momentum-resolved spectral density \( A(x, E, q) \) and the DOS \( \rho(x, E) \) are given by the standard relations

\[ A(x, E, q) = -\frac{1}{\pi} \text{Im} \left\{ \text{Tr} \hat{G}_{ee}^\dagger(x, x, E, q) \right\}, \]

\[ \rho(x, E) = \int dq A(x, E, q). \]

In this work, we analyze the transport properties of some junctions with two and three different regions. The differential conductance of a system such as the presented in figure 2 is given by \( \sigma = \partial I/\partial V \), with \( V \) the applied bias voltage and \( I \) the stationary current through the junction [64–67]

\[ I = \frac{e}{2\hbar} \int dq dE \text{Tr} \left( \tau_c \left[ \hat{G}_{q \delta L}^++(E) - i \hat{G}_{q \delta R}^+(E) \right] \right), \]

where \( i \equiv \Sigma_{LR} \) and the \( \hat{G}_{ik}^+(E) \) are the non-local Keldysh (or non-equilibrium) Green’s functions evaluated at the edges of the \( L \) and \( R \) regions, which are related to the equilibrium Green’s functions of the system as shown in detail in appendix C for a three-region system.

3. Examples: two-region junctions

To illustrate the implementation and validity of our method, two systems previously studied in the literature were considered, the FF and FS junctions. The emphasis is focused on the interface states and momentum-resolved spectral density. The details of the calculations are presented in appendix B.

3.1. FF junction

First, the case of an FF junction was considered, where the surface of a topological insulator is placed in contact with two adjacent ferromagnetic regions with polarized magnetization in \( z \) direction as illustrated in figure 3(a). In this system, a magnetization perpendicular to the TI surface induces a gap in the energy spectrum of the system and now the surface state constitutes the QAHE topological phase. The surface exhibits a chiral edge state at a magnetic domain wall with associated Hall conductance \( \sigma_y = \text{sgn} (M_R) e^2/h \). In turn, this conductance is proportional to the Chern number, a topological invariant for symmetry class A [21–25].

This system can be modeled as a junction between two semi-infinite ferromagnetic regions perfectly coupled at \( x_0 = 0 \). The Green’s function of the compound system at the interface is obtained by the Dyson equation (8) [see equation (B1)]. The Green’s functions poles contain information of the bound states present in the FF interface. There are no subgap solutions for zero doping in both regions and \( M_L = M_L \), while for \( M_R = -M_L \) (domain wall configuration) we obtain the linear dispersion relation \( E = \text{sgn} (M_R) \hbar v_F q \) for the QAHE chiral edge states. The interface momentum-resolved spectral density for this configuration is shown in panel (b) of figure 3. This illustrates that our approach leads to well-known results in the literature [21, 22, 25]. At the same time, it allows the derivation of the dispersion relation of the IBS, as well as the direct calculation of the momentum-resolved spectral density at the interface.

3.2. FS junction

Now the case of a FS junction is considered. There, the right ferromagnetic insulator of the FF junction is replaced by a conventional s-wave superconductor as shown in figure 3(c). At the weak-coupling limit, the proximity effect between an s-wave superconductor and the TI surface gives rise to an effective spinless \( p_x + ip_y \) superconducting order parameter. Here, the Andreev bound states at FS interfaces are chiral Majorana modes [28–31]. The local Green’s function of the coupled system at the interface is also given by (B1) with the right unperturbed Green’s function presented in (B9). The poles of this coupled Green’s function lead to the dispersion relation of a
chiral Majorana mode [figure 3(d)]

\[ E(M_L, q) = \frac{-\text{sgn}(M_L)|\Delta|\hbar v_F q}{\sqrt{(|\Delta| + M_L)^2 + (\hbar v_F q)^2}} \]  

\[ (13) \]

The information associated with the chirality of this Majorana IBS is contained in factors of the full spectral density, as in the case of IBS in graphene [65]. In panel (d) of figure 3 there are a couple of subgap interface states with opposite chirality. These states correspond to the remaining IBS modes with energy \( E(-M_L, q) \), which are suppressed in the magnetic gap region. This occurs due to the chiral effect of the magnetization direction in the spin polarization of the helical surface states. Again, the formalism implemented here leads to results reported in the literature [28, 33, 36].

4. Three-region junctions: geometrical effects

In this section we analyze the local spectral density and differential conductance of junctions with a finite intermediate region, by following the Green’s function approach exposed in the previous sections. In these systems, the finite size of the central region results in the appearance of Fabry–Pérot resonances (FPR’s) that are manifested in the transport properties of the system.

4.1. NFN junction

The NFN junction consists of an infinite surface of a topological insulator with a ferromagnetic region of finite width \( d \) as illustrated in figure 4(a). The spectral density of the system at the FN interface (\( \chi_0 = 0 \)) is similar to the case of an infinite NF junction for small doping of the normal lateral regions (\( E_{FL/R} / M \sim 0 \)). It exhibits a Dirac cone with vertex at \( E = -E_{FC} = 0 \) and a chiral edge state associated with the QAHE [figure 3(b)]. However, the spectral density presents a pattern of faint ‘parabolic’ undulations inside the cone from \( |E| > |M| \), whose number increases in proportion to the width of the ferromagnetic region, evidencing its geometric character. These undulations correspond to weak quasi-bound modes or FPR’s that occur within the ferromagnetic region due to specular reflection processes at the interfaces. The introduction of the mass term in the Dirac Hamiltonian (associated with the magnetization vector perpendicular to the surface) reduces the transmission probability and introduces reflected modes at the interfaces [71, 72], even though Klein tunneling ensures perfect transmission at normal incidence between normal surfaces [72, 73]. Since these modes propagate in \( x \) direction, they appreciably contribute to the differential conductance of the junction as shown in figure 4(d) for several widths of the magnetic region. Besides, this is suppressed in the range \( |eV| < |M| \) due to the absence of transport channels inside the magnetic gap, and the suppression effect is proportional to the size of the ferromagnetic region. Also, the conductance exhibits a series of undulations in the regions \( |eV| > |M| \) due to the formation of quasi-bound modes.

Even though the chiral edge state characteristic of zero doping cases disappears for non-zero doping of the lateral regions [figure 4(c)], the spectral density still retains a chiral character. Besides, it has two overlapping cones: the first is a Dirac cone...
Figure 5. (a) A Bi$_2$Se$_3$ block in interfacial contact with a ferromagnetic insulator of finite width $d$ and a conventional superconductor ($E_{FL} = 0$ and $E_{FR} = 100\Delta$). Panels (b) and (c) show the momentum-resolved spectral density of the junction at the FS interface for two different widths $d$ and $E_{FC} = 0$. Differential conductance of the NFS junction for (d) different values of the magnetization and $d \sim \xi$ (e) for different widths of the central region and $M = 0.5\Delta$ ($\xi = \Delta/\hbar v_F$).

with a vertex at $E = -E_{EL/R}$ that correspond to the normal lateral regions and the second is a ‘gapped cone’ associated with the ferromagnetic central region. The later presents a pattern of parabolic undulations for $E > 0$ (as in the case with zero doping), while for $E < 0$ presents a series of clearly defined parabolic FPR bands that fade when entering the Dirac cone of the lateral regions. The FPR’s significantly contribute to transverse transport as shown in figure 4(e).

4.2. NFS junction

In the case of the NFS junction, the normal region at the right of the NFN junction is placed in contact with an s-wave superconductor as seen in figure 5, panel (a). The spectral density at the FS interface is presented in panels (b) and (c). For a width $d \sim \xi$ [figure 5(b)], the system exhibits a pair of subgap bands, a negative-slope band corresponding to the chiral Majorana mode (13) and a positive-slope band associated with the IBS solution $E(-M, q)$. The later is attenuated in the vicinity of $q \sim 0$ due to the selective effect of the magnetization vector in the spin polarization of the helical surface states. This situation is analogous to that found for the FS junction of the previous section, except for the attenuation region that turns smaller due to the finite size of the ferromagnetic region. In contrast, for $d = 15\xi$ [figure 5(c)] there is an evident attenuation region in the range $|E| < |M|$ as in the case of the FS junction. In this case, there is a pattern of undulations inside the paraboloid (with gap $2M$) associated with the central region.

Regarding the longitudinal conductance for low doping levels of the left electrode, a ferromagnetic region with $d \sim \xi$ results in a reduction of transport proportional to the induced magnetization in the range $0 < |eV| < |\Delta|$ [figure 5(d)]. A zero-energy conductance peak (ZBCP) is preserved due to the presence of a chiral Majorana mode at the NS interface. However, this state rapidly decays in the $x$ direction and for $d > 5\xi$, the ZBCP begins to drop whereas some undulations start to emerge for $|eV| > |M|$. These oscillations are associated with the weak FPR bands inside the paraboloid due to the finite size of the ferromagnetic region [figure 5(e)].

4.3. FNS junction

Finally, we consider the case of the FNS junction shown in figure 6(a). Panels (b) and (c) of this figure show the spectral density evaluated at the NS interface for two different values of $d$ and $M_L (E_{FC} = 0)$, where the chiral IBS’s at the FS interface
are observed, including the chiral Majorana mode of \( E(M_\perp, q) \) \((13)\), now accompanied by FPR bands originated by the formation of Andreev quasi-bound states inside the central normal region. These bound states are the result of the constructive superposition of propagating states scattered at the interfaces of the central region. Hence, incoming electron-like quasiparticles from the left ferromagnetic electrode are Andreev-reflected as hole-like quasiparticles at the NS interface, and are partially transmitted and reflected at the FN interface, depending on the angle of incidence and the value of \( M \) (equivalently for incoming hole-like states reflected as electron-like states at the NS interface).

As noted in the previous case, these FPR bands are attenuated outside the gap and its number is proportional to the width of the central region (as in the case of the Andreev quasi-bound states present in NINS junctions \([65, 74]\)). However, in this case, the transmission at normal incidence (associated with Klein tunneling) is not reduced by an insulating contact or an imperfect coupling, but due to the presence of the magnetic-mass term in the surface Hamiltonian. This effect gives rise to reflected waves at the FN interface, even at normal incidence as stated above for the NFN junction. All this geometrical effects could be observed in spectroscopy experiments as ARPES or scanning tunneling spectroscopy (STS).

In the absence of magnetization and for \( E_{\text{FC}} = E_{\text{EL}} \), the system becomes an NS junction and its differential conductance presents the specular Andreev reflections profile. This is characterized by a zero conductance minimum located at \( eV = -E_F \) that corresponds with the minimum of the DOS associated with the Dirac point of the N region \([32]\) [figure 6(d)]. Nevertheless, for the FNS junction case, the presence of the ferromagnetic insulator at the surface of the left electrode, with a finite normal region in the middle, has interesting effects in the longitudinal conductance.

First, the longitudinal differential conductance [figure 6(e)] shows zero conductance region \( |eV| < |M| \) for all the doping levels due to the absence of transport channels inside the magnetic gap of the left semi-infinite electrode. As mentioned in the section above, the suppressor effect of \( M \) is proportional to the size of the ferromagnetic region and is total for an infinite-size electrode. Second, there is a minimum at \( eV = -E_F \) associated with the vertex of the Dirac cone of the central region, that separates specular and retro-Andreev reflection regimes [figure 6(d)]. However, in this case this minimum is attenuated due to the contribution of some FPR bands at the Fermi level of the N region. Third, for high doping levels, parabolic FPR bands manifest in the conductance as a series of small peaks whose number is proportional to the width of the central N region. As in a graphene-based NINS junction \([65, 75]\), these conductance resonances have a higher intensity when increasing the doping of the central region as shows figure 6(e). This effect is because by increasing the doping of the central normal region, the reflection processes at the NS interface transit from the specular to the retro-Andreev reflections regime, that, in a semi-classical perspective favors the formation of closed paths for Andreev bound states \([74, 75]\).

5. Conclusion

In this paper, we adapted the asymptotic-solutions Green’s functions approach for the case of junctions on the surface of strong TI’s with ferromagnetic and s-wave superconducting interfaces. This method has been successfully implemented for 2D systems with multiple coupled regions like graphene-based superconducting junctions. For the construction of the Green’s functions of each region, artificial boundary conditions were adopted, so that all the junction interfaces had perfect transparency when coupled with the Dyson equation. This method allows the study of the transport properties of a wide variety of junctions with the same basic elements. Besides, it also permits the direct calculation of the momentum-resolved spectral densities at the interfaces, which could be of interest for the identification and analysis of topological IBS.

The results obtained for junctions of two regions are consistent with those found in literature. In our study, the FF junction presents the characteristic chiral bound state of the QAHE for opposite magnetizations and a gapped spectrum for parallel magnetizations. On the other hand, for the FS junction the chiral IBS and Majorana modes were found. The properties of some junctions with three regions were also studied. Regarding the NFN junction, the QAHE chiral edge state is observed for \( E_F = 0 \) along with some FPR’s. These resonances are originated in the reflection process at the interfaces and their number is proportional to the width of the central region. With respect to the NFS junction, IBS and Majorana chiral modes are observed in addition to some weak FPR’s. Respect to the longitudinal transport of this junction, the increase in magnetization reduces the subgap conductance except by a small peak for \( eV = 0 \) associated with the chiral Majorana mode, which finally decays for widths of the central regions greater than the superconducting coherence length, while the number of peaks associated with the FPR’s becomes relevant.

Respect to the FNS junction, this also presents chiral IBS and Majorana modes at the NS interface for zero doping of the central region, in addition to some strong subgap FPR bands associated with the Andreev bound states confined by conventional and Andreev reflection process at the interfaces. The number of these resonances also increases with the width of the central region and the associated conductance peaks become appreciable for high doping levels of the central region. On the other hand, due to the large size of the ferromagnetic left electrode, the conductance is suppressed for \( |eV| < |M| \). For low doping of the central region, the subgap conductance structure resembles the characteristic profile of specular Andreev reflection of an NS junction in Dirac 2D systems. Finally, we expect this method to become a useful tool in further studies on electronic and transport properties of junctions and nanostructures on the TI’s surface and other 2D similar systems, specially for the sake of the experimental identification and characterization of new topological phases and IBS present in these types of structures, either through ARPES or transport measurements.
Appendix A. Green’s functions for uncoupled regions

In this appendix, we present the calculation of the equilibrium Green’s functions of the uncoupled normal-ferromagnetic and superconducting regions by the asymptotic solutions method. Then, these Green functions can be coupled by using the Dyson equation to obtain the equilibrium Green’s function of a system composed of several regions, as illustrated in appendix B.

A.1. Normal and ferromagnetic regions

First, to calculate the asymptotic solutions of normal and ferromagnetic regions, it was necessary to find the eigenvalues and eigenvectors of Hamiltonian (1) for \( M = M_L \) and \( \Delta_0 = 0 \). The spectrum is given by

\[
E_{\epsilon/h} = \pm \left( \sqrt{(h_{\text{VF}} | k |)^2 + M^2} - E_F \right),
\]

(A1)

with eigenspinors

\[
\psi_\epsilon^e (r) = e^{i\epsilon x} e^{i\epsilon k_x x} (\varphi_\epsilon^e, 0)^T,
\]

(A2)

\[
\psi_\epsilon^h (r) = e^{i\epsilon x} e^{i\epsilon k_x x} (0, \varphi_\epsilon^h)^T,
\]

(A3)

where \( \varphi_\epsilon^e (r) \) (with \( \mu = e, h \)) are the eigenspinors of the electrons/holes matrix sectors of Hamiltonian (1)

\[
\varphi_\epsilon^e = \left( M_\epsilon^e, -e^{i\epsilon x} e^{i\epsilon k_x x} \right)^T / \sqrt{2},
\]

(A4)

\[
\varphi_\epsilon^h = \left( e^{i\epsilon x} e^{i\epsilon k_x x}, M_\epsilon^h \right)^T / \sqrt{2},
\]

(A5)

\[
M_\epsilon^e = \sqrt{E + E_F + M} / \sqrt{E + E_F},
\]

(A6)

\[
M_\epsilon^h = \sqrt{E_F - E + M} / \sqrt{E_F - E},
\]

(A7)

\[
e^{i\epsilon x} = h_{\text{VF}} (k_x + i) / (E_F + E),
\]

(A8)

and wave number in \( x \)

\[
k_{\epsilon/h} = \text{sgn} (E_F + E) \sqrt{(E_F + E)^2 - M^2} / h_{\text{VF}} - q_\epsilon^2,
\]

(A9)

where the sign-function sets the correct sign for the valence band. For the adopted ‘zigzag-type’ artificial boundary conditions for spin \( \psi^e_L (x_L) |_{L+} = \psi^h_R (x_R) |_{R+} = 0 \), the reflection coefficients in (5) are given by

\[
\hat{r}_{\epsilon/h}^{1/e} (R, L) = -e^{2ik_{\epsilon/h} x_R} e^{2ik_{\epsilon/h} x_L},
\]

(A10)

\[
\hat{r}_{\epsilon/h}^{1/e} (L, R) = e^{-2ik_{\epsilon/h} x_R} e^{-2ik_{\epsilon/h} x_L},
\]

(A11)

\[
\hat{r}_{\epsilon/h}^{1/e} (L, R) = -e^{2ik_{\epsilon/h} x_R},
\]

(A12)

\[
\hat{r}_{\epsilon/h}^{1/e} (R, L) = e^{2i k_{\epsilon/h} x_R} e^{2i k_{\epsilon/h} x_L}.
\]

(A13)

Integrating the equation (2) in \( x \) over an infinitesimal region around \( x' \) we obtain the following auxiliary relation

\[
\hat{g} (x' + 0^+, x') - \hat{g} (x' - 0^+, x') = \frac{i}{h_{\text{VF}}} (\tau_e \otimes \sigma_y),
\]

(A14)

which allows to obtain the coefficient matrices \( \hat{C}_{\mu \nu} \). In this case, by grouping similar terms in the constraint condition (A14) we found that the only non-zero coefficient matrices are \( \hat{C}_{\mu \mu} = \hat{C}_{\mu \mu} \) (since there is not coupling between electrons and holes), and if we assume electron–hole symmetry \( \hat{C}_{ee} = \hat{C}_{hh} \) we have

\[
\hat{C}_{ee} = \frac{-iN_e}{2h_{\text{VF}}} \cos \alpha_e 1 - r_R^2 E_L^2 + \frac{-iN_h}{2h_{\text{VF}}} \cos \alpha_h 1 - r_R^2 E_L^2.
\]

(A15)

By substituting the above expressions in (3), the Green’s function for ferromagnetic and normal regions \( (M = 0) \) is obtained

\[
\hat{g}_{ee/hh} (x, x') = -\frac{i}{h_{\text{VF}}} \left( \begin{array}{cc} \hat{g}_{ee} (x, x') & 0 \\ 0 & \hat{g}_{hh} (x, x') \end{array} \right),
\]

(A16)

where the Green’s functions for electrons and holes sectors are given by

\[
\hat{g}_{ee/hh} (x, x') = \left( \begin{array}{c} -i N_e h e^{i(\epsilon' - \epsilon)x} e^{-i\epsilon x} \cos \alpha_e \cosh \tau_e \tau_h \\ 2(1 - r_R^2 E_L^2) \end{array} \right) \times \left( \begin{array}{cc} M_e^e E & ±iM_e^e e^{-i\epsilon x} J_L \\ ±iM_e^h e^{-i\epsilon x} J_L M_e^h \end{array} \right),
\]

(A17)

with the parameters

\[
I_e = 1 - r_L^e e^{2ik_e x}, J_e = 1 - r_L^e e^{-2ik_e x},
\]

(A18)

\[
J_e = 1 - r_L^e e^{2ik_e x}, J_h = 1 + r_L^h e^{-2ik_h x},
\]

(A19)

\[
K_e = 1 - r_L^e e^{-2ik_e x}, K_h = 1 - r_L^h e^{2ik_h x},
\]

(A20)

\[
L_e = 1 - r_L^e e^{-2ik_e x}, L_h = 1 + r_L^h e^{2ik_h x},
\]

(A21)

\[
N_{e/h} (E_F ± E) / \sqrt{(E_F ± E)^2 - M_e^2} = \sqrt{(E_F ± E)^2 - M_e^2}.
\]

(A22)

where \( s = 1 \) for \( x < x' \), while \( s = -1 \) for \( x' < x \) and the subscripts are exchanged in the reflection coefficients of the previous expressions \( (R \leftrightarrow L) \). In the case of a semi-infinite left (right) surface, the Green’s functions are obtained from (A16) by making \( r_L^e = 0 \) \( (r_L^h = 0) \) since there are no reflection processes for open boundary conditions.

A.2. Superconducting regions

Analogously, asymptotic solutions for the superconducting regions are calculated using the eigenvectors of the Hamiltonian (1) and the reflection coefficients associated with the boundary conditions (6). For the superconducting case and \( M = 0 \) the Hamiltonian (1) has the spectrum

\[
E = ± \sqrt{(h_{\text{VF}} | k | - E_F)^2 + \Delta_0^2},
\]

(A19)

\[
\hat{g} (x' + 0^+, x') - \hat{g} (x' - 0^+, x') = \frac{i}{h_{\text{VF}}} (\tau_e \otimes \sigma_y),
\]

(A14)
and eigenstates of the form
\[
\psi^\pm(x) = e^{i\mathcal{K}_{\pm}x}(u_0\varphi^\pm + iv_0\sigma_y\varphi^\pm)^T,
\]
where the coherence factors are given by
\[
u_0 = \sqrt{\frac{1}{2}(1 + \Omega/E)}, \quad v_0 = \sqrt{\frac{1}{2}(1 - \Omega/E)},
\]
and the eigenstates of the form \(\psi^\pm(x)\) (\(\pm = qe, qh\)) by the expressions
\[
\varphi^q = (1, -\epsilon e^{i\theta^q})^T / \sqrt{2},
\]
\[
\varphi^h = (\epsilon e^{i\theta^h}, 1)^T / \sqrt{2},
\]
with wave number in \(x\)
\[
k_{qe/qh} = \text{sgn}(E_F \mp \Omega) \sqrt{\frac{(E_F \pm \Omega)^2}{h^2c^2} - q^2}.
\]
In this case the reflection coefficients in (5) for the boundary conditions \(\psi^\pm_L(x_L)|_L = \psi^\pm_R(x_R)|_R = 0\) are \((\Gamma\alpha = v_0/u_0)\)
\[
\begin{align*}
\alpha^{ab}_{L} &= \pm \frac{\epsilon^{\mp i\theta^q} - \Gamma_{0}^{2}\delta^{\mp i\theta^q}}{\epsilon^{\pm i\theta^q} + \Gamma_{0}^{2}\delta^{\pm i\theta^q}} e^{\pm 2i\mathcal{K}_{q}^{fe}/\mathcal{K}_{0}}, \\
\alpha^{ab}_{R} &= \pm \frac{\epsilon^{\mp i\theta^h} - \Gamma_{0}^{2}\delta^{\pm i\theta^h}}{\epsilon^{\pm i\theta^h} + \Gamma_{0}^{2}\delta^{\pm i\theta^h}} e^{\pm 2i\mathcal{K}_{h}/\mathcal{K}_{0}}, \\
\alpha^{cd}_{L} &= \pm \frac{2\Gamma_{0}^{2} \cos \theta^q e^{i(k_{q} - k_{h})u}}{e^{\pm i\theta^q} + \Gamma_{0}^{2}\delta^{\pm i\theta^q}}, \\
\alpha^{cd}_{R} &= \pm \frac{2\Gamma_{0}^{2} \cos \theta^h e^{i(k_{h} - k_{q})u}}{e^{\pm i\theta^h} + \Gamma_{0}^{2}\delta^{\pm i\theta^h}},
\end{align*}
\]
and for the alternate boundary conditions \(\psi^\pm_L(x_L)|_L = \psi^\pm_R(x_R)|_R = 0\)
\[
\begin{align*}
\alpha^{ab}_{L} &= \pm \frac{\epsilon^{\mp i\theta^q} - \Gamma_{0}^{2}\delta^{\mp i\theta^q}}{\epsilon^{\pm i\theta^q} + \Gamma_{0}^{2}\delta^{\pm i\theta^q}} e^{\pm 2i\mathcal{K}_{q}^{fe}/\mathcal{K}_{0}}, \\
\alpha^{ab}_{R} &= \pm \frac{\epsilon^{\mp i\theta^h} - \Gamma_{0}^{2}\delta^{\pm i\theta^h}}{\epsilon^{\pm i\theta^h} + \Gamma_{0}^{2}\delta^{\pm i\theta^h}} e^{\pm 2i\mathcal{K}_{h}/\mathcal{K}_{0}}, \\
\alpha^{cd}_{L} &= \pm \frac{2\Gamma_{0}^{2} \cos \theta^q e^{i(k_{q} - k_{h})u}}{e^{\pm i\theta^q} + \Gamma_{0}^{2}\delta^{\pm i\theta^q}}, \\
\alpha^{cd}_{R} &= \pm \frac{2\Gamma_{0}^{2} \cos \theta^h e^{i(k_{h} - k_{q})u}}{e^{\pm i\theta^h} + \Gamma_{0}^{2}\delta^{\pm i\theta^h}},
\end{align*}
\]
The Green’s functions of the superconducting system are given by the general expression (3), and the constraint condition \((A14)\) leads to the following relations for the coefficient matrices
\[
\mathcal{C}_{\mu\nu} = \mathcal{C}_{\mu\nu}, \quad \mathcal{C}_{\mu\nu} = \mathcal{X}\mathcal{C}_{\mu\nu},
\]
\[
\mathcal{C}_{\mu\nu} = Y\mathcal{C}_{\mu\nu}, \quad \mathcal{C}_{\mu\nu} = Z\mathcal{C}_{\mu\nu},
\]
where the proportionality factors \(X, Y\) and \(Z\) depend only on the reflection coefficients
\[
X = \frac{\left(\frac{r_{L}^{q} r_{R}^{q} + r_{L}^{h} r_{R}^{h}}{r_{L}^{q} r_{R}^{q} + r_{L}^{h} r_{R}^{h}} - 1\right)}{\left(\frac{r_{L}^{q} r_{R}^{q} + r_{L}^{h} r_{R}^{h}}{r_{L}^{q} r_{R}^{q} + r_{L}^{h} r_{R}^{h}} - 1\right)},
\]
\[
Y = \frac{\left(\frac{r_{L}^{q} r_{R}^{q} + r_{L}^{h} r_{R}^{h}}{r_{L}^{q} r_{R}^{q} + r_{L}^{h} r_{R}^{h}} - 1\right)}{\left(\frac{r_{L}^{q} r_{R}^{q} + r_{L}^{h} r_{R}^{h}}{r_{L}^{q} r_{R}^{q} + r_{L}^{h} r_{R}^{h}} - 1\right)},
\]
\[
Z = \frac{\left(\frac{r_{L}^{q} r_{R}^{q} + r_{L}^{h} r_{R}^{h}}{1 - r_{L}^{q} r_{R}^{q} - r_{L}^{h} r_{R}^{h}}\right)}{1 - r_{L}^{q} r_{R}^{q} - r_{L}^{h} r_{R}^{h}},
\]
and the matrix \(\mathcal{C}_{\mu\nu}\) is given by the expression
\[
\mathcal{C}_{\mu\nu} = -\frac{2i}{\hbar v_F\mu_0} \frac{1}{Q^2 - PR} \begin{pmatrix} R & 0 & 0 & Q \\ 0 & R & -Q & 0 \\ Q & -P & 0 \\ -P & 0 & -P \end{pmatrix},
\]
with the parameters
\[
P = A + XD + YG + ZI, \quad Q = B + XE + YH + ZK, \quad R = C + XF + YI + ZL,
\]
\[
A = \left(1 - r_{L}^{q} r_{R}^{q}\right) \cos \alpha_{qg} + \Gamma_{0}^{2} r_{L}^{q} r_{R}^{q} \cos \alpha_{qh},
\]
\[
B = -\Gamma_{0} \left(\left(1 - r_{L}^{q} r_{R}^{q}\right) \cos \alpha_{qg} + r_{L}^{q} r_{R}^{q} \cos \alpha_{qh}\right),
\]
\[
C = \Gamma_{0}^{2} \left(1 - r_{L}^{q} r_{R}^{q}\right) \cos \alpha_{qg} + r_{L}^{q} r_{R}^{q} \cos \alpha_{qh},
\]
\[
D = -\Gamma_{0} \left(1 - r_{L}^{h} r_{R}^{h}\right) \cos \alpha_{qg} - r_{L}^{h} r_{R}^{h} \cos \alpha_{qh},
\]
\[
E = \Gamma_{0} \left(\left(1 - r_{L}^{h} r_{R}^{h}\right) \cos \alpha_{qg} + r_{L}^{h} r_{R}^{h} \cos \alpha_{qh}\right),
\]
\[
F = -\left(1 - r_{L}^{h} r_{R}^{h}\right) \cos \alpha_{qg} - r_{L}^{h} r_{R}^{h} \cos \alpha_{qh},
\]
\[
G = \Gamma_{0} \left(1 - r_{L}^{q} r_{R}^{q}\right) \cos \alpha_{qg} - r_{L}^{q} r_{R}^{q} \cos \alpha_{qh},
\]
\[
H = -\Gamma_{0} \left(1 - r_{L}^{h} r_{R}^{h}\right) \cos \alpha_{qg} - r_{L}^{h} r_{R}^{h} \cos \alpha_{qh},
\]
\[
I = r_{L}^{h} r_{R}^{h} \cos \alpha_{qg} - \Gamma_{0}^{2} r_{L}^{h} r_{R}^{h} \cos \alpha_{qh},
\]
\[
J = \Gamma_{0} \left(1 - r_{L}^{h} r_{R}^{h}\right) \cos \alpha_{qg} - r_{L}^{h} r_{R}^{h} \cos \alpha_{qh},
\]
\[
K = -\Gamma_{0} \left(1 - r_{L}^{q} r_{R}^{q}\right) \cos \alpha_{qg} - r_{L}^{q} r_{R}^{q} \cos \alpha_{qh},
\]
\[
L = r_{L}^{q} r_{R}^{q} \cos \alpha_{qg} - \Gamma_{0}^{2} r_{L}^{q} r_{R}^{q} \cos \alpha_{qh}.
\]
Appendix B. Dyson equation for coupling adjacent regions: Green’s functions for FF and FS junctions

The equilibrium Green’s functions of a system, evaluated at the interface $x_0$ between two coupled regions (figure 2) is obtained by the Dyson equation (8), which can be written in the simple form \[64, 66\]

$$
\hat{G}_{L/R} = \hat{g}_{L/R} + \hat{g}(x_{L/R}, x_0 \mp \varepsilon^\pm) \hat{\Sigma}_{L/R/L},
$$

$$
\hat{G}_{L/R/L} = \hat{g}(x_{L/R}, x_0 \mp \varepsilon^\pm) \hat{\Sigma}_{L/R/L},
$$

where $\varepsilon^\pm$ are infinitesimal scalars such that $0 < \varepsilon^- < \varepsilon^+ \ll 1$, and were used the following abbreviated notation: \(\hat{G}_{L/R} = \hat{G}(x_{L/R}, x'_{L/R})\), \(\hat{G}_{L/R/L} = \hat{G}(x_{L/R}, x'_{L/R/L})\).

As a first example, consider the case of the FF junction. The Green’s functions of the decoupled regions $\hat{g}_{L/R}$ around $x_0 = 0$ can be obtained from (A16) by making $r'_{L/R} = 0$ for left/right region. Hence, the Green’s functions of the e/h sectors (A17) for the left region take the form

$$
\hat{g}_{ee/hh}(-\varepsilon^+, -\varepsilon^-) = \left( \begin{array}{cc} 0 & \pm iL_{e}e^{-i\Omega} \\ 0 & 0 \end{array} \right) \frac{\mp i}{\hbar v_F},
$$

$$
\hat{g}_{ee/hh}(-\varepsilon^-, -\varepsilon^+) = \left( \begin{array}{cc} 0 & 0 \\ \pm iL_{e}e^{i\Omega} & 0 \end{array} \right) \frac{\mp i}{\hbar v_F},
$$

and for the right region

$$
\hat{g}_{ee/hh}(\varepsilon^+, \varepsilon^-) = \left( \begin{array}{cc} iL_{e}e^{i\Omega} & 0 \\ \pm iL_{e}e^{-i\Omega} & 0 \end{array} \right) \frac{\mp i}{\hbar v_F},
$$

with the factors

$$
L_{e,h}/h = \frac{E_{FL} \pm E - M_{L}}{\sqrt{(E \pm E_{FL})^2 - M_{L}^2}},
$$

$$
L_{R,e/h} = \frac{E_{FR} \pm E - M_{R}}{\sqrt{(E \pm E_{FR})^2 - M_{R}^2}}.
$$

Thus, the Green’s function of the coupled system given by \(B1\) takes the form

$$
\hat{G}(-\varepsilon^+, -\varepsilon^-) = \left( \begin{array}{cc} G_{ee} & 0 \\ 0 & G_{hh} \end{array} \right),
$$

where $G_{ee}$ and $G_{hh}$ are the Green’s functions of the left and right regions, respectively.

For the subsequent analytical calculation, the high doping limit for the superconducting region will be assumed ($e^{i\Omega}$ $\sim$ 1). Then, the Green’s function of the coupled system takes the form

$$
\hat{G}(-\varepsilon^+, -\varepsilon^-) = \left( \begin{array}{cc} i(1 - \Gamma_0^2) & -\frac{i}{\hbar v_F} \hat{g}_{ee/hh} \hat{g}_{hh} \\ -\frac{i}{\hbar v_F} \hat{g}_{eh} \hat{g}_{he} & i(1 - \Gamma_0^2) \end{array} \right),
$$

where $\Gamma_0$ is the coupling constant between the e/h subsystems.

For the case of the FS junction, the Green’s function at the right of the interface $\hat{g}_{hh}(\varepsilon^+, \varepsilon^-)$ is replaced by the Green’s function of the superconducting case with $r'_{L/R} = 0$

$$
\hat{g}_{hh}(\varepsilon^+, \varepsilon^-) = \left( \begin{array}{cc} 0 & \frac{i}{\hbar v_F} \hat{g}_{eh} \hat{g}_{he} \\ -\frac{i}{\hbar v_F} \hat{g}_{he} \hat{g}_{eh} & 0 \end{array} \right),
$$

and the denominator $D$ by

$$
D = E (L_{e,h}e^{-i\Omega}e^{-i\Omega} + 1) + \Omega (L_{e,h}e^{-i\Omega} + L_{e,h}e^{i\Omega}).
$$

This reduces to the expression (13) for zero doping levels of the two regions \[66\]. For the case of junctions with more than two regions, the Dyson equation can be implemented sequentially to each interface to obtain the equilibrium Green’s functions of the entire system. Figure 7 illustrates the coupling process for the case of a junction of three regions. For the first interface at $x = 0$, the equilibrium Green’s functions of the left (L) and central (C) regions are the ‘left’ and ‘right’ inputs in equations \(B1\) and \(B2\) to obtain the coupled Green’s functions of the L-C subsystem. Following the same procedure for

\[\text{et al.} \]
Figure 7. Schematic representation of the equilibrium Green’s functions calculation for a junction with a finite central region and two semi-infinite lateral leads. First, the Green’s functions of the L and C regions are coupled with the Dyson equation. Then, the resulting Green’s functions are taken as the new left-input for a second Dyson equation to finally obtain the Green’s functions of the complete system.

the second interface at $x = d$, the Green’s functions of the L-C subsystem and those of the right region (R) are the new ‘left’ and ‘right’ inputs in the same equations, obtaining the total equilibrium Green’s functions of the junction.

Appendix C. Differential conductance derivation

For a system consisting of three regions as showed in figure 7, the Hamiltonian has the form [65–67]

$$H = H_L + H_C + H_R + H_{L_C} + H_{C_R},$$  \hspace{1cm} (C1)

with $H_{L,C,R}$ the Hamiltonians of the three decoupled regions (left (L), central (C) and right (R)) and $H_{L_C,R}$ the tunneling Hamiltonians (7) for the left and right interfaces

$$H_{L_C}(\tau) = t \int d\mathbf{q} e^{i\phi_{L_C}(\tau)/2} c_{\downarrow}^\dagger \mathbf{q}_{L_C} \hat{b}_{\downarrow} \mathbf{q}_{L_C} + \text{h.c.},$$  \hspace{1cm} (C2)

$$H_{C_R}(\tau) = t \int d\mathbf{q} e^{i\phi_{C_R}(\tau)/2} c_{\downarrow}^\dagger \mathbf{q}_{C_R} \hat{b}_{\downarrow} \mathbf{q}_{C_R} + \text{h.c.},$$  \hspace{1cm} (C3)

where $t = \hbar v_F$, $\phi_{L_R}(\tau) = \phi_0 + 2(\mu_{L_R} - \mu_L)\tau/\hbar$ the gauge phases induced by the gradient of the chemical potential, the $\hat{c}_{\mathbf{q}_{L,R}}$, with $\nu = L, R$ and $\sigma = \uparrow, \downarrow$, are the annihilation operators for electrons at the edges of the left and right regions with wave number $\mathbf{q}$ and the $\hat{b}_{\mathbf{q}_{L,R}}$ are the annihilation operators at the edges of the central region. In the Heisenberg picture, the average current at the left interface is given by

$$I(\tau) = -e \left\langle \frac{d}{dt} N_L(\tau) \right\rangle$$  

$$= it \frac{e}{h} \int d\mathbf{q} \left[ \left\langle \hat{c}_{L_C}(\tau) \hat{b}_{L_C}(\tau) \right\rangle - \left\langle \hat{b}_{L_C}^\dagger(\tau) \hat{c}_{L_C}(\tau) \right\rangle \right],$$  \hspace{1cm} (C4)

which can be expressed in terms of Keldysh Green’s functions as

$$\bar{G}_{\alpha\beta}^{\alpha\beta}(\tau_\alpha, \tau_\beta) = -i \left\langle T_\tau \left[ D_{\alpha\beta}(\tau_\alpha) D_{\alpha\beta}^\dagger(\tau_\beta) \right] \right\rangle,$$  \hspace{1cm} (C5)

where $i, j = L, C, C', R$ are the border indexes of each region, $\alpha, \beta$ indicate the Keldysh temporal branches, $T_\tau$ is the Keldysh time-ordering operator and where the following vector operators were defined

$$\hat{D}_{\alpha\beta}(\tau) = \left( \hat{d}_{\alpha\beta}(\tau), \hat{d}_{\alpha\beta}(\tau), \hat{d}_{\alpha\beta}(\tau), \hat{d}_{\alpha\beta}(\tau) \right)^T,$$  \hspace{1cm} (C6)

$$\hat{D}_{\alpha\beta}^\dagger(\tau) = \left( \hat{d}_{\alpha\beta}(\tau), \hat{d}_{\alpha\beta}(\tau), \hat{d}_{\alpha\beta}(\tau), \hat{d}_{\alpha\beta}(\tau) \right).$$  \hspace{1cm} (C7)

According to relations $\hat{d}_{\alpha\beta}(\tau) = \hat{d}_{\alpha\beta}(\tau)$, $\hat{d}_{\alpha\beta}(\tau) = \hat{b}_{\alpha\beta}(\tau)$, $\hat{d}_{\alpha\beta}(\tau) = \hat{b}_{\alpha\beta}(\tau)$, $\hat{d}_{\alpha\beta}(\tau) = \hat{c}_{\alpha\beta}(\tau)$.

Considering a stationary situation, the average current can be written in energy space as ($i = \Sigma_{L,R}$)

$$I = \frac{e}{2\hbar} \int dE d\mathbf{q} \text{Tr} \left( \tau_L \left[ g_{\alpha\beta}^{++}(E) \right] g_{\alpha\beta}^{++}(E) \right),$$  \hspace{1cm} (C8)

This expression can also be applied for a two-region system with a single interface, by considering the union of regions $R$ and $C$ as a new region $R$, as explained in the previous section for Green’s functions (this equation coincides with equation (12) by changing index $C$ by $R$). By using the following Dyson equations

$$\bar{G}_{\alpha\beta}^{++}(E) = \bar{G}_{\alpha\beta}^{++}(E) + \bar{G}_{\alpha\beta}^{++}(E) \bar{G}_{\alpha\beta}^{++}(E) \bar{G}_{\alpha\beta}^{++}(E),$$  \hspace{1cm} (C9)

$$\bar{G}_{\alpha\beta}^{++}(E) = \bar{G}_{\alpha\beta}^{++}(E) \bar{G}_{\alpha\beta}^{++}(E) \bar{G}_{\alpha\beta}^{++}(E),$$  \hspace{1cm} (C10)

the average current can be written in terms of local Green’s functions as

$$I = \frac{e}{2\hbar} \int dE d\mathbf{q} \text{Tr} \left( \tau_L \left[ g_{\alpha\beta}^{++}(E) g_{\alpha\beta}^{++}(E) \right] \right),$$  \hspace{1cm} (C11)

where the unperturbed Keldysh Green’s functions are given by the relations

$$\hat{b}_{\alpha\beta}^{--}(E) = 2\pi i \rho_{\beta\alpha}(E) \hat{n}_{\beta}(E),$$  \hspace{1cm} (C12)

$$\hat{b}_{\alpha\beta}^{+-}(E) = -2\pi i \rho_{\alpha\beta}(E) (\tau_\alpha - \hat{n}_{\alpha}(E)),$$  \hspace{1cm} (C13)

being $\hat{n}_{\alpha}(E) = \text{Im}(\bar{G}_{\alpha\alpha}^{++}(E))/\pi$ the DOS matrix of the $i$ electrode and $\hat{n}_i$ the quasiparticle occupation matrix

$$\hat{n}_i(E) = \text{diag}(n_{i0}(E)\tau_0, n_{i0}(E)\tau_0),$$  \hspace{1cm} (C14)

with $n_{i0}(E) = \left[ 1 + e^{(E_i - E_0)/\hbar}) \right]^{-1}$ the Fermi–Dirac functions for electrons/holes (from here we will consider the limit $T \to 0$). By means of the following Dyson equation

$$\bar{G}_{\alpha\beta}^{++}(E) = \bar{G}_{\alpha\beta}^{++}(E) \bar{G}_{\alpha\beta}^{++}(E) \bar{G}_{\alpha\beta}^{++}(E) \bar{G}_{\alpha\beta}^{++}(E),$$  \hspace{1cm} (C15)

the expression for the electrical current takes the form

$$I = \frac{2\pi^2 e}{h} \int dE d\mathbf{q} \text{Tr} \left( \tau_L \left[ \hat{r}_{\alpha\beta} \hat{n}_{\alpha\beta} \right] \right),$$  \hspace{1cm} (C16)
This current incorporates the contribution of transport processes between states with spin $\uparrow$ on the left and spin $\downarrow$ to the right of each contact ($L \leftarrow R$). However, under normal conditions on the surface of a TI, both spin projections symmetrically contribute to the transport. Then, it is necessary to consider the contribution of the opposite-spin processes ($L \leftarrow R$), which introduces an additional factor of 2. Again, the electric potential $V$ is introduced as a shift between the chemical potentials of the electrodes ($\mu_L = E_{FL} + eV$ and $\mu_R = E_{FR}$) and the Fermi levels of the regions are controlled independently through gates. The normalized differential conductance is given by

$$\sigma = \sigma_Q + \sigma_A,$$

$$\sigma_Q = \frac{4e^2}{\hbar \sigma_0} \int dq \, \text{Tr} \left[ \hat{\rho}_{qL} \hat{G}^{\prime}_{q,C,C} \hat{\rho}_{qR} \hat{G}^{\prime}_{q,C,C} \right],$$

$$\sigma_A = \frac{4e^2}{\hbar \sigma_0} \int dq \, \text{Tr} \left( \hat{\rho}_{qL} \hat{G}^{\prime}_{q,C,C} \hat{\rho}_{qR} \hat{G}^{\prime}_{q,C,C} \hat{\tau}_z \right),$$

(C17)

and in terms the Nambu space components

$$\sigma_Q = \frac{4e^2}{\hbar \sigma_0} \int dq \, \text{Tr} \left\{ \hat{\rho}_{q,Lee} \left[ \hat{G}^{\prime}_{q,C,C,ee} \hat{\rho}_{q,Reh} \hat{G}^{\prime}_{q,C,C,ee} - \hat{\rho}_{q,Reh} \hat{G}^{\prime}_{q,C,C,ee} \hat{\rho}_{q,Lee} \right] - \hat{G}^{\prime}_{q,C,C,ch} \left[ \hat{\rho}_{q,Lee} \hat{G}^{\prime}_{q,C,C,ee} - \hat{\rho}_{q,Reh} \hat{G}^{\prime}_{q,C,C,ee} \hat{\rho}_{q,Lee} \right] \right\},$$

$$\sigma_A = \frac{8e^2}{\hbar \sigma_0} \int dq \, \text{Tr} \left\{ \hat{\rho}_{q,Lee} \hat{G}^{\prime}_{q,C,C,ch} \hat{\rho}_{q,Lhh} \hat{G}^{\prime}_{q,C,C,ee} \right\}.$$ 

Here, the following matrices were defined

$$\hat{\rho}_{qL} \equiv \pi I \hat{\rho}_{qL} I, \quad \hat{\rho}_{qR} \equiv \pi I \hat{\rho}_{qR} I,$$

(C18)

and the two components have been normalized to ballistic conductance per unit of surface length of a TI, $\sigma_0 (V) = 2e^2 (E_F + eV) / h \pi N_{1d}$. This expression for the conductance can be approximated to those of the case of two coupled semi-infinite regions, at the limit when the width of the central region tends to zero ($d \rightarrow 0$), and by making the parameters of this region equal to those of any of the electrodes. For example, for a normal left region and superconducting right region, the component $\sigma_A$ includes terms that involve the DOS of both electrodes and is generally associated with electron–electron transport processes by direct transport ($\times \hat{\rho}_{q,Lee} \hat{\rho}_{q,Reh}$) or by pair-creation/annihilation process as intermediate state ($\times \hat{\rho}_{q,Lee} \hat{\rho}_{q,Reh}$/), in addition to electron–hole conversion processes in the superconductor ($\times \hat{\rho}_{q,Lee} \hat{\rho}_{q,Lhh}$) by branch crossing. On the other hand, the product $\hat{\rho}_{q,Lee} \hat{\rho}_{q,Lhh}$ in the second component involves only the left electrode and is associated with electron–hole conversion processes such as Andreev reflections with a probability proportional to $|\hat{G}^{\prime}_{q,C,C,ee}|^2$ [67].

References

[1] Qi X-L and Zhang S-C 2011 Topological insulators and superconductors Rev. Mod. Phys. 83 1057–110
[2] Hasan M Z and Kane C L 2010 Colloquium: topological insulators Rev. Mod. Phys. 82 3045–67
[3] Ando Y 2013 Topological insulator materials J. Phys. Soc. Japan 82 102001
[4] Andrei Bernevig B and Hughes T L 2013 Topological Insulators and Topological Superconductors Student edn (Princeton, NJ: Princeton University Press)
[5] Yokoyama T and Murakami S 2014 Spintronics and spincaloritronics in topological insulators Physica E 55 1–8
[6] Zhang H, Liu C-X, Qi X-L, Dai X, Fang Z and Zhang S-C 2009 Topological insulators in Bi2Se3, Bi2Te3, and Sb2Te3 with a single Dirac cone on the surface Nat. Phys. 5 438
[7] Liu C-X, Qi X-L, Zhang H J, Dai X, Zhong F and Zhang S-C 2010 Model Hamiltonian for topological insulators Phys. Rev. B 82 045122
[8] Silvestrov P G, Brouwer P W and Mishchenko E G 2012 Spin and charge structure of the surface states in topological insulators Phys. Rev. B 86 075302
[9] Xia Y et al 2009 Observation of a large-gap topological-insulator class with a single Dirac cone on the surface Nat. Phys. 5 398
[10] Chen Y L et al 2009 Experimental realization of a three-dimensional topological insulator, Bi2Te3 Science 325 178–81
[11] Chen J et al 2010 Gate-voltage control of chemical potential and weak antilocalization in Bi2Se3 Phys. Rev. Lett. 105 176602
[12] Chen J, He X Y, Wu K H, Ji Z Q, Lu L, Shi J R, Smet J H and Li Y Q 2011 Tunable surface conductivity in Bi2Se3 revealed in diffusive electron transport Phys. Rev. B 83 241304
[13] Steinberg H, Laloe J-B, Fatemi V, Moodera J S and Jarillo-Herrero P 2011 Electrically tunable surface-to-bulk coherent coupling in topological insulator thin films Phys. Rev. B 84 233101
[14] Kim Y S et al 2011 Thickness-dependent bulk properties and weak antilocalization effect in topological insulator Bi2Se3 Phys. Rev. B 84 073109
[15] Cha J, Kong D, Hong S-S, Analytis J G, Lai K and Cui Y 2012 Weak antilocalization in Bi2Se3: Sb nanoribbons and nanoplanes Nano Lett. 12 1107–11
[16] Zhang Z-D, Wang Z-H and Gao X P A 2010 Topological insulators and their heterostructures Chin. Phys. B 27 109701
[17] Xiong J, Luo Y, Khou Y H, Jia S, Cava R J and Ong N P 2012 High-field Shubnikov–de Haas oscillations in the topological insulator Bi2Te2Se Phys. Rev. B 86 045314
[18] Shrestha K, Marinova V, Lorenz B, Paul C and Chu W 2014 Shubnikov–de Haas oscillations from topological surface states of metallic Bi2Se2Te9 Phys. Rev. B 90 241111
[19] de Vries E K, Pezzini S, Meijer M J, Koirala N, Salehi M, Moon J, Oh S, Wiedmann S and Banerjee T 2017 Coexistence of bulk and surface states probed by Shubnikov–de Haas oscillations in the topological insulator Bi2Se3 Phys. Rev. B 96 045433
[20] Akiyama R, Sumida K, Ichinokura S, Nakanishi R, Kimura A, Kohk K A, Tereshchenko O E and Hasegawa S 2018 Shubnikov–de Haas oscillations in p and n-type topological insulator (Bi,Sb)2Te3 J. Phys.: Condens. Matter 30 265001
[21] Qi X-L, Hughes T L and Zhang S-C 2008 Topological field theory of time-reversal invariant insulators Phys. Rev. B 78 195424
[22] Yokoyama T, Tanaka Y and Nagaosa N 2010 Anomalous magnetoresistance of a two-dimensional ferromagnet-ferromagnet junction on the surface of a topological insulator Phys. Rev. B 81 121401
[23] Chang C-Z et al 2013 Experimental observation of the quantum anomalous Hall effect in a magnetic topological insulator Science 340 167–70
[24] Xu Y et al 2014 Observation of topological surface state quantum Hall effect in an intrinsic three-dimensional topological insulator Nat. Phys. 10 956
[25] Brey L and Fertig H A 2014 Electronic states of wires and slabs of topological insulators: quantum Hall effects and edge transport Phys. Rev. B 89 085305
[26] Yoshihara R, Tsukazaki A, Kozuka Y, Falson J, Takahashi K S, Chechelsky J G, Nagaosa N, Kawasaki M and Tokura Y 2015 Quantum Hall effect on top and bottom surface states of topological insulator (Bi₁₋ₓSbx)₂Te₃ films Nat. Commun. 6 6627
[27] Kubota Y et al 2016 Interface electronic structure at the topological insulator-ferromagnetic insulator junction J. Phys.: Condens. Matter 29 055002
[28] Fu L and Kane C L 2008 Superconducting proximity effect and Majorana fermions at the surface of a topological insulator Phys. Rev. Lett. 100 096407
[29] Xu J-P et al 2015 Experimental detection of a Majorana mode in the core of a magnetic vortex inside a topological insulator-supercollider Bi₂Te₃/NbSe₂ heterostructure Phys. Rev. Lett. 114 017001
[30] Sun H-H et al 2016 Majorana zero mode detected with spin selective Andreev reflection in the vortex of a topological superconductor Phys. Rev. Lett. 116 257003
[31] Sun H-H and Jia J-F 2017 Detection of Majorana zero mode in the vortex npj Quantum Mater. 2 34
[32] Beenakker C W J 2006 Specular Andreev reflection in graphene Phys. Rev. Lett. 97 067007
[33] Linder J, Tanaka Y, Yokoyama T, Sudbø A and Nagaosa N 2010 Interplay between superconductivity and ferromagnetism on a topological insulator Phys. Rev. B 81 184525
[34] Bercioux D and Lucignano P 2018 Quasiparticle cooling using a topological insulator-supercollider hybrid junction Eur. Phys. J. Spec. Top. 227 1361–75
[35] Fu L and Kane C L 2009 Josephson current and noise at a superconductor/quantum-spin-Hall-insulator/superconductor junction Phys. Rev. B 79 164508
[36] Tanaka Y, Yokoyama T and Nagaosa N 2009 Manipulation of the Majorana fermion, Andreev reflection, and Josephson current on topological insulators Phys. Rev. Lett. 103 107002
[37] Linder J, Tanaka Y, Yokoyama T, Sudbø A and Nagaosa N 2010 Unconventional superconductivity on a topological insulator Phys. Rev. Lett. 104 067001
[38] Mondal S, Sen D, Sengupta K and Shankar R 2010 Magnetotransport of Dirac fermions on the surface of a topological insulator Phys. Rev. B 82 045120
[39] Soodchomshom B 2010 Magnetic gap effect on the tunneling conductance in a topological insulator ferromagnet/superconductor junction Phys. Lett. A 374 1561–6
[40] Yokoyama T 2012 Josephson and proximity effects on the surface of a topological insulator Phys. Rev. B 86 075410
[41] Lababidi M and Zhao E 2012 Nearly flat Andreev bound states in superconductor-topological insulator hybrid structures Phys. Rev. B 86 161108
[42] Snelder M, Veldhorst M, Golubov A A and Brinkman A 2013 Andreev bound states and current-phase relations in three-dimensional topological insulators Phys. Rev. B 87 104507
[43] Cheng Q, Chen C and Jin B 2014 Majorana fermions, Andreev reflection and magnetoresistance effect in three-dimensional topological insulators Physica B 449 199–203
[44] Suwanvarangkoon A, Tang I-M, Hoosawat R and Soodchomshom B 2011 Tunneling conductance on surface of topological insulator ferromagnet/insulator/(s- or d-wave) superconductor junction: effect of magnetically-induced relativistic mass Physica E 43 1867–73
[45] Vali R and Vali M 2012 Conductance properties of topological insulator based ferromagnetic insulator/ d-wave superconductor and normal metal/ferromagnetic insulator/d-wave superconductor junctions J. Appl. Phys. 112 083911
[46] Vali R and Vali M 2012 Tunneling transport in topological insulator normal metal/insulator/d-wave superconductor junctions J. Phys.: Condens. Matter 24 325702
[47] Niu Z P 2010 Crossed Andreev reflection on a topological insulator J. Appl. Phys. 108 103904
[48] Tkachov G and Hankiewicz E M 2013 Helical Andreev bound states and superconducting Klein tunneling in topological insulator Josephson junctions Phys. Rev. B 88 075401
[49] Yang Y, Wei K-W and Bai C 2014 Magnetoresistance through a ferromagnet/superconductor/ferromagnet junction on the surface of a topological insulator Appl. Phys. Express 7 023001
[50] Vali R and Khouzestani H F 2014 Coherent conductance and magnetoresistance in a topological insulator ferromagnet/superconductor/ferrimagnet junction Solid State Commun. 187 23–7
[51] Vali R and Khouzestani H F 2014 Nonlocal transport properties of topological insulator F/ISC/F/F junction with perpendicular magnetization Eur. Phys. J. B 87 25
[52] Zhang K and Cheng Q 2018 Electrically tunable crossed Andreev reflection in a ferromagnet-superconductor-ferromagnet junction on a topological insulator Supercond. Sci. Technol. 31 075001
[53] Li D, Rosenstein B, Shapiro B Y and Shapiro I 2014 Quantum critical point in the superconducting transition on the surface of a topological insulator Phys. Rev. B 90 054517
[54] Lu B, Yada K, Golubov A A and Tanaka Y 2015 Anomalous Josephson effect in d-wave superconductor junctions on a topological insulator surface Phys. Rev. B 92 100503
[55] Snelder M, Golubov A A, Asano Y and Brinkman A 2015 Observability of surface Andreev bound states in a topological insulator in proximity to ans-wave superconductor J. Phys.: Condens. Matter 27 315701
[56] Burset P, Lu B, Tkachov G, Tanaka Y, Hankiewicz E M and Trauzettel B 2015 Superconducting proximity effect in three-dimensional topological insulators in the presence of a magnetic field Phys. Rev. B 92 205424
[57] Acero S, Brey L, Herrera W J and Levy Yeyati A 2015 Transport in selectively magnetically doped topological insulator wires Phys. Rev. B 92 235445
[58] Alexander Z, Alidoust M and Daniel L 2016 Josephson junction through a disordered topological insulator with helical magnetization Phys. Rev. B 93 214502
[59] Bobkova I V, Bobkov A M, Zyuzin A A and Alidoust M 2016 Magnetoelectrics in disordered topological insulator Josephson junctions Phys. Rev. B 94 134506
[60] Alidoust M and Hamzehpour H 2017 Spontaneous supercurrent and φ0 phase shift parallel to magnetized topological insulator interfaces Phys. Rev. B 96 165422
[61] Lu B and Tanaka Y 2018 Study on Green’s function on topological insulator surface Phil. Trans. R. Soc. A 376 20150246
[62] McMillan W L 1968 Theory of superconductor-normal-metal interfaces Phys. Rev. B 175 559–68
[63] Herrera W J, Burset P and Levy Yeyati A 2010 A Green function approach to graphene-superconductor junctions with well-defined edges J. Phys.: Condens. Matter 22 275304
[64] Gomez S 2011 Transporte eléctrico en superconductores no convencionales www.bdigital.unal.edu.co/8020/
[65] Casas O E, Páez S G, Levy Yeyati A, Burset P and Herrera W J 2019 Subgap states in two-dimensional spectroscopy of graphene-based superconducting hybrid junctions Phys. Rev. B 99 144502
[66] Casas O E 2019 Transporte eléctrico en nanoestructuras topológicas www.bdigital.unal.edu.co/73258/
[67] Cuevas J C, Martín-Rodero A and Levy Yeyati A 1996 Hamiltonian approach to the transport properties of superconducting quantum point contacts Phys. Rev. B 54 7366–79
[68] Páez S G, Camilo Martínez W J H, Levy Yeyati A and Burset P 2019 Dirac point formation revealed by Andreev tunneling in superlattice-graphene/superconductor junctions Phys. Rev. B 100 205429
[69] Butkov E 1968 Mathematical Physics (New York: Addison Wesley)

[70] Jan L and Öhrn Y 1973 Propagators in Quantum Chemistry (London: Academic)
[71] Setare M R and Jahani D 2010 Klein tunneling of massive Dirac fermions in single-layer graphene Physica B 405 1433–6
[72] Xie Y, Tan Y and Ghosh A W 2017 Spintronic signatures of Klein tunneling in topological insulators Phys. Rev. B 96 205151
[73] Lee S et al 2019 Perfect Andreev reflection due to the Klein paradox in a topological superconducting state Nature 570 344–8
[74] Löfwander T, Shumeiko V S and Wendin G 2001 Andreev bound states in high-tc superconducting junctions Supercond. Sci. Technol. 14 R53
[75] Zhang Z-Y 2008 Differential conductance through a NINS junction on graphene J. Phys.: Condens. Matter 20 445220
[76] Burset P, Herrera W and Levy Yeyati A 2009 Proximity-induced interface bound states in superconductor-graphene junctions Phys. Rev. B 80 041402