General framework for transport in spin-orbit coupled superconducting heterostructures: Non-uniform spin-orbit coupling and spin-orbit-active interfaces

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Electronic spin-orbit coupling (SOC) is essential for various newly discovered phenomena in condensed-matter systems. In particular, one-dimensional topological heterostructures with SOC have been widely investigated in both theory and experiment for their distinct transport signatures indicating the presence of emergent Majorana fermions. However, a general framework for the SOC-affectected transport in superconducting heterostructures, especially with the consideration of interfacial effects, has not been developed even regardless of the topological aspects. We hereby provide one for an effectively one-dimensional superconductor-normal heterostructure with non-uniform magnitude and direction of both Rashba and Dresselhaus SOC as well as a spin-orbit-active interface. We extend the Blonder-Tinkham-Klapwijk treatment to analyze the current-voltage relation and obtain a rich range of transport behaviors. Our work provides a basis for characterizing fundamental physics arising from spin-orbit interactions in heterostructures and its implications for topological systems, spintronic applications and a whole variety of experimental set-ups.

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Introduction: The interplay between electronic spin and orbital degrees of freedom, or spin-orbit coupling (SOC), has played a crucial role in various aspects of condensed-matter physics, including the study on semiconductors, ferromagnets, superconductors and materials with exotic orders \cite{1–13} as well as the application on building quantum electronic or spintronic devices \cite{14, 15}. Recently, great interest has been stimulated in exploring topological states of matter \cite{16, 17}, whose experimental realization and detection strongly rely on transport or STM measurements of artificially engineered heterostructures with SOC. Among them, those with building blocks such as semiconductor/topological-insulator wire with SOC and conventional superconductor \cite{18–22} (used to induce a proximity gap) or 1D ferromagnet combined with a bulk superconductors with SOC \cite{23–27} are of particular interest to explore emerging Majorana fermions (MFs) \cite{28–33}. Most theoretical studies have focused on either effective models or employed SOC as a uniform model parameter \cite{34–45}. However, the set-up of interest usually has only a segment or end point of the 1D element in contact with a (bulk) superconductor due to either the experimental constraints or an explicit interest in studying (topological) heterostructures \cite{22, 38, 46, 47}.

In this letter, we develop a framework to study an (effectively) 1D normal (N)–superconductor (S) set-up (see Fig. 1) that is general enough to capture the effects of SOC in a wide range of (emergent) heterostructures. We allow for both Rashba \cite{48} and Dresselhaus \cite{49} SOC with arbitrary relative strengths on each side as well as at the interface (I) which could also be a thin insulating layer. Furthermore, we allow the SOC to have a different magnitude as well as direction in N, S and I regions. Non-uniform SOC is in fact bound to arise for a variety of reasons including difference in the chemical composition, crystallographic direction, or direction of electric field \cite{48, 49} and may be relevant also for practical implementations of topological quantum computing schemes \cite{50, 51}. SOC in the interface can even simply arise due to a lack of “left-right” symmetry \cite{52, 53}. We start by analyzing the appropriate Bogoliubov–de Gennes (BdG) Hamiltonian and develope a generalized Blonder-Tinkham-Klapwijk formalism to calculate the current-voltage characteristics for our general set-up. We phenomenologically model what we call the spin-orbit-active interface as a generalization of a spin-active interface \cite{55–70}, which itself is a generalization of a single Z-parameter used in the original BTK approach. We find that the rich physics emanating from

![Fig. 1](image-url)
non-uniform SOC and/or spin-orbit-active interface is not only of fundamental interest but also highly relevant for interpreting the results of experiments. For example, it can effectively lower the interfacial barrier, drastically change the zero-bias conductance and determine between re-entrant or monotonic temperature dependence. Our results also underline the danger in using a single Z-parameter fit to extract the interface properties in experiments and offer a more accurate picture.

**Model and Hamiltonian:** As illustrated in Fig. 1, our effectively 1D system comprises of N (x < 0) and S (x > 0) regions with an arbitrary SOC on each side, intersecting at I (x = 0). The Hamiltonian \( H_{j=N,S} \) in corresponding basis \( \Psi_j = (\psi_{\uparrow j}, \psi_{\downarrow j}, \psi_{\uparrow j}' T - \psi_{\downarrow j}')^T \) reads

\[
H_N = \tau_\sigma \otimes (E_p \mathbb{1} + \alpha_N p \sigma_y + \beta_N p \sigma_x), \\
H_S = \tau_\sigma \otimes (E_p \mathbb{1} + \alpha_S p \sigma_y + \beta_S p \sigma_x) - \Delta \tau_\sigma \otimes \mathbb{1},
\]

where \( E_p = \frac{\gamma_\sigma^2}{2m} - \mu \) is the free spectrum with chemical potential \( \mu \), \( \sigma_j \) (\( \beta_j \)) are Rashba (Dresselhaus) SOC on j side, \( \Delta \) (taken real for convenience) is the s-wave (possibly proximity-induced) superconducting gap, \( \sigma \) and \( \tau \) are Pauli matrices spanned in spin and particle-hole basis, respectively, and \( \mathbb{1} \) is the \( 2 \times 2 \) identity matrix. The spin basis on both sides can differ by an Euler rotation \( \Psi_S = (1 \otimes e^{-i\sigma} \eta_{N(3)} \) \( e^{-i\sigma} \eta_{N(3)} \) \( e^{-i\sigma} \eta_{N(3)} \)) \( \Psi_S = U_{NS} \Psi_N \).

The two SOCs can be combined as a complex factor \( \gamma_j e^{i\varphi_j} = \beta_j + i\alpha_j \). We rotate the Hamiltonians into an isospin basis \( \Psi_{\phi'} \) under transformation \( H_{j'} = U_{j'j} H_j U_{j'j}^\dagger \), where \( U_{j,j'} = \frac{1}{\sqrt{2}} \mathbb{1} \otimes \begin{pmatrix} e^{-i\varphi_j} & 1 \\ -1 & e^{i\varphi_j} \end{pmatrix} \) and obtain a diagonal \( H_{N'} \) and block-diagonal \( H_{S'} \) as

\[
H_{N'} = \tau_\sigma \otimes (E_p \mathbb{1} - \gamma_N \tau p \sigma_x), \\
H_{S'} = \tau_\sigma \otimes (E_p \mathbb{1} - \gamma_S \tau p \sigma_x) - \Delta \tau_\sigma \otimes \mathbb{1}.
\]

The spectra of \( H_{N'} \) and \( H_{S'} \) show particle and hole bands, denoted by \( \sigma = \pm \). Each band has two isospin branches denoted by \( \phi = \pm \). At a given energy \( E \), there are eight corresponding eigenfunctions \( \chi_{\sigma \phi}^\tau e^{i(xp_\sigma + \gamma \sigma \phi)x} \) for \( H_{N'} \) and the other eight \( \chi_{\eta \phi}^\tau e^{i(xp_\eta + \gamma \phi \phi)x} \) for \( H_{S'} \), where \( p_\sigma^\tau = \sqrt{2m(\mu' - m\gamma^2 + \tau E)} \) and \( k_\sigma^\tau = \sqrt{2m(\mu' + m\gamma^2 + \tau E - 2\Delta)} \) with \( \mu' = \mu + m(\nabla_\gamma^2 + \nabla_\phi^2)/4 \) and \( \psi_\gamma^\tau \). The particle-hole band and isospin states have representations as \( \chi_{\sigma \phi}^{\tau} = (\delta_{\phi} \delta_{\phi} + \delta_{\phi} \delta_{\phi} - \delta_{\phi} \delta_{\phi} - \delta_{\phi} \delta_{\phi})^T \) and \( \chi_{\eta \phi}^{\tau} = u(\delta_{\phi} \delta_{\phi} + \delta_{\phi} \delta_{\phi} + \delta_{\phi} \delta_{\phi} + \delta_{\phi} \delta_{\phi})^T + v(\delta_{\phi} \delta_{\phi} + \delta_{\phi} \delta_{\phi} - \delta_{\phi} \delta_{\phi} - \delta_{\phi} \delta_{\phi})^T \), where \( u^2 = 1 - \psi_\phi^2 = \frac{1}{2} \left(1 + \frac{2\Delta}{\sqrt{2m(\mu' - \Delta)}} \right) \) and \( \delta \) is the delta function. Below we drop \( h \) in all equations for convenience and take \( \mu' \) and \( \sqrt{2mp_\sigma^\tau} \) to be natural energy and momentum units, respectively (so \( \nabla_\gamma^2 + \nabla_\phi^2 \) causes no qualitative change but energy rescaling). The presence of \( \psi_\phi^2 \) induces charge carrier imbalance between both sides. Note that we consider energy range in which the hole excitations have real momenta [71].

In a BTK treatment, the interface is phenomenologically modeled by Hamiltonian \( H_\delta(x) \), which generally has the same \( 4 \times 4 \) representation as the bulk Hamiltonian. The matrix components reflect the interfacial properties as well as the physical discontinuity between both sides and specify transport processes through the interface. The original BTK model adopts one parameter \( Z_0 \tau z \otimes \mathbb{1} \) to describe barrier effects from an oxide layer or local disorder [54]. For ferromagnet–superconductor heterostructures, \( H_1 \) can be modeled as a Zeeman form \( \mathbb{1} \otimes Z_h (\mathbb{\hat{n}} \cdot \mathbb{\hat{\sigma}}) \) with unit direction \( \mathbb{\hat{n}} = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta) \), which accounts for various spin-active processes such as spin-flip scattering, spin-dependent phase shift, and spin-related Andreev reflection [57–70]. In our case, we expect that the discontinuity of the bulk SOC and the interfacial SOC itself would play an active role in the transport. This effect is modeled by Rashba \( Z_\alpha \tau z \otimes \sigma_y \) and Dresselhaus \( Z_\alpha \tau z \otimes \sigma_y \) components. To capture the most general interplay with spins, we incorporate all the factors above and write down our spin-orbit-active interface,

\[
H_1 = \tau_\sigma \otimes (Z_0 \mathbb{1} + Z_\alpha \sigma_y + Z_{\beta} \sigma_x) + 1 \otimes Z_h (\mathbb{\hat{n}} \cdot \mathbb{\hat{\sigma}}).
\]

In general, the spin basis of \( H_1 \) and \( H_N \) differ by another Euler rotation \( U_{N1} = (1 \otimes e^{-i\sigma} \eta_{N(3)} \) \( e^{-i\sigma} \eta_{N(3)} \) \( e^{-i\sigma} \eta_{N(3)} \)) \( \Psi_N \) and we write the rotated \( H_1 \) in a suggestive form as

\[
U_{N1} H_1 U_{N1}^T = \begin{pmatrix}
Z_0 - Z_1 & Z_2 e^{-i\gamma} & 0 & 0 \\
Z_2 e^{i\gamma} & Z_0 + Z_1 & 0 & 0 \\
0 & 0 & -Z_0 - Z_3 & -Z_4 e^{i(\gamma + \phi')} \\
0 & 0 & -Z_4 e^{i(\gamma + \phi')} & -Z_0 + Z_3
\end{pmatrix}.
\]

There are relations \( Z_1^2 + Z_3^2 + Z_4^2 + Z_2^2 = Z_0^2 + Z_2^2 \) and \( Z_1^2 + Z_3^2 - Z_2^2 - Z_4^2 = 2Z_0 Z_3 \sin \theta \cos (\phi - \varphi_1) \) that are independent of the Euler angles. Comparing Eq. (3) and Eq. (6), one can see that the 3 Euler angles effectively generate one additional variable.

In brief, the key ingredients on our system, the bulk SOCs \( \alpha_{\beta} \sigma_y \) and \( \beta_{\beta} \sigma_x \) as well as the interfacial parameters \( Z_\alpha \sigma_y, Z_{\beta} \sigma_x \), and \( Z_\alpha \mathbb{\hat{n}} \cdot \mathbb{\hat{\sigma}} \), can be characterized by different vectors in spin space in the corresponding regions, as illustrated in Fig. 1. Below we study the system’s transport properties as a function of these vectors.

**BTK calculations:** Here we apply the BTK treatment to compute current–voltage relations of the system. Considering an incoming wave \( \Psi_{\text{in}}^{\tau \sigma} = \chi_{\sigma}^{\tau} e^{i(xp_\sigma + \gamma \phi \phi)} \) with energy \( E \) on the N side that propagates toward the interface (positive group velocity) and scatters through, we incorporate all possible outgoing waves and write down the following equations on N and S sides, as \( \Psi_L = U_{NN} \chi_{\sigma}^{\tau \sigma} + \sum_{\eta} e^{i\sigma \gamma N} (b_\eta \chi_{\eta}^{\tau \sigma} e^{-i\eta \phi} + a_\eta \chi_{\eta}^{\tau \sigma} e^{i\eta \phi}) \) and
\[ \Psi_R = U_{NS} U_{SS} \sum_\sigma e^{i0\gamma_3} (c_\sigma \chi_0^{\sigma} e^{ik^+_x} + d_\sigma \chi_0^{-\sigma} e^{-ik^-_x}) \]

respectively (all wavefunctions are represented in the real spin basis of \( H_N \)). Because reflections (transmissions) should have the group velocity direction opposite to (same as) the incoming wave, only eight states are considered (see Insets in Fig. 1). For an incoming electron \((\tau = +)\), the amplitudes \( b, a, c, \) and \( d \) correspond to normal reflection, Andreev reflection [72], quasi-particle transmission and quasi-hole transmission, respectively, while for an incoming hole \((-)\), \( a \) and \( b \) reverse their roles. The subscript \( \sigma \) of the amplitudes describes in-branch (cross-branch) processes if its sign is the same as (opposite to) the incoming wave. These amplitudes can be determined by two boundary conditions at the interface. The first one is the continuity of the wavefunction \( \Psi_L(0) = \Psi_R(0) \), while the second one can be obtained by integrating the BdG equation over an infinitesimal interval across the interface,

\[ \int_0^x \frac{1}{2}[H_N \theta(-x) + U_{NS} H_S \Upsilon_{NS}(x) + h.c.] + U_{NS} H_1 \Upsilon_{NS}(x)] \Psi dx = 0, \]

where \( \theta(x) \) is the step function and \( \Psi(0^-) = \Psi_{R/L}(0) \). We carefully keep the Hamiltonian hermitian when it is expressed using the step function [73].

The probability current \( J \) is calculated from its definition \( \partial_t \Psi^\dagger \Psi = -\partial_x J \). For each incoming wave \( \Psi_{in}^\dagger \), we calculate \( J \) corresponding to different scattering processes normalized by the incoming current and obtain combined currents carried by the in- and cross-branch normal (Andreev) reflections together, \( J_{NR,\sigma}^R, J_{AR,\sigma}^R \), as well as those carried by all the transmissions together, \( J_{\tau,\sigma}^T = 1 - J_{NR,\sigma}^R - J_{AR,\sigma}^R \) due to the probability conservation. Following the standard BTK treatment, the net charge current \( I \) induced by a voltage drop \( V \) across the junction can be evaluated as

\[ I = \sum_{\tau,\sigma} A e \int_0^\infty dE \{ [1 - J_{NR,\sigma}^R] [f(E - \tau eV) - f(E)] + J_{AR,\sigma}^R [f(E) - f(E + \tau eV)] \}, \]

where \( A \) is a constant associated with density of states, Fermi velocity, as well as an effective cross-sectional area, and \( f(E) = \exp(E/k_B T) + 1 \)^{-1} is the Fermi distribution function at temperature \( T \). We compute the \( I-V \) relation and normalized differential conductance (NDC) \( G/G_0 \), where \( G = \frac{2e^2}{h} \) and

\[ G_0 = \frac{dI(\Delta=0)}{dV} \]

is a reference value when the S side is normal.

**Results:** We first find that \( \sum_{\tau,\sigma} J_{\tau,\sigma}^{NR/AR/T} \) and hence \( I(V) \) are independent of the Euler angles \( \eta_{NS}^{(i)} \). Therefore, parameters such as \( \varphi_N \) and \( \varphi_S \) that rely on the relative spin coordinate (RSC) between both sides should play no role on the transport either. We numerically confirm this independence by varying the ratio of Rashba and Dresselhaus SOC on each side. For the interface, \( I(V) \) is independent of \( \eta_{NS}^{(i)} \) if one of \( Z_0 \) and \( Z_1 \) in Eq. (5) is zero, so \( \tilde{n} \) or \( \varphi_S \) has no effect given \( Z_0 = 0 \) or \( Z_1 = 0 \), respectively. We find that the scattering amplitude and probability current for each channel sensitively vary with RSC, but they compensate in the summation for \( I(V) \). This implies that RSC may affect \( I(V) \) as a result of interference in a multi-channel or multi-terminal system [69, 70] and also open interesting possibilities for spintronics.

In Fig. 2a we plot zero-bias NDC in the \( Z_0-Z_\gamma \) plane for a purely spin-orbit-active interface \( (Z_h = 0) \). We see that NDC reaches a high value when \( Z_\gamma \) is close to \( Z_0 \) and exhibits a symmetry under the exchange between \( Z_0 \) and \( Z_\gamma \). To explain this, one can Euler rotate \( H_1 \) to its eigenspin basis. The eigenvalues can be regarded as a set of characteristic barrier strengths \( |Z_0 \pm Z_\gamma| \) that determine the BTK results. Such set is invariant under \( Z_0 \leftrightarrow Z_\gamma \) and hence leads to the symmetry. To understand the NDC peaks, one can look at the scattering of the eigenspin states. At \( Z_\gamma = Z_0 \), electrons of one spin direction and holes of the opposite both see a clean interface \( |Z_0 - Z_\gamma| = 0 \), which maximizes the Andreev current as well as NDC. In other words, the presence of interfacial SOC can effectively lower the original BTK barrier \( (|Z_0 - Z_\gamma| < Z_0) \) [74]. In Fig. 2b we plot NDC in the \( Z_0-Z_h \) plane for a purely spin-active interface \( Z_\gamma = 0 \) for comparison. We see that there is no symmetry under \( Z_0 \leftrightarrow Z_h \) and no conductance peak along the \( Z_0 = Z_h \) line. Such differences illustrate the interfacial SOC effects that the original spin-active picture does not capture.

With the coexistence of Zeeman and SOC effects at the interface, the Euler angles \( \eta_{NS}^{(i)} \) are no longer irrelevant. We consider the general Hamiltonian of Eq. (6) and find that \( I(V) \) is independent of \( \zeta \). The relevant variables are the 5 strength parameters \( Z_{0,1,2,3,4} \) and the phase difference \( \zeta' \) between off-diagonal elements of the particle and hole blocks. Notice that the role of \( \zeta' \) is special: (1) it comes from the interplay between \( Z_h \) and \( Z_\gamma \), and (2) it does not alter the eigenvalues of the interfacial Hamiltonian. Therefore, its effects on the transport can be attributed to the interference between particle and hole channels. In Fig. 3a–c, we plot NDC vs \( V \) at various \( \zeta' \) and \( Z_0 \) (we set \( Z_1 = Z_3 = 0 \) and \( Z_2 = Z_4 = 0.5 \) for illustrating the salient features from the interplay between \( \zeta' \) and \( Z_0 \)). At \( Z_0 = 0 \) (a), the curves are all...
above 1 and show a qualitative change from center-dent to center-peak types as \( \zeta' \) goes through 0 (diamonds), 0.25\( \pi \) (triangles), 0.5\( \pi \) (squares), 0.75\( \pi \) (circles), and \( \pi \) (crosses). In this half period, the zero-bias NDC monotonically increases with \( \zeta' \). From \( \zeta' = \pi \) to \( \zeta' = 2\pi \), the deformation of curves completes the other half period and reverses back to the \( \zeta' = 0 \) case. As \( Z_0 \) increases, the center-peak curves drastically deform toward the center-dent type, and the trend of zero-bias NDC vs \( \zeta' \) also reverses. At \( Z_0 = 0.66 \) (b), the \( \zeta' = \pi \) curve has the lowest zero-bias NDC \( \approx 1 \). At \( Z_0 = 1.5 \) (c), the center-dent curves remains and are well below 1 at low bias due to the suppression of transmissions and Andreev reflections (tunneling limit in the BTK model). The role of \( \zeta' \) is not significant in this case. We turn to show one way to independently tune \( \zeta' \) via the tuning of parameters in Eq. (5). Assuming the same spin basis on the N side and the interface \( (\eta_{\text{NI}}^{(i)} = 0) \) and the interfacial Zeeman components tuned as \( m = \pi/2 \), \( Z_k \cos \phi = Z_2 \sin^2 \varphi_1 / \cos \varphi_1 \), and \( Z_k \sin \phi = -Z_2 \sin \varphi_1 \), we obtain \( Z_1 = Z_3 = 0, Z_2 = Z_4 = Z_3 / \cos \varphi_1, \) and \( \zeta' = -2\gamma_0 \) by equating Eqs. (5) and (6). In this case, \( \zeta' \) is associated with the ratio of Rashba and Dresselhaus components at the interface with properly controlled Zeeman components.

All the results above are for cases of balanced charge carriers between N and S sides (\( \gamma_N = \gamma_S \)). In Figure 3(d–f) we explore effects of nonuniform SOC induced imbalance (\( \delta \gamma^2 \neq 0 \)) and its interplay with the interfacial parameters. At \( \zeta' = 0 \), the curves are all of the center-dent type and roughly display symmetry between positive and negative imbalance. The zero-bias NDC is far below 1 in the highly imbalanced cases. As \( \zeta' \) increases, the \( \delta \gamma^2 \) ≤ 0 curves deform more drastically than the \( \delta \gamma^2 > 0 \) ones. At \( \zeta' = 0.65\pi \), the \( m\delta \gamma^2 = -0.5 \) curve develops a plateau around \( V = 0 \), indicating an incipience of a center peak. The \( m\delta \gamma^2 = -0.975 \) curve develops minimums around \( eV = \Delta \). At \( \zeta' = \pi \), the \( m\delta \gamma^2 = -0.5 \) and 0 curves show a center-peak structure, and the double minimums of the \( m\delta \gamma^2 = -0.975 \) curves become more significant. The range of zero-bias NDC as a function of \( \delta \gamma^2 \) also maximizes. These rich behaviors can be attributed to the high mismatch between the quasi-particle momenta on both sides and the interfacial phase difference \( \zeta' \) between particle and hole channels, which together alter the scattering amplitudes in the BTK calculations.

Finally we discuss the temperature dependence of the transport. In Fig. 4 we plot zero-bias NDC vs \( T/T_c \) \( (T_c \) is the superconducting transition temperature) at various \( \zeta' \) [(a), same convention and setting as Fig. 3a] or \( \delta \gamma^2 \) [(b), same as Fig. 3c]. The curves can exhibit three types of behavior: (1) monotonic increase, (2) monotonic decrease, and (3) first increase and then decrease (a reentrant phenomenon). These rich behaviors come from the same reason as the case of NDC vs \( V \) do, because high-energy excitations play a more important role at higher temperature. As a result, the conductance as a function of temperature is also sensitive to the bulk SOC and spin-orbit-active interface.

In conclusion, a general framework for superconducting heterostructures with SOC is developed and analyzed by generalizing the BTK scheme. Study of the conductance reveals the crucial role spin-orbit-active interface and non-uniform SOC play in determining the transport properties. In addition to being directly relevant for underpinning the physics of a range of hybrid systems of relevance to various fields including topological matter and spintronics, our work opens up many future research directions.
avenues. One is to apply and extend our transport analysis to other heterostructures, for example, to study the interplay with magnetic fields or ferromagnetism and also to uncover the interference effects in multi-terminal setups. Other is to analyze the impact on pairing symmetry, such as the possibility of p-wave pairing [75], and its consequences. Finally, another important direction is to explore the consequences of non-uniformity and boundary/interface behaviors of SOC in ultracold atoms [76] by leveraging their tunability and amenability for probing the dynamics.

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In the high imbalance limit $\delta\gamma^2 \to \pm1$, the hole excitations have imaginary momenta in a wide range of $E$ and thus become ill-defined in the BdG scenario.